



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 09:31 AM UTC

PDB ID : 8IB6 / pdb_00008ib6
EMDB ID : EMD-35333
Title : Respiratory complex Membrane domain of CI, focus-refined of type IA, Wild type mouse under cold temperature
Authors : Shin, Y.-C.; Liao, M.
Deposited on : 2023-02-09
Resolution : 3.30 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

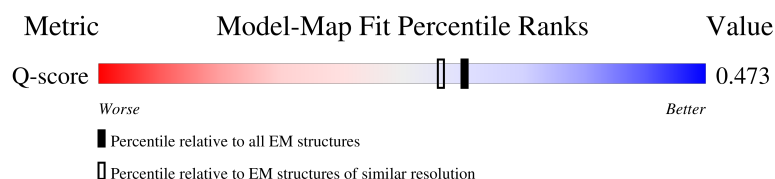
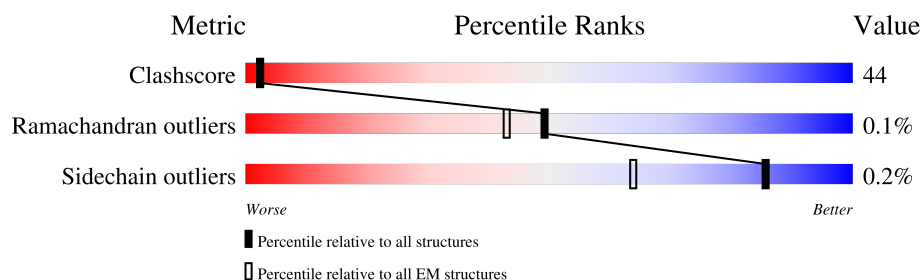
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	D	463	
2	J	172	
3	K	98	
4	L	607	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	M	459	
6	N	345	
7	O	355	
8	U	156	
9	X	172	
10	Y	143	
11	c	76	
12	d	120	
13	e	106	
14	f	57	
15	g	151	
16	h	189	
17	i	128	
18	j	105	
19	k	104	
20	l	186	
21	m	129	
22	n	179	
23	o	137	
24	p	176	

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
25	3PE	L	701	-	-	X	-

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 31822 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	38	Total	C	N	O	S	0	0
			320	208	53	58	1		

- Molecule 2 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	J	159	Total	C	N	O	S	0	0
			1205	814	171	205	15		

- Molecule 3 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	97	Total	C	N	O	S	0	0
			729	473	111	135	10		

- Molecule 4 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	606	Total	C	N	O	S	0	0
			4798	3181	746	826	45		

- Molecule 5 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	458	Total	C	N	O	S	0	0
			3622	2402	566	615	39		

- Molecule 6 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	344	Total	C	N	O	S	0	0
			2694	1790	416	451	37		

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	319	Total	C	N	O	S	0	0
			2599	1668	430	491	10		

- Molecule 8 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	U	84	Total	C	N	O	S	0	0
			678	438	100	135	5		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	X	27	Total	C	N	O	0	0
			221	146	39	36		

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Y	139	Total	C	N	O	S	0	0
			1030	657	174	191	8		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	c	47	Total	C	N	O	S	0	0
			389	255	67	66	1		

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	d	119	Total	C	N	O	S	0	0
			988	646	170	164	8		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	e	104	Total	C	N	O	S	0	0
			863	546	158	151	8		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	f	55	Total	C	N	O	S	0	0
			475	310	84	79	2		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	g	102	Total	C	N	O	S	0	0
			858	553	137	164	4		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	h	136	Total	C	N	O	S	0	0
			1146	754	191	198	3		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	i	94	Total	C	N	O	S	0	0
			796	520	139	134	3		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	j	65	Total	C	N	O	S	0	0
			563	369	93	100	1		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	k	71	Total	C	N	O	S	0	0
			569	375	99	93	2		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	l	158	Total	C	N	O	S	0	0
			1328	858	221	238	11		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	m	127	Total	C	N	O	S	0	0
			1054	678	190	186			

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	n	178	Total	C	N	O	S	0	0
			1541	985	276	269	11		

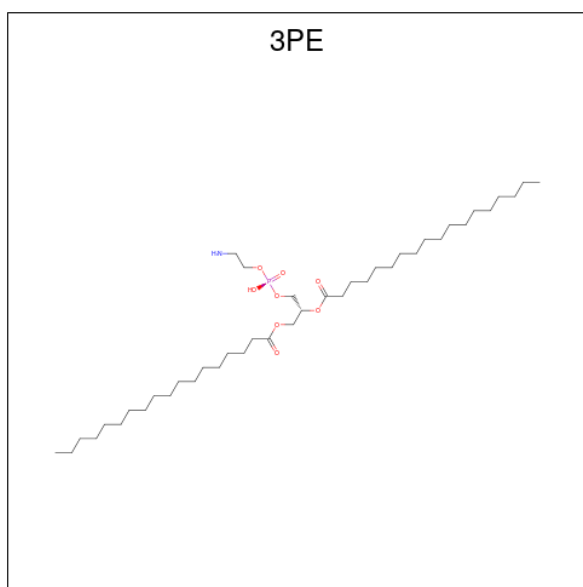
- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	o	120	Total	C	N	O	S	0	0
			1027	647	192	179	9		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

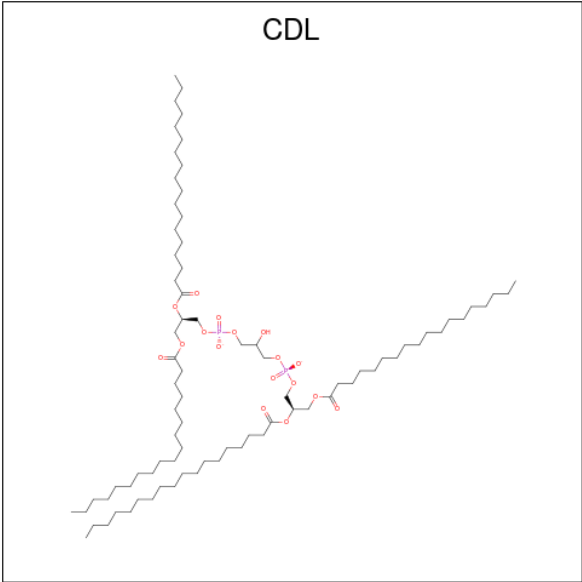
Mol	Chain	Residues	Atoms					AltConf	Trace
24	p	170	Total	C	N	O	S	0	0
			1438	904	258	268	8		

- Molecule 25 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C₄₁H₈₂NO₈P) (labeled as "Ligand of Interest" by depositor).



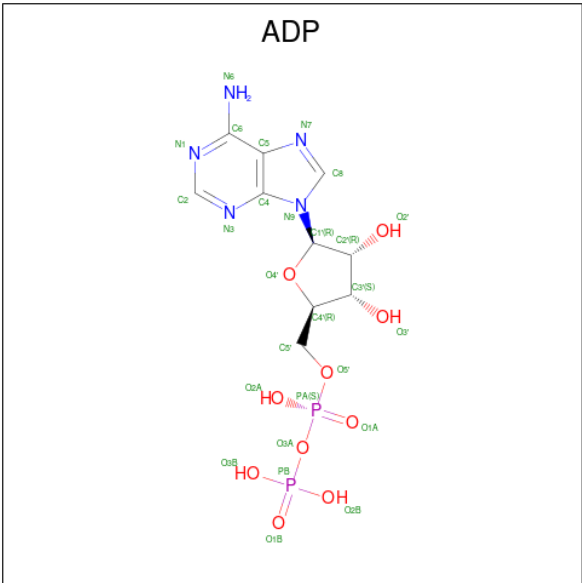
Mol	Chain	Residues	Atoms					AltConf
25	J	1	Total	C	N	O	P	0
			46	36	1	8	1	
25	L	1	Total	C	N	O	P	0
			42	32	1	8	1	
25	L	1	Total	C	N	O	P	0
			40	30	1	8	1	
25	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
25	L	1	Total	C	N	O	P	0
			47	37	1	8	1	
25	L	1	Total	C	N	O	P	0
			45	35	1	8	1	
25	M	1	Total	C	N	O	P	0
			51	41	1	8	1	
25	M	1	Total	C	N	O	P	0
			51	41	1	8	1	
25	M	1	Total	C	N	O	P	0
			51	41	1	8	1	
25	N	1	Total	C	N	O	P	0
			37	27	1	8	1	
25	O	1	Total	C	N	O	P	0
			31	21	1	8	1	
25	Y	1	Total	C	N	O	P	0
			40	30	1	8	1	

- Molecule 26 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



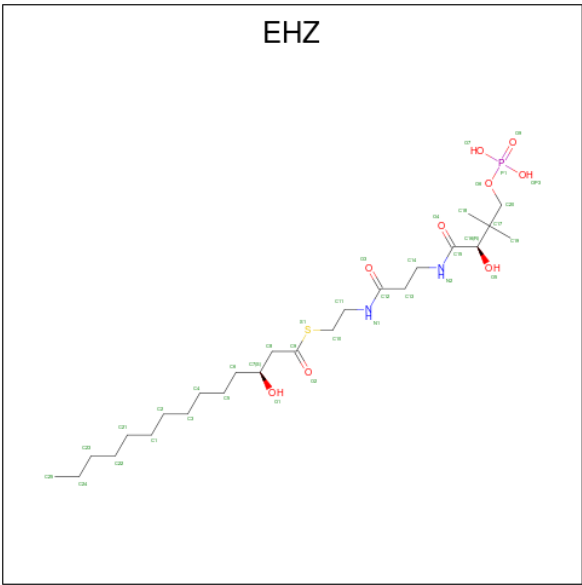
Mol	Chain	Residues	Atoms				AltConf
26	L	1	Total	C	O	P	0
			77	58	17	2	
26	L	1	Total	C	O	P	0
			86	67	17	2	
26	X	1	Total	C	O	P	0
			67	48	17	2	
26	h	1	Total	C	O	P	0
			70	51	17	2	

- Molecule 27 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
27	O	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 28 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: C₂₅H₄₉N₂O₉PS) (labeled as "Ligand of Interest" by depositor).

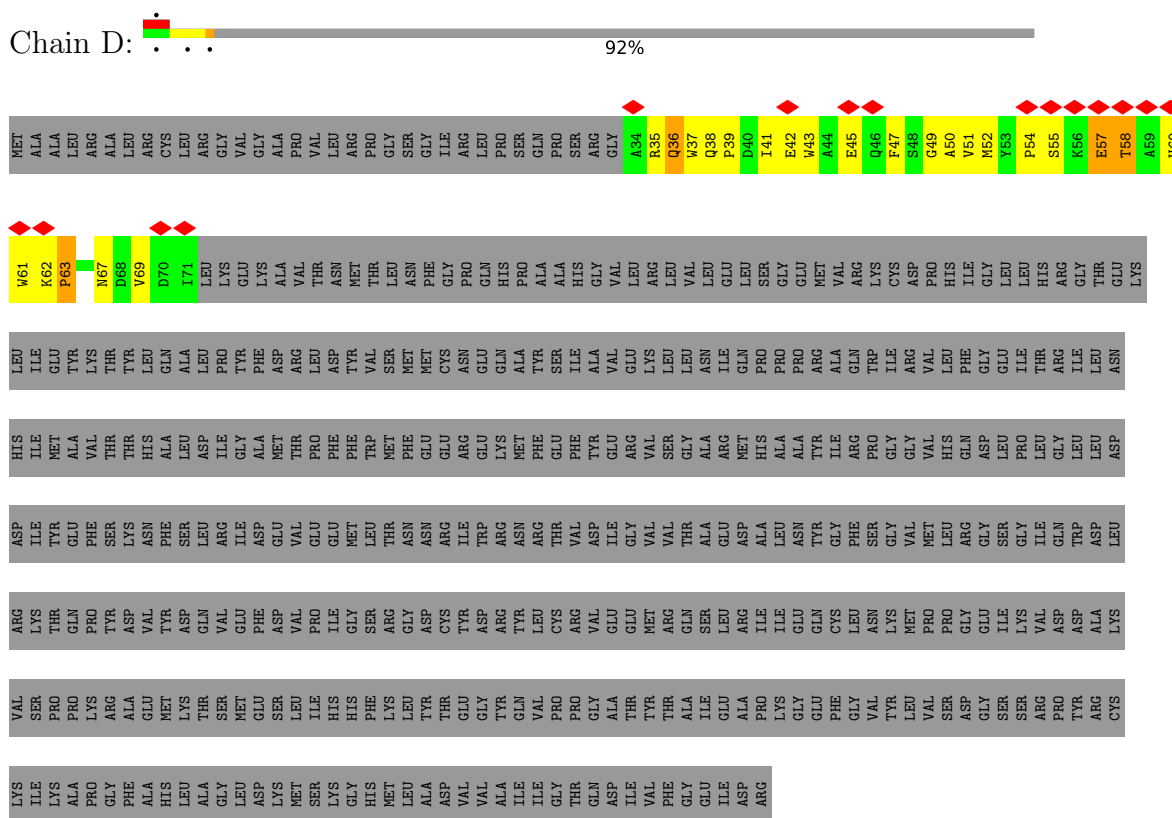


Mol	Chain	Residues	Atoms						AltConf
28	n	1	Total	C	N	O	P	S	0
			32	19	2	9	1	1	

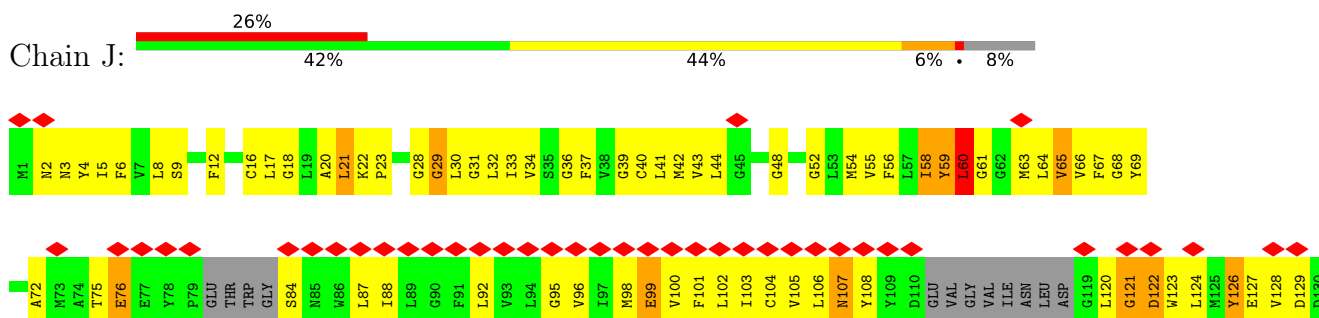
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

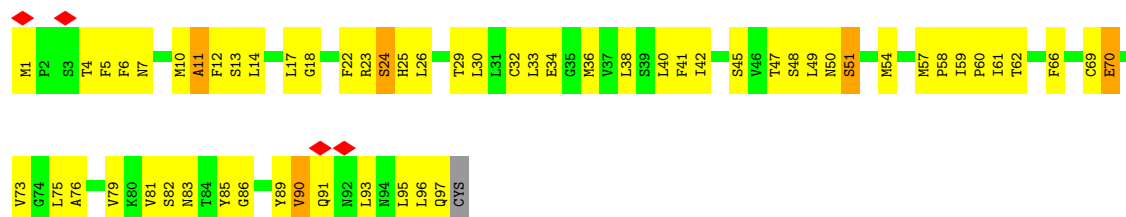


- Molecule 2: NADH-ubiquinone oxidoreductase chain 6

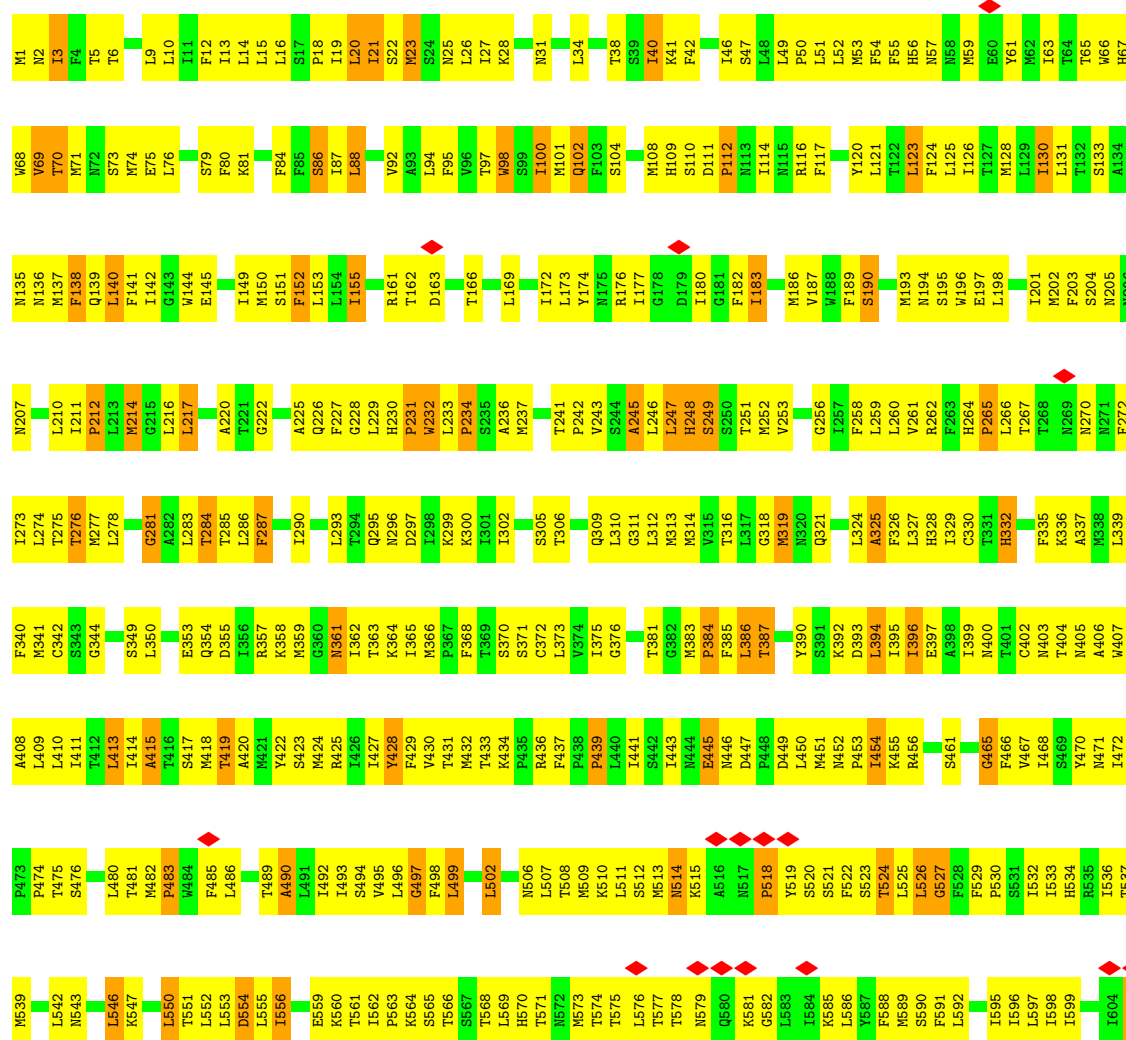




• Molecule 3: NADH-ubiquinone oxidoreductase chain 4L



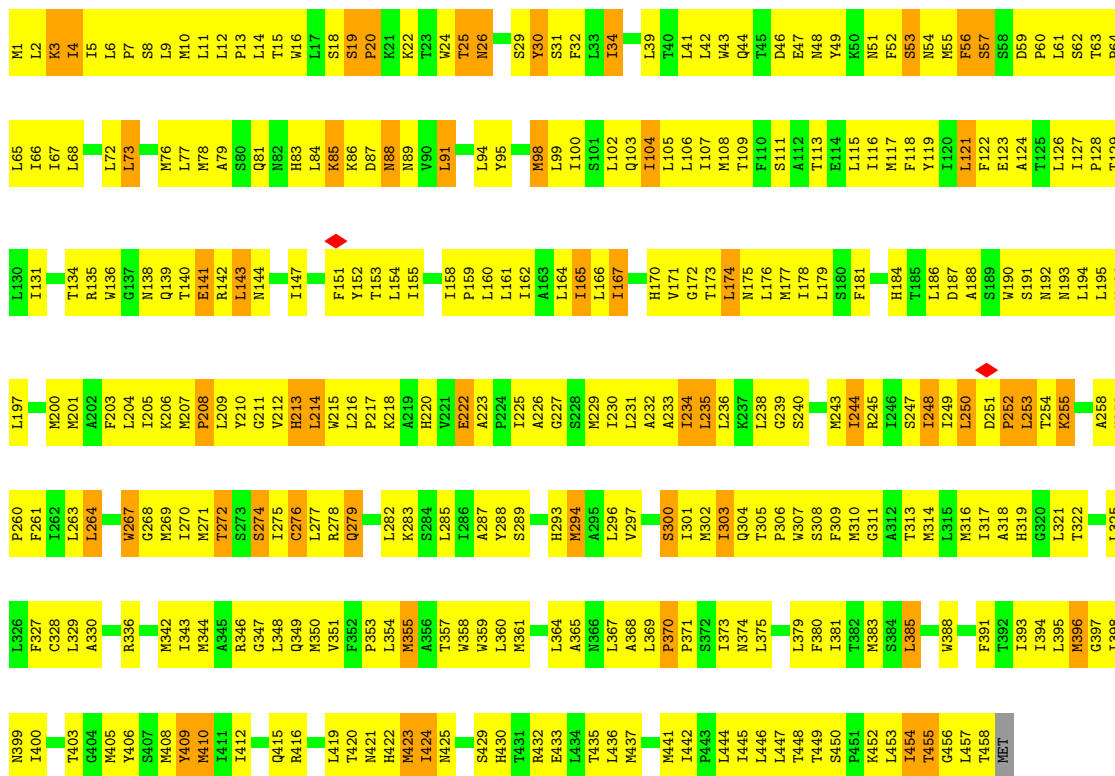
• Molecule 4: NADH-ubiquinone oxidoreductase chain 5



GLU

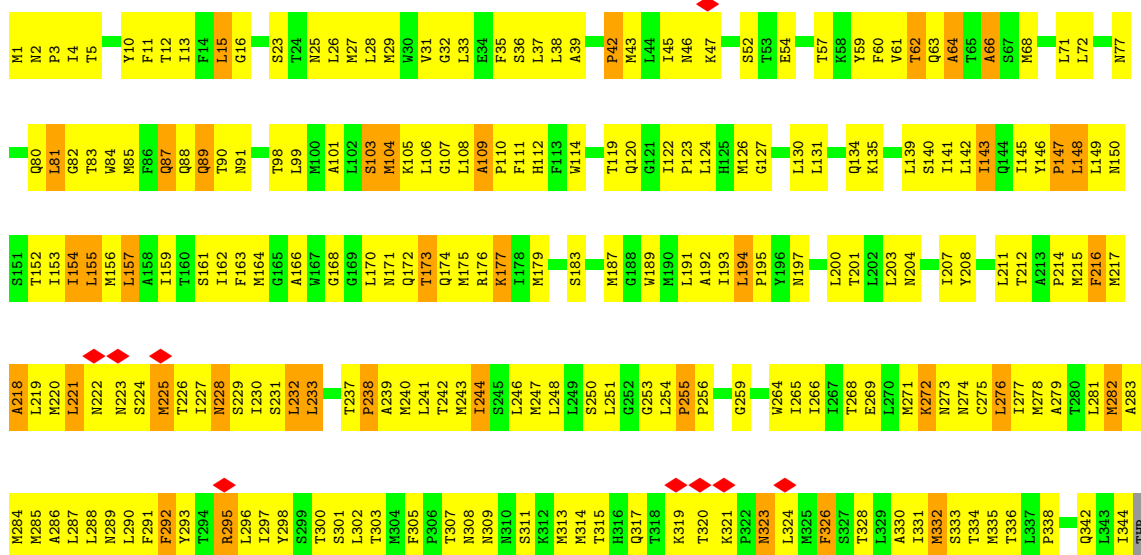
- Molecule 5: NADH-ubiquinone oxidoreductase chain 4

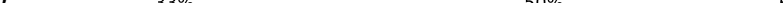
Chain M: 28% 60% 12%

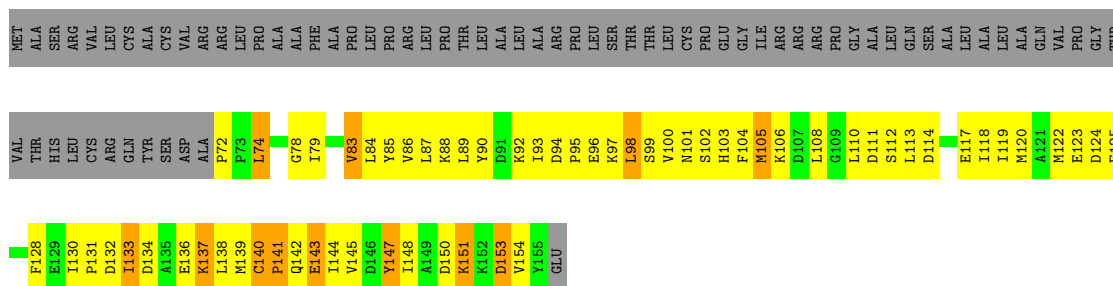
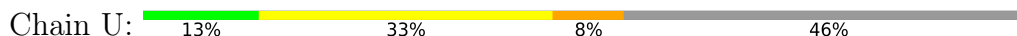


- Molecule 6: NADH-ubiquinone oxidoreductase chain 2

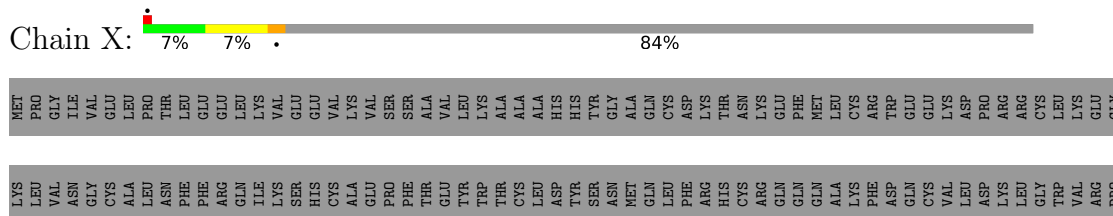
Chain N: 33% 55% 11%

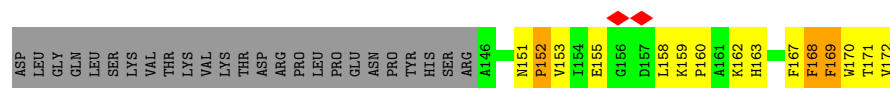


- Chain O: 

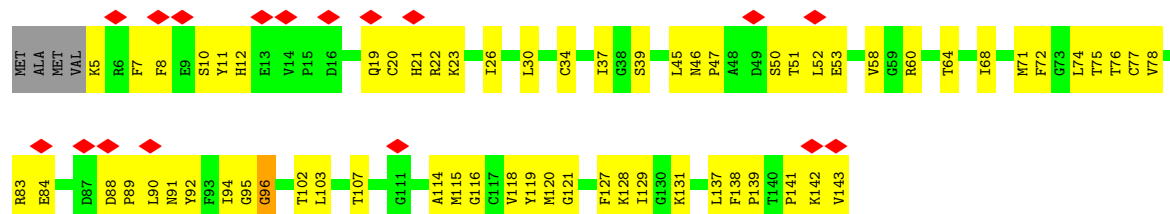


- Molecule 9: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

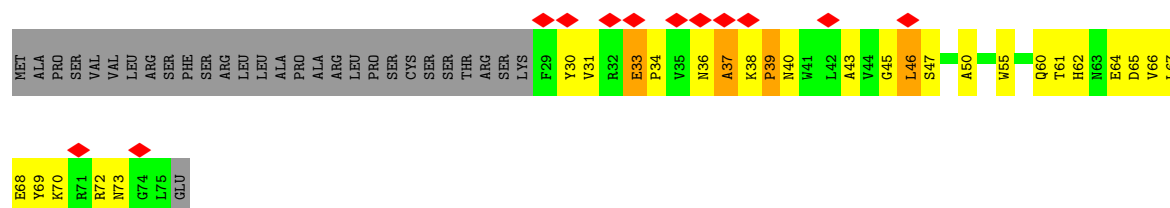
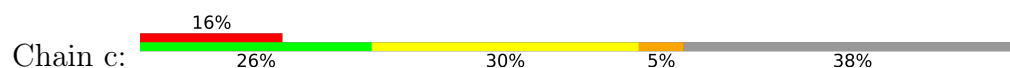




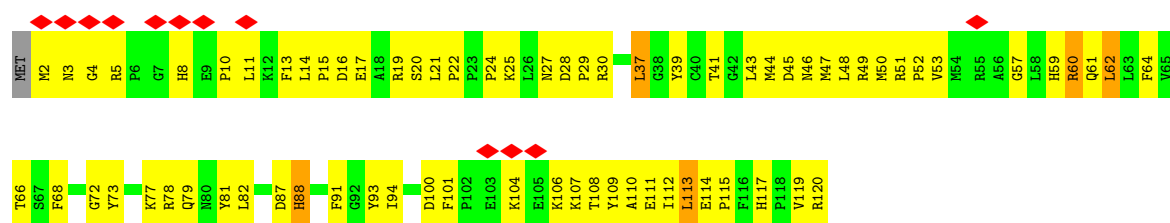
- Molecule 10: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



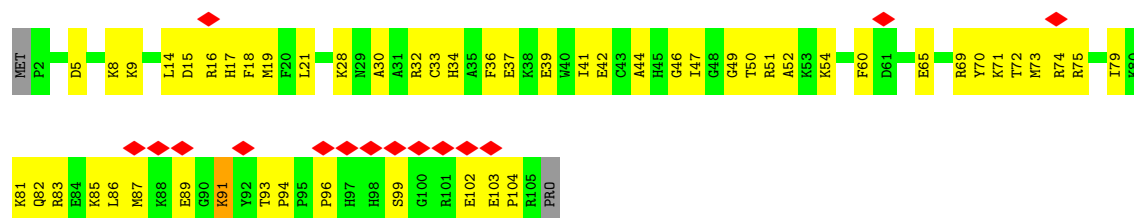
- Molecule 11: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



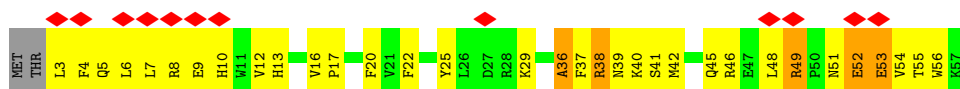
- Molecule 12: NADH dehydrogenase [ubiquinone] 1 subunit C2



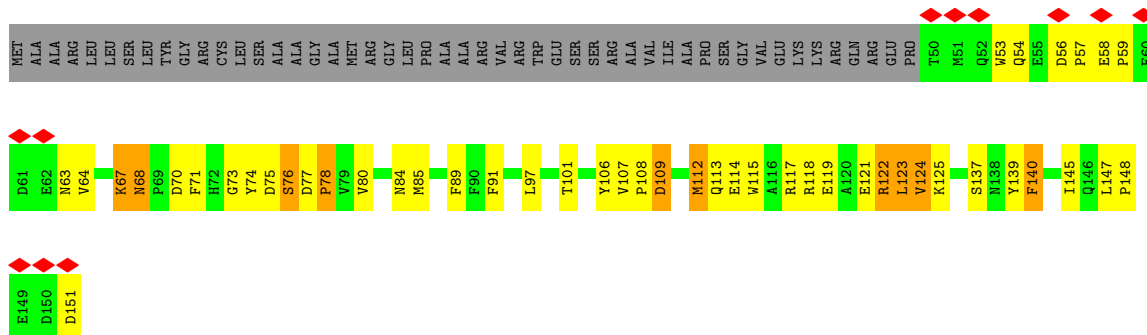
- Molecule 13: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



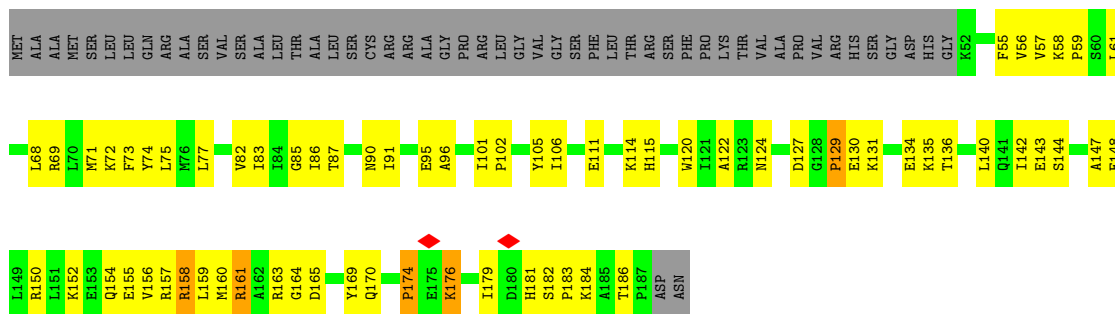
- Molecule 14: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



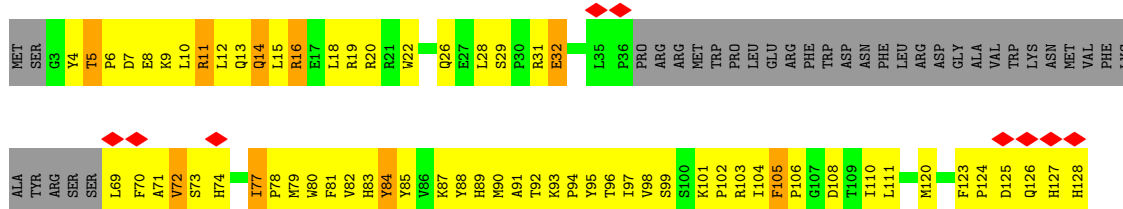
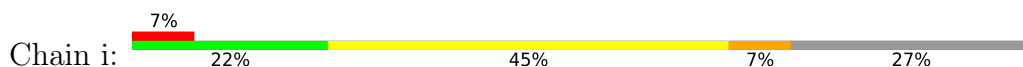
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



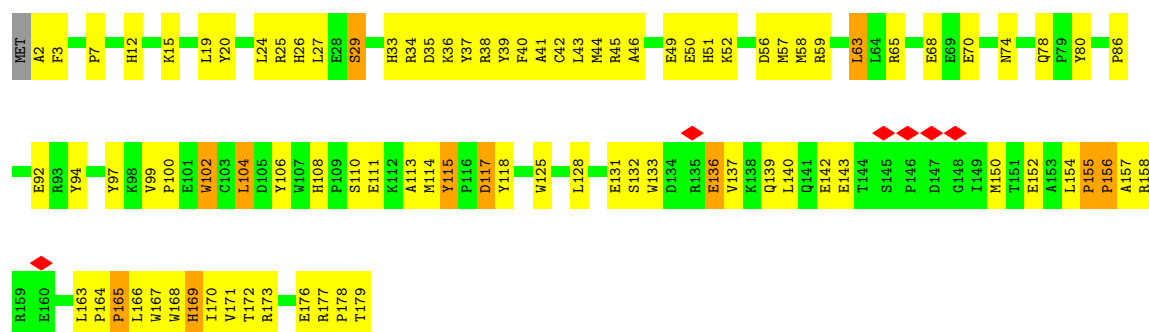
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



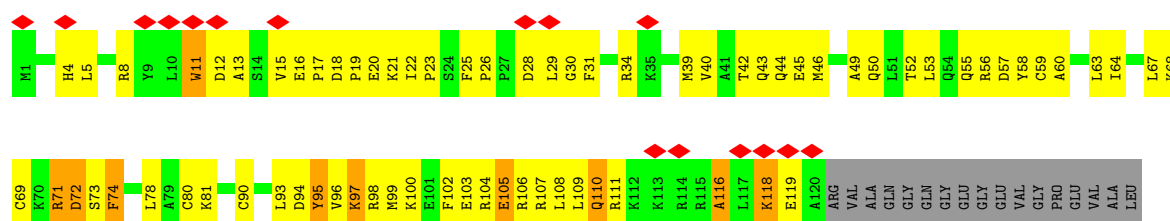
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



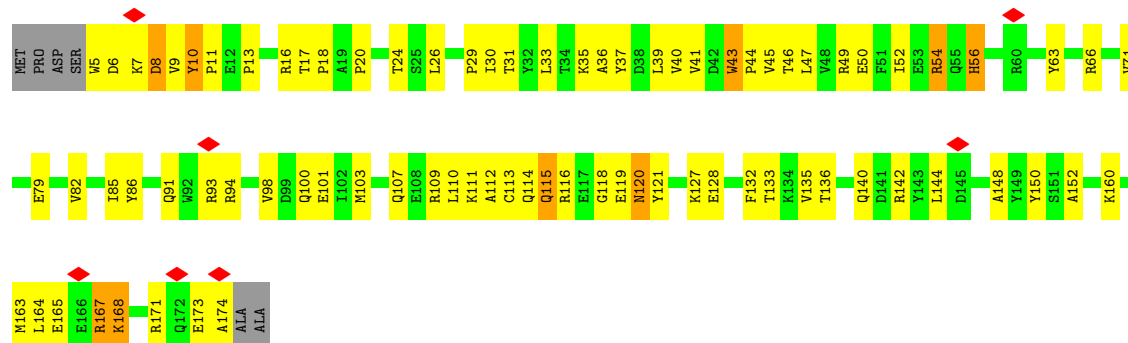
- Molecule 18: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	151188	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	46.1, 45.9	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k), GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.877	Depositor
Minimum map value	-1.712	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.089	Depositor
Recommended contour level	0.55	Depositor
Map size ($\text{\AA}$)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3PE, ADP, CDL, EH2

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	D	0.73	1/335 (0.3%)	1.20	4/461 (0.9%)
2	J	0.78	0/1233	1.35	16/1672 (1.0%)
3	K	0.90	0/740	1.54	13/1005 (1.3%)
4	L	0.99	8/4921 (0.2%)	1.59	114/6696 (1.7%)
5	M	1.01	7/3709 (0.2%)	1.56	85/5052 (1.7%)
6	N	1.01	4/2756 (0.1%)	1.56	62/3751 (1.7%)
7	O	1.02	9/2666 (0.3%)	1.44	43/3615 (1.2%)
8	U	0.96	1/690 (0.1%)	1.49	22/931 (2.4%)
9	X	1.03	1/230 (0.4%)	1.30	4/313 (1.3%)
10	Y	0.88	0/1054	0.97	2/1429 (0.1%)
11	c	0.92	1/400 (0.2%)	1.48	13/544 (2.4%)
12	d	1.02	2/1020 (0.2%)	1.15	11/1377 (0.8%)
13	e	0.63	0/885	0.91	1/1178 (0.1%)
14	f	0.92	1/488 (0.2%)	1.30	10/657 (1.5%)
15	g	0.88	3/886 (0.3%)	1.35	20/1207 (1.7%)
16	h	0.76	1/1181 (0.1%)	1.27	8/1599 (0.5%)
17	i	0.79	0/823	1.31	13/1119 (1.2%)
18	j	0.82	0/588	1.32	8/805 (1.0%)
19	k	0.86	0/587	1.40	11/794 (1.4%)
20	l	0.97	3/1384 (0.2%)	1.24	11/1889 (0.6%)
21	m	0.79	1/1083 (0.1%)	1.17	14/1468 (1.0%)
22	n	0.89	1/1596 (0.1%)	1.27	17/2162 (0.8%)
23	o	0.83	0/1052	1.29	14/1411 (1.0%)
24	p	0.64	1/1471 (0.1%)	1.03	15/1988 (0.8%)
All	All	0.92	45/31778 (0.1%)	1.39	531/43123 (1.2%)

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	O	247	PRO	N-CD	16.66	1.71	1.47
12	d	115	PRO	N-CD	-13.98	1.28	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	265	PRO	N-CD	13.84	1.67	1.47
6	N	255	PRO	N-CD	-13.54	1.28	1.47
11	c	39	PRO	N-CD	-13.32	1.29	1.47
7	O	315	PRO	N-CD	-12.05	1.30	1.47
4	L	234	PRO	N-CD	11.17	1.63	1.47
6	N	123	PRO	N-CD	-10.91	1.32	1.47
5	M	370	PRO	N-CD	-10.55	1.32	1.47
7	O	210	PRO	N-CD	-10.49	1.33	1.47
7	O	224	PRO	N-CD	-10.22	1.33	1.47
9	X	152	PRO	N-CD	-10.14	1.33	1.47
15	g	78	PRO	N-CD	-9.52	1.34	1.47
12	d	15	PRO	N-CD	-9.41	1.34	1.47
7	O	212	PRO	N-CD	-8.89	1.35	1.47
5	M	20	PRO	N-CD	8.60	1.59	1.47
4	L	212	PRO	N-CD	-8.28	1.36	1.47
22	n	155	PRO	N-CD	8.09	1.59	1.47
4	L	513	MET	C-N	7.89	1.43	1.33
4	L	525	LEU	CA-C	7.81	1.62	1.53
20	l	104	PRO	N-CD	-7.21	1.37	1.47
7	O	83	MET	C-N	7.20	1.43	1.33
5	M	208	PRO	N-CD	7.11	1.57	1.47
6	N	238	PRO	N-CD	-7.08	1.37	1.47
7	O	211	VAL	CA-C	6.95	1.60	1.52
6	N	147	PRO	N-CD	-6.77	1.38	1.47
15	g	113	GLN	CA-C	6.55	1.61	1.52
4	L	384	PRO	N-CD	6.41	1.56	1.47
15	g	137	SER	C-O	-6.09	1.16	1.24
4	L	514	ASN	C-N	-6.06	1.24	1.33
24	p	10	TYR	CA-C	-5.99	1.46	1.52
4	L	112	PRO	N-CD	5.90	1.56	1.47
21	m	72	ARG	CA-C	5.85	1.60	1.52
20	l	45	PRO	N-CD	-5.83	1.39	1.47
7	O	87	PRO	N-CD	-5.71	1.39	1.47
5	M	454	ILE	CA-C	5.68	1.60	1.52
5	M	252	PRO	N-CD	-5.61	1.40	1.47
20	l	119	THR	CA-C	-5.53	1.45	1.53
7	O	103	PRO	N-CD	-5.32	1.40	1.47
5	M	424	ILE	CA-C	-5.17	1.45	1.52
16	h	174	PRO	N-CD	-5.15	1.40	1.47
14	f	38	ARG	CA-C	-5.13	1.46	1.52
8	U	140	CYS	C-O	-5.07	1.17	1.23
1	D	63	PRO	N-CD	-5.04	1.40	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	159	PRO	N-CD	5.04	1.54	1.47

All (531) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	N	255	PRO	N-CA-C	14.59	128.50	110.70
5	M	370	PRO	N-CA-C	14.59	128.50	110.70
7	O	83	MET	O-C-N	14.43	140.50	122.89
7	O	118	TYR	N-CA-C	13.88	125.92	111.07
7	O	83	MET	CA-C-N	-13.70	100.06	120.75
7	O	83	MET	C-N-CA	-13.70	100.06	120.75
22	n	165	PRO	N-CA-C	13.37	130.45	111.33
23	o	118	LYS	N-CA-C	-12.86	97.31	111.07
24	p	128	GLU	N-CA-C	12.55	125.04	111.36
7	O	157	VAL	N-CA-C	11.68	124.46	108.11
5	M	424	ILE	N-CA-C	-11.66	94.03	109.30
17	i	14	GLN	N-CA-C	11.59	123.91	111.28
5	M	104	ILE	N-CA-C	-11.49	99.15	110.30
7	O	114	LEU	N-CA-C	-11.47	98.86	111.36
4	L	194	ASN	N-CA-C	11.41	125.31	109.11
6	N	244	ILE	N-CA-C	-11.36	99.25	110.72
4	L	278	LEU	N-CA-C	-11.26	98.98	111.14
3	K	83	ASN	N-CA-C	-11.15	100.21	114.04
5	M	455	THR	N-CA-C	-10.96	95.44	110.35
4	L	582	GLY	N-CA-C	-10.83	99.47	114.64
4	L	556	ILE	N-CA-C	10.76	121.42	110.23
18	j	82	GLY	N-CA-C	-10.74	91.03	111.02
4	L	231	PRO	N-CA-C	10.71	127.76	113.84
16	h	101	ILE	N-CA-C	-10.53	98.63	108.95
7	O	96	THR	N-CA-C	-10.36	100.07	111.36
2	J	122	ASP	N-CA-C	-10.35	98.81	111.33
5	M	276	CYS	N-CA-C	-10.34	100.01	111.28
7	O	247	PRO	N-CA-CB	10.22	114.29	103.15
20	l	170	ARG	N-CA-C	-10.13	101.56	113.21
5	M	117	MET	N-CA-C	-9.99	100.39	111.28
5	M	423	MET	N-CA-C	-9.78	96.86	110.35
3	K	90	VAL	N-CA-C	-9.77	100.35	112.76
6	N	255	PRO	CA-N-CD	9.70	125.58	112.00
6	N	286	ALA	N-CA-C	-9.66	100.75	111.28
5	M	83	HIS	N-CA-C	-9.64	97.23	110.35
22	n	29	SER	N-CA-C	-9.52	101.56	113.55
4	L	375	ILE	N-CA-C	-9.52	101.28	110.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	d	115	PRO	N-CA-CB	-9.50	95.09	103.35
2	J	36	GLY	N-CA-C	-9.46	101.04	112.49
6	N	228	ASN	N-CA-C	-9.45	100.96	111.07
24	p	56	HIS	N-CA-C	9.44	121.56	111.28
14	f	51	ASN	CB-CA-C	-9.37	97.35	112.06
5	M	104	ILE	N-CA-CB	9.35	120.81	110.62
12	d	115	PRO	CA-N-CD	9.34	125.08	112.00
4	L	394	LEU	N-CA-C	-9.30	101.12	111.07
19	k	60	MET	N-CA-C	9.28	121.09	110.97
19	k	56	ALA	N-CA-C	9.26	121.45	111.36
4	L	40	ILE	N-CA-C	-9.23	101.40	110.72
4	L	467	VAL	N-CA-C	9.17	119.22	110.42
21	m	48	LEU	N-CA-C	9.16	124.01	113.01
4	L	483	PRO	N-CA-C	-9.16	96.81	111.38
6	N	326	PHE	N-CA-C	-9.15	101.28	111.07
6	N	87	GLN	N-CA-C	9.10	123.25	109.41
7	O	247	PRO	CA-N-CD	-9.09	99.27	112.00
5	M	442	ILE	N-CA-CB	9.09	117.54	110.45
11	c	64	GLU	N-CA-C	-9.07	101.36	111.07
11	c	39	PRO	N-CA-CB	-9.05	95.28	103.25
4	L	524	THR	N-CA-C	8.99	122.25	111.82
23	o	97	LYS	N-CA-C	-8.97	101.47	111.07
24	p	115	GLN	N-CA-C	-8.95	102.88	113.88
3	K	70	GLU	N-CA-C	-8.93	100.39	111.11
4	L	406	ALA	N-CA-C	-8.90	101.65	111.36
2	J	43	VAL	N-CA-C	-8.89	101.55	110.62
4	L	344	GLY	N-CA-C	-8.87	102.21	112.50
6	N	233	LEU	N-CA-C	-8.86	101.62	111.28
7	O	183	CYS	N-CA-C	-8.86	100.48	111.11
7	O	206	TYR	N-CA-CB	-8.83	92.81	110.64
22	n	70	GLU	N-CA-C	-8.79	101.67	111.07
5	M	255	LYS	N-CA-C	-8.77	101.68	111.07
6	N	255	PRO	N-CA-CB	-8.76	94.58	103.08
4	L	526	LEU	N-CA-CB	-8.75	99.00	112.30
23	o	72	ASP	N-CA-C	-8.73	99.01	110.53
6	N	81	LEU	N-CA-C	-8.71	94.44	108.55
17	i	12	LEU	N-CA-C	-8.60	101.11	111.69
5	M	248	ILE	N-CA-C	-8.60	102.17	110.42
2	J	29	GLY	N-CA-C	-8.59	102.25	112.64
4	L	212	PRO	N-CA-C	8.57	125.73	113.47
7	O	315	PRO	CA-N-CD	8.52	123.93	112.00
8	U	154	VAL	N-CA-C	8.47	119.75	106.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	N	221	LEU	N-CA-C	-8.43	101.13	111.33
4	L	281	GLY	N-CA-C	-8.42	102.73	112.50
7	O	212	PRO	N-CA-C	8.38	126.24	113.75
6	N	272	LYS	N-CA-C	-8.38	102.15	111.28
4	L	287	PHE	N-CA-C	-8.36	102.13	111.07
22	n	19	LEU	N-CA-C	-8.33	103.25	113.41
6	N	157	LEU	N-CA-C	-8.32	102.16	111.07
6	N	218	ALA	N-CA-C	-8.25	98.93	111.56
4	L	88	LEU	N-CA-C	-8.19	102.29	111.14
5	M	274	SER	N-CA-C	8.18	120.19	111.28
5	M	26	ASN	N-CA-C	-8.17	102.31	111.14
7	O	245	PHE	N-CA-C	8.15	120.17	111.28
4	L	169	LEU	N-CA-C	-8.15	102.48	111.36
6	N	32	GLY	N-CA-C	-8.13	103.07	112.50
4	L	151	SER	N-CA-C	-8.12	102.51	111.36
7	O	217	ARG	N-CA-C	-8.09	102.42	111.07
19	k	38	VAL	N-CA-C	-8.08	102.56	110.72
12	d	15	PRO	N-CA-CB	-8.08	96.32	103.35
22	n	170	ILE	N-CA-C	-8.07	103.03	111.58
5	M	205	ILE	N-CA-C	8.03	118.13	110.42
8	U	74	LEU	N-CA-C	8.03	122.04	108.23
4	L	276	THR	N-CA-CB	8.01	121.62	110.01
5	M	385	LEU	N-CA-C	-8.00	102.56	111.28
1	D	36	GLN	N-CA-C	-7.99	98.49	110.24
2	J	60	LEU	N-CA-C	7.95	120.72	111.02
11	c	39	PRO	CA-N-CD	7.94	123.11	112.00
5	M	141	GLU	N-CA-C	7.89	122.75	113.20
17	i	10	LEU	N-CA-C	-7.89	104.14	114.31
11	c	45	GLY	N-CA-C	7.86	123.53	113.24
24	p	128	GLU	N-CA-CB	-7.84	98.56	110.16
5	M	85	LYS	N-CA-C	-7.81	101.38	113.02
3	K	51	SER	N-CA-C	-7.81	102.84	113.30
4	L	265	PRO	N-CA-CB	7.81	111.66	103.15
21	m	50	GLN	N-CA-C	-7.80	102.78	114.64
4	L	111	ASP	N-CA-C	-7.78	100.28	109.93
4	L	265	PRO	CA-N-CD	-7.77	101.13	112.00
5	M	330	ALA	N-CA-C	-7.76	102.75	111.14
4	L	265	PRO	N-CA-C	-7.70	101.31	113.78
4	L	415	ALA	N-CA-C	-7.68	102.91	111.28
2	J	124	LEU	N-CA-C	-7.64	103.81	113.43
14	f	48	LEU	N-CA-C	7.63	121.75	110.30
14	f	51	ASN	N-CA-C	7.63	121.94	111.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	g	124	VAL	N-CA-C	-7.59	103.05	110.72
8	U	147	TYR	N-CA-C	-7.54	102.99	111.14
4	L	245	ALA	N-CA-C	7.54	119.14	111.07
23	o	81	LYS	N-CA-C	-7.54	104.61	113.88
4	L	605	ASN	N-CA-CB	7.53	121.39	110.47
13	e	46	GLY	N-CA-C	-7.50	104.92	114.37
3	K	14	LEU	N-CA-C	-7.44	103.25	111.36
4	L	392	LYS	N-CA-C	7.43	119.02	111.07
4	L	138	PHE	N-CA-C	-7.40	103.21	111.28
4	L	123	LEU	N-CA-C	-7.39	103.30	111.36
12	d	113	LEU	N-CA-CB	-7.38	99.94	111.23
20	l	36	MET	N-CA-C	-7.37	103.42	113.30
4	L	21	ILE	N-CA-CB	7.37	121.63	110.58
4	L	19	ILE	N-CA-C	7.36	117.49	110.42
20	l	97	LEU	N-CA-C	-7.36	103.89	113.17
4	L	526	LEU	N-CA-C	7.36	121.66	112.24
21	m	72	ARG	N-CA-C	7.36	122.55	113.50
5	M	250	LEU	N-CA-C	-7.35	103.61	112.58
4	L	28	LYS	N-CA-C	-7.34	103.28	111.28
9	X	152	PRO	N-CA-CB	-7.31	96.52	103.39
11	c	37	ALA	N-CA-C	7.28	119.84	111.11
5	M	289	SER	N-CA-C	-7.27	103.29	111.07
23	o	118	LYS	N-CA-CB	7.27	120.55	110.01
22	n	165	PRO	CB-CA-C	-7.27	100.21	111.40
16	h	174	PRO	N-CA-C	7.26	122.66	111.11
4	L	527	GLY	N-CA-C	-7.25	105.71	115.36
7	O	224	PRO	N-CA-CB	-7.22	96.75	103.46
6	N	332	MET	N-CA-C	-7.21	103.36	111.07
2	J	121	GLY	N-CA-C	-7.20	106.28	115.42
8	U	136	GLU	N-CA-C	-7.20	104.49	113.20
2	J	21	LEU	N-CA-C	-7.18	104.61	113.15
3	K	81	VAL	N-CA-C	7.18	117.94	110.62
3	K	24	SER	CB-CA-C	-7.17	107.48	117.23
19	k	73	ILE	N-CA-C	-7.17	103.31	110.62
7	O	210	PRO	CA-N-CD	7.15	122.01	112.00
18	j	78	ASP	N-CA-C	-7.12	103.16	112.41
24	p	168	LYS	N-CA-C	-7.11	104.23	113.12
22	n	102	TRP	N-CA-C	-7.10	104.98	112.93
4	L	554	ASP	N-CA-CB	7.08	121.19	110.42
5	M	244	ILE	N-CA-C	7.08	117.84	110.62
5	M	325	LEU	N-CA-C	-7.08	103.50	111.07
3	K	48	SER	N-CA-C	-7.07	103.58	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	O	210	PRO	N-CA-C	7.05	122.27	111.34
6	N	103	SER	N-CA-C	-7.04	103.65	111.82
4	L	319	MET	N-CA-C	-7.03	104.70	112.72
5	M	365	ALA	N-CA-C	-7.02	103.70	111.36
18	j	65	MET	N-CA-C	-7.02	103.56	111.07
18	j	81	LEU	CA-C-O	7.02	126.02	119.00
5	M	34	ILE	N-CA-C	-7.01	103.47	110.62
4	L	546	LEU	N-CA-C	6.98	119.53	111.02
5	M	264	LEU	N-CA-C	-6.97	103.61	111.07
5	M	213	HIS	CB-CA-C	-6.97	96.88	110.11
4	L	100	ILE	N-CA-C	6.96	119.75	111.05
4	L	471	ASN	N-CA-C	6.95	118.93	111.36
5	M	91	LEU	N-CA-C	-6.94	103.81	112.90
7	O	231	SER	N-CA-C	-6.92	103.82	111.36
4	L	86	SER	N-CA-C	6.91	118.46	111.07
5	M	235	LEU	N-CA-C	6.88	119.36	111.11
4	L	26	LEU	N-CA-C	6.88	119.62	111.71
22	n	117	ASP	N-CA-C	-6.87	103.85	111.82
15	g	78	PRO	CA-N-CD	6.87	121.61	112.00
5	M	276	CYS	N-CA-CB	6.86	120.20	110.12
5	M	442	ILE	N-CA-C	-6.86	104.12	112.35
3	K	83	ASN	N-CA-CB	6.85	120.95	110.81
5	M	165	ILE	N-CA-C	-6.85	102.53	111.09
19	k	59	TYR	N-CA-CB	-6.85	98.90	110.41
6	N	194	LEU	CA-C-N	-6.80	112.69	120.04
6	N	194	LEU	C-N-CA	-6.80	112.69	120.04
3	K	70	GLU	N-CA-CB	6.80	120.07	109.94
4	L	547	LYS	N-CA-C	6.79	118.68	111.28
21	m	127	ILE	N-CA-C	-6.79	106.18	112.43
2	J	58	ILE	N-CA-C	6.79	117.40	111.56
7	O	93	TYR	N-CA-C	-6.79	103.96	111.36
6	N	162	ILE	N-CA-C	-6.79	103.91	110.42
18	j	79	ALA	N-CA-C	-6.78	103.98	111.36
17	i	5	THR	N-CA-C	-6.77	101.82	109.60
12	d	88	HIS	N-CA-C	-6.76	102.99	111.11
5	M	374	ASN	N-CA-C	-6.73	103.87	111.07
23	o	11	TRP	CB-CA-C	-6.73	108.80	116.54
15	g	76	SER	N-CA-C	6.72	118.26	111.07
8	U	140	CYS	N-CA-C	-6.72	100.81	110.08
5	M	248	ILE	N-CA-CB	6.71	118.40	110.55
8	U	150	ASP	CB-CA-C	6.71	121.93	110.79
7	O	207	ILE	N-CA-C	-6.70	97.28	107.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	95	PHE	N-CA-C	-6.69	103.91	111.07
8	U	151	LYS	N-CA-C	6.68	119.13	111.11
20	l	86	ARG	N-CA-C	-6.68	99.64	110.20
7	O	224	PRO	CA-N-CD	6.67	121.34	112.00
8	U	140	CYS	CA-C-N	-6.67	114.03	120.83
8	U	140	CYS	C-N-CA	-6.67	114.03	120.83
6	N	228	ASN	N-CA-CB	6.67	119.68	110.01
5	M	410	MET	N-CA-C	-6.66	103.94	111.07
4	L	499	LEU	N-CA-C	-6.66	103.71	110.97
3	K	76	ALA	N-CA-C	-6.64	104.12	111.36
7	O	315	PRO	N-CA-CB	-6.64	96.02	103.33
5	M	143	LEU	N-CA-C	-6.62	103.98	111.07
6	N	323	ASN	N-CA-C	6.62	119.35	110.35
8	U	98	LEU	N-CA-C	-6.60	100.40	110.30
5	M	303	ILE	N-CA-C	-6.58	104.07	110.72
19	k	57	TRP	N-CA-C	-6.57	104.52	112.54
7	O	140	LEU	N-CA-C	-6.56	104.05	111.07
21	m	51	TYR	N-CA-C	-6.56	105.58	113.97
4	L	130	ILE	N-CA-C	-6.54	103.94	110.62
6	N	173	THR	N-CA-C	-6.54	105.02	114.12
4	L	232	TRP	N-CA-C	6.54	120.52	112.54
22	n	115	TYR	N-CA-CB	6.53	122.00	110.37
24	p	54	ARG	N-CA-C	-6.52	103.67	111.69
5	M	161	LEU	N-CA-C	-6.50	104.12	111.07
9	X	152	PRO	CA-N-CD	6.50	121.10	112.00
7	O	118	TYR	N-CA-CB	-6.49	100.59	110.01
6	N	315	THR	N-CA-C	-6.47	104.22	111.28
4	L	423	SER	N-CA-C	-6.47	104.14	111.07
8	U	153	ASP	N-CA-CB	-6.46	101.54	111.74
4	L	329	ILE	N-CA-C	-6.46	104.22	110.42
10	Y	96	GLY	N-CA-C	-6.44	104.53	112.77
7	O	320	GLY	N-CA-C	-6.43	96.63	111.04
9	X	168	PHE	CB-CA-C	-6.42	101.91	109.80
6	N	145	ILE	N-CA-C	-6.41	106.20	111.91
5	M	455	THR	N-CA-CB	6.41	119.46	110.04
4	L	325	ALA	N-CA-C	-6.40	104.31	111.28
3	K	11	ALA	N-CA-C	-6.38	104.24	111.07
4	L	234	PRO	CA-N-CD	-6.38	103.07	112.00
15	g	112	MET	N-CA-C	6.36	120.82	113.38
4	L	70	THR	N-CA-C	-6.36	103.87	111.69
4	L	387	THR	N-CA-C	6.35	119.01	111.71
12	d	15	PRO	CA-N-CD	6.34	120.88	112.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	32	PHE	N-CA-C	-6.34	104.29	111.07
4	L	439	PRO	N-CA-C	6.33	122.33	113.53
17	i	32	GLU	CA-C-N	-6.33	111.92	119.84
17	i	32	GLU	C-N-CA	-6.33	111.92	119.84
7	O	98	THR	N-CA-C	6.33	120.59	109.96
5	M	26	ASN	N-CA-CB	6.31	119.22	110.07
4	L	490	ALA	N-CA-C	-6.30	104.32	111.07
4	L	337	ALA	N-CA-C	-6.29	104.42	111.28
6	N	89	GLN	N-CA-C	6.29	120.51	112.34
21	m	17	THR	N-CA-C	-6.28	102.24	110.53
20	l	105	ILE	CA-C-O	-6.27	115.13	121.59
11	c	47	SER	N-CA-CB	6.27	120.87	110.33
5	M	317	ILE	N-CA-C	-6.27	104.64	110.53
14	f	52	GLU	N-CA-CB	6.26	121.10	110.71
2	J	126	TYR	N-CA-C	6.24	119.02	111.40
6	N	46	ASN	N-CA-C	-6.23	105.70	113.55
15	g	123	LEU	N-CA-CB	6.22	119.09	110.07
7	O	113	SER	N-CA-C	6.22	118.55	108.41
8	U	137	LYS	CA-C-N	-6.21	113.66	122.41
8	U	137	LYS	C-N-CA	-6.21	113.66	122.41
4	L	502	LEU	N-CA-C	-6.20	104.52	111.28
8	U	105	MET	N-CA-C	6.20	119.31	111.69
6	N	216	PHE	N-CA-C	6.19	118.11	111.36
6	N	276	LEU	N-CA-C	-6.19	105.37	113.17
6	N	91	ASN	N-CA-CB	6.18	119.06	109.97
19	k	59	TYR	N-CA-C	6.18	120.66	113.18
21	m	72	ARG	CA-C-O	6.17	125.92	119.14
23	o	110	GLN	N-CA-C	-6.17	104.64	111.36
4	L	98	TRP	N-CA-C	-6.14	104.67	111.36
16	h	101	ILE	N-CA-CB	6.14	115.79	110.08
14	f	49	ARG	N-CA-CB	6.13	119.06	110.11
22	n	63	LEU	N-CA-C	-6.13	104.15	111.69
6	N	47	LYS	N-CA-C	-6.12	104.72	111.82
1	D	57	GLU	N-CA-CB	-6.12	102.84	112.08
19	k	30	ILE	N-CA-C	6.12	118.74	111.09
4	L	361	ASN	CB-CA-C	-6.12	102.87	111.80
5	M	4	ILE	N-CA-C	-6.12	104.00	112.50
23	o	105	GLU	N-CA-C	-6.12	104.69	111.36
5	M	121	LEU	N-CA-C	-6.10	104.71	111.36
7	O	210	PRO	N-CA-CB	-6.10	97.66	103.39
4	L	287	PHE	N-CA-CB	6.09	118.85	110.01
6	N	91	ASN	N-CA-C	-6.09	101.26	110.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	c	33	GLU	CA-C-N	-6.09	114.00	120.03
11	c	33	GLU	C-N-CA	-6.09	114.00	120.03
14	f	39	ASN	N-CA-C	-6.08	104.02	112.30
15	g	109	ASP	CA-CB-CG	6.07	118.67	112.60
5	M	57	SER	N-CA-C	6.06	119.08	109.50
23	o	116	ALA	N-CA-C	6.06	118.66	111.33
15	g	123	LEU	N-CA-C	-6.06	104.60	111.14
16	h	142	ILE	N-CA-C	-6.04	104.62	110.42
4	L	140	LEU	N-CA-C	-6.04	104.70	111.28
4	L	454	ILE	N-CA-C	-6.03	104.47	110.62
5	M	3	LYS	N-CA-C	-6.03	106.06	113.41
5	M	213	HIS	N-CA-C	6.03	120.49	113.20
15	g	78	PRO	N-CA-C	6.02	121.90	113.53
5	M	396	MET	N-CA-C	-6.02	105.92	113.20
7	O	234	LEU	N-CA-C	-6.01	104.81	111.36
4	L	234	PRO	N-CA-CB	6.01	109.66	103.23
11	c	47	SER	N-CA-C	-6.01	104.69	112.68
4	L	102	GLN	N-CA-C	-6.00	104.81	111.36
6	N	295	ARG	N-CA-C	-6.00	104.73	111.28
7	O	183	CYS	N-CA-CB	5.99	118.87	109.94
5	M	370	PRO	CA-N-CD	5.98	120.38	112.00
5	M	88	ASN	N-CA-C	5.98	120.20	113.02
5	M	222	GLU	N-CA-C	5.98	120.42	113.18
24	p	127	LYS	N-CA-C	-5.97	104.12	111.40
5	M	300	SER	N-CA-C	-5.96	106.99	114.56
24	p	8	ASP	N-CA-C	5.95	120.61	113.23
7	O	181	LYS	N-CA-C	5.94	117.43	111.07
6	N	98	THR	N-CA-C	-5.94	104.81	111.28
5	M	234	ILE	N-CA-CB	-5.92	104.90	111.41
6	N	140	SER	N-CA-C	-5.91	104.92	111.36
14	f	53	GLU	N-CA-CB	-5.91	101.39	110.20
4	L	112	PRO	CB-CA-C	-5.91	103.05	111.68
4	L	278	LEU	N-CA-CB	5.91	118.64	110.07
5	M	253	LEU	N-CA-C	5.90	117.71	111.28
4	L	248	HIS	CB-CA-C	5.90	120.88	110.85
4	L	247	LEU	N-CA-CB	5.90	120.60	110.34
4	L	88	LEU	N-CA-CB	5.89	118.61	110.07
2	J	155	ALA	N-CA-C	-5.89	104.94	111.36
19	k	80	GLY	N-CA-C	-5.89	105.67	112.50
6	N	66	ALA	N-CA-C	-5.88	104.95	111.36
7	O	130	ARG	N-CA-C	-5.88	104.87	111.28
8	U	143	GLU	N-CA-C	-5.88	104.23	111.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	N	16	GLY	CA-C-N	-5.87	112.45	118.85
6	N	16	GLY	C-N-CA	-5.87	112.45	118.85
4	L	387	THR	CB-CA-C	-5.87	99.77	110.63
1	D	58	THR	N-CA-C	-5.87	105.88	114.39
21	m	116	ILE	N-CA-C	-5.87	104.79	110.42
7	O	221	LYS	N-CA-C	-5.85	101.75	110.23
7	O	222	GLY	N-CA-C	5.84	120.25	112.77
8	U	153	ASP	CB-CA-C	5.83	120.63	112.11
22	n	27	LEU	N-CA-C	-5.83	106.14	113.72
19	k	50	PRO	N-CA-C	5.83	121.63	113.53
7	O	217	ARG	N-CA-CB	5.82	118.45	110.01
14	f	52	GLU	N-CA-C	-5.82	98.01	108.48
19	k	82	ALA	N-CA-C	-5.82	104.94	111.28
7	O	262	GLU	N-CA-C	-5.82	104.94	111.28
5	M	272	THR	N-CA-C	-5.80	105.04	111.36
4	L	428	TYR	N-CA-C	-5.79	104.88	111.14
12	d	62	LEU	N-CA-C	5.79	117.59	111.28
22	n	52	LYS	N-CA-C	-5.78	105.89	113.12
20	l	186	ILE	N-CA-CB	-5.78	101.68	111.50
8	U	83	VAL	N-CA-C	-5.76	104.90	110.72
4	L	23	MET	N-CA-CB	5.76	118.36	110.01
6	N	15	LEU	N-CA-C	-5.75	105.76	112.89
12	d	53	VAL	N-CA-C	5.75	116.40	110.36
18	j	73	PHE	N-CA-C	-5.75	104.92	111.07
2	J	76	GLU	N-CA-C	-5.74	105.61	113.30
4	L	467	VAL	N-CA-CB	-5.74	103.84	110.55
4	L	495	VAL	N-CA-C	5.74	115.93	110.42
23	o	71	ARG	N-CA-C	-5.73	104.41	111.40
5	M	124	ALA	N-CA-C	-5.73	105.12	111.36
15	g	78	PRO	N-CA-CB	-5.73	97.03	103.33
4	L	177	ILE	N-CA-C	-5.72	104.78	110.62
5	M	19	SER	N-CA-C	5.72	117.80	109.84
4	L	605	ASN	N-CA-C	-5.72	106.16	113.02
15	g	67	LYS	N-CA-C	-5.71	102.01	110.46
12	d	4	GLY	N-CA-C	-5.70	108.18	115.42
5	M	424	ILE	O-C-N	5.69	128.31	122.79
5	M	279	GLN	N-CA-C	-5.69	98.62	108.69
14	f	36	ALA	N-CA-C	-5.69	103.41	110.41
6	N	232	LEU	N-CA-C	-5.68	106.57	112.93
2	J	107	ASN	N-CA-C	-5.68	105.23	111.82
4	L	371	SER	N-CA-C	-5.67	105.02	111.14
4	L	419	THR	N-CA-C	-5.67	105.10	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	i	5	THR	N-CA-CB	5.66	118.07	109.75
17	i	14	GLN	N-CA-CB	-5.66	101.81	110.12
6	N	148	LEU	N-CA-C	5.65	117.52	111.36
21	m	104	VAL	N-CA-C	-5.65	105.59	111.58
17	i	84	TYR	N-CA-C	-5.65	105.12	111.28
5	M	214	LEU	N-CA-C	-5.64	105.65	112.54
20	l	49	ALA	N-CA-C	-5.64	106.56	113.50
20	l	119	THR	N-CA-C	-5.64	95.76	107.67
7	O	214	VAL	N-CA-CB	5.64	119.05	110.58
4	L	342	CYS	N-CA-CB	5.63	118.18	110.01
4	L	151	SER	N-CA-CB	5.63	118.49	110.16
21	m	60	ILE	N-CA-C	-5.62	101.94	109.30
4	L	20	LEU	N-CA-C	5.61	119.84	112.89
15	g	122	ARG	N-CA-C	5.60	118.32	111.82
4	L	234	PRO	N-CA-C	-5.60	105.47	113.47
15	g	107	VAL	N-CA-C	-5.59	102.86	108.96
24	p	115	GLN	N-CA-CB	5.59	118.03	110.59
4	L	214	MET	N-CA-C	-5.59	105.27	111.36
6	N	192	ALA	N-CA-C	-5.58	105.20	111.28
15	g	113	GLN	CA-C-O	5.58	126.25	119.11
4	L	445	GLU	CB-CA-C	-5.58	101.98	111.02
6	N	251	LEU	N-CA-C	-5.56	105.22	111.28
15	g	140	PHE	N-CA-CB	5.56	118.27	109.71
8	U	154	VAL	CB-CA-C	-5.55	104.20	111.81
4	L	155	ILE	N-CA-C	-5.55	105.31	110.53
6	N	36	SER	N-CA-C	-5.55	105.23	111.28
24	p	120	ASN	N-CA-C	-5.54	105.14	113.89
21	m	46	GLU	N-CA-C	-5.53	106.53	113.72
4	L	394	LEU	N-CA-CB	5.51	118.00	110.01
5	M	355	MET	N-CA-C	-5.51	104.66	111.33
4	L	465	GLY	N-CA-C	-5.51	105.72	112.77
6	N	123	PRO	CA-N-CD	5.50	119.71	112.00
24	p	94	ARG	N-CA-C	5.50	116.96	111.07
4	L	370	SER	N-CA-C	-5.50	105.37	111.36
5	M	223	ALA	N-CA-CB	5.50	118.13	110.11
4	L	152	PHE	N-CA-C	-5.49	105.19	111.07
5	M	370	PRO	N-CA-CB	-5.49	97.75	103.08
11	c	64	GLU	N-CA-CB	5.49	117.97	110.01
5	M	234	ILE	N-CA-C	5.49	116.28	111.56
5	M	73	LEU	N-CA-C	-5.48	105.30	112.75
6	N	62	THR	N-CA-C	-5.46	105.23	111.07
4	L	543	ASN	N-CA-C	-5.46	105.33	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	194	ASN	CB-CA-C	-5.45	103.38	111.72
22	n	136	GLU	CB-CA-C	5.45	121.26	110.42
15	g	137	SER	N-CA-CB	-5.44	101.27	110.41
4	L	550	LEU	CA-C-O	-5.43	115.19	120.89
5	M	174	LEU	N-CA-C	-5.42	106.45	112.57
6	N	177	LYS	N-CA-C	-5.42	105.38	111.28
23	o	74	PHE	CA-C-N	-5.41	114.04	119.56
23	o	74	PHE	C-N-CA	-5.41	114.04	119.56
4	L	21	ILE	N-CA-C	-5.41	105.25	110.72
4	L	183	ILE	N-CA-C	-5.41	105.10	110.62
7	O	175	ASN	N-CA-C	-5.41	105.39	111.28
15	g	80	VAL	N-CA-C	-5.40	105.24	110.42
17	i	77	ILE	CB-CA-C	-5.40	108.63	114.35
6	N	89	GLN	N-CA-CB	-5.39	100.47	110.18
9	X	169	PHE	N-CA-C	5.39	119.44	112.86
21	m	52	ASN	N-CA-C	-5.39	105.15	112.26
4	L	311	GLY	N-CA-C	-5.38	106.28	112.73
6	N	143	ILE	N-CA-C	-5.38	105.29	110.72
6	N	155	LEU	N-CA-CB	5.38	117.81	110.01
2	J	133	VAL	N-CA-C	-5.37	107.89	113.10
18	j	64	LEU	N-CA-C	-5.37	105.51	111.36
5	M	409	TYR	N-CA-C	-5.37	105.59	111.82
22	n	104	LEU	N-CA-C	-5.36	106.77	113.15
5	M	53	SER	N-CA-C	5.36	115.61	108.38
4	L	415	ALA	N-CA-CB	5.35	117.99	110.12
2	J	99	GLU	N-CA-C	-5.35	105.45	111.28
4	L	386	LEU	N-CA-C	-5.35	101.00	108.96
4	L	413	LEU	N-CA-C	5.34	117.10	111.28
5	M	25	THR	CB-CA-C	-5.34	100.41	110.67
5	M	117	MET	N-CA-CB	5.34	117.97	110.12
4	L	137	MET	N-CA-C	5.34	119.41	113.01
8	U	141	PRO	N-CA-C	-5.32	109.14	114.68
4	L	231	PRO	CB-CA-C	-5.32	104.30	111.85
5	M	343	ILE	N-CA-C	5.32	116.04	110.62
5	M	167	ILE	N-CA-C	5.31	117.69	111.05
4	L	494	SER	N-CA-C	-5.30	105.42	111.14
6	N	218	ALA	N-CA-CB	5.30	118.41	110.14
7	O	219	GLN	N-CA-C	5.30	117.47	111.11
7	O	264	GLU	N-CA-C	-5.28	107.20	113.38
4	L	190	SER	N-CA-C	-5.27	106.70	113.23
7	O	206	TYR	N-CA-C	5.27	118.87	107.49
22	n	26	HIS	N-CA-C	-5.26	106.44	112.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	N	154	ILE	CB-CA-C	-5.26	103.73	112.26
15	g	68	ASN	N-CA-CB	5.25	119.02	111.51
5	M	294	MET	N-CA-C	-5.25	106.90	113.72
8	U	133	ILE	CB-CA-C	-5.24	104.03	112.16
22	n	12	HIS	N-CA-C	-5.24	105.00	111.40
6	N	155	LEU	N-CA-C	-5.24	105.46	111.07
6	N	326	PHE	N-CA-CB	5.23	117.60	110.01
6	N	104	MET	N-CA-C	-5.23	105.47	111.07
4	L	375	ILE	N-CA-CB	5.23	116.67	110.55
16	h	129	PRO	N-CA-C	-5.23	106.72	113.57
17	i	105	PHE	N-CA-CB	-5.22	101.05	110.39
5	M	212	VAL	CB-CA-C	-5.22	105.21	112.36
5	M	20	PRO	N-CA-C	-5.21	106.28	113.53
4	L	497	GLY	N-CA-C	-5.21	106.46	112.50
16	h	158	ARG	N-CA-C	-5.21	105.52	111.14
24	p	167	ARG	CB-CA-C	5.21	117.25	109.13
4	L	396	ILE	O-C-N	5.20	127.00	121.91
5	M	317	ILE	N-CA-CB	5.18	117.20	110.57
4	L	332	HIS	N-CA-C	-5.18	105.64	111.28
5	M	98	MET	N-CA-C	-5.18	105.53	111.07
8	U	133	ILE	N-CA-C	5.18	117.52	111.05
4	L	284	THR	N-CA-C	-5.17	105.73	111.36
4	L	485	PHE	N-CA-CB	5.17	117.50	110.01
20	l	37	LEU	N-CA-C	-5.17	102.64	110.50
6	N	90	THR	N-CA-C	5.17	117.58	110.35
18	j	76	ASP	CB-CA-C	-5.16	104.71	112.09
6	N	225	MET	N-CA-C	-5.16	106.58	112.92
12	d	37	LEU	N-CA-C	-5.15	105.66	111.28
4	L	217	LEU	N-CA-C	-5.15	105.67	111.28
6	N	222	ASN	N-CA-C	-5.15	106.23	112.88
24	p	13	PRO	O-C-N	5.14	123.56	121.15
21	m	61	GLU	N-CA-C	5.14	119.63	112.90
16	h	176	LYS	N-CA-C	-5.13	105.86	111.82
4	L	386	LEU	CA-C-O	-5.13	115.96	121.45
23	o	95	TYR	N-CA-C	-5.12	105.59	111.07
4	L	249	SER	N-CA-C	5.12	116.66	111.14
11	c	60	GLN	N-CA-C	-5.11	105.60	111.07
23	o	11	TRP	N-CA-C	5.11	116.08	108.31
14	f	55	THR	N-CA-C	5.10	116.53	110.97
21	m	47	TYR	N-CA-C	-5.10	105.89	112.68
24	p	43	TRP	CA-C-N	-5.09	113.67	118.97
24	p	43	TRP	C-N-CA	-5.09	113.67	118.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	N	292	PHE	CA-CB-CG	5.08	118.88	113.80
20	l	168	LEU	N-CA-C	-5.08	105.65	111.14
1	D	63	PRO	N-CA-C	5.08	116.90	110.70
10	Y	72	PHE	N-CA-C	-5.08	105.64	111.07
5	M	56	PHE	N-CA-C	5.08	116.80	108.52
5	M	86	LYS	N-CA-C	-5.08	106.33	112.88
5	M	30	TYR	N-CA-C	5.07	116.81	111.28
5	M	330	ALA	N-CA-CB	5.07	117.43	110.07
17	i	11	ARG	N-CA-C	-5.07	105.45	111.69
15	g	137	SER	N-CA-C	5.07	119.31	113.18
6	N	42	PRO	CB-CA-C	-5.07	105.01	113.06
17	i	16	ARG	N-CA-C	-5.06	105.76	111.28
5	M	32	PHE	N-CA-CB	5.06	117.35	110.01
6	N	282	MET	N-CA-C	-5.05	105.66	111.07
22	n	169	HIS	CB-CA-C	5.05	118.71	110.17
8	U	132	ASP	N-CA-C	5.05	117.18	111.02
11	c	39	PRO	N-CA-C	5.04	119.12	111.15
4	L	384	PRO	N-CA-CB	5.04	107.73	103.35
11	c	46	LEU	CA-C-O	5.04	125.18	119.18
20	l	45	PRO	N-CA-C	5.04	120.45	113.65
15	g	109	ASP	CB-CA-C	5.04	119.04	111.89
5	M	234	ILE	CB-CA-C	5.03	116.22	111.44
7	O	212	PRO	CA-N-CD	5.03	119.04	112.00
12	d	60	ARG	N-CA-C	-5.03	105.71	111.14
5	M	229	MET	N-CA-C	-5.02	105.70	111.07
6	N	64	ALA	N-CA-C	5.01	116.43	111.07
15	g	124	VAL	N-CA-CB	5.01	118.09	110.58
4	L	212	PRO	CA-N-CD	5.01	119.01	112.00
16	h	161	ARG	N-CA-C	-5.01	105.51	110.97
3	K	48	SER	N-CA-CB	5.00	117.48	110.12
2	J	59	TYR	N-CA-C	-5.00	105.30	111.40
5	M	267	TRP	N-CA-C	-5.00	105.91	111.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	320	0	287	41	0
2	J	1205	0	1229	125	0
3	K	729	0	764	94	0
4	L	4798	0	4986	623	0
5	M	3622	0	3845	543	0
6	N	2694	0	2896	399	0
7	O	2599	0	2552	265	0
8	U	678	0	677	90	0
9	X	221	0	215	21	0
10	Y	1030	0	1015	82	0
11	c	389	0	385	27	0
12	d	988	0	989	90	0
13	e	863	0	850	75	0
14	f	475	0	472	42	0
15	g	858	0	787	70	0
16	h	1146	0	1153	121	0
17	i	796	0	797	122	0
18	j	563	0	510	67	0
19	k	569	0	568	53	0
20	l	1328	0	1218	89	0
21	m	1054	0	1064	96	0
22	n	1541	0	1470	138	0
23	o	1027	0	1018	101	0
24	p	1438	0	1404	124	0
25	J	46	0	66	5	0
25	L	225	0	332	54	0
25	M	153	0	246	26	0
25	N	37	0	48	14	0
25	O	31	0	36	5	0
25	Y	40	0	54	20	0
26	L	163	0	217	38	0
26	X	67	0	81	9	0
26	h	70	0	87	15	0
27	O	27	0	12	6	0
28	n	32	0	0	0	0
All	All	31822	0	32330	2849	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 44.

All (2849) 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)
7:O:247:PRO:CD	7:O:247:PRO:N	1.71	1.39
4:L:302:ILE:HG22	4:L:340:PHE:CZ	1.64	1.31
3:K:66:PHE:HZ	6:N:35:PHE:CZ	1.49	1.29
4:L:358:LYS:HG3	22:n:80:TYR:CZ	1.66	1.29
7:O:168:VAL:HG21	7:O:241:TYR:CZ	1.66	1.29
3:K:66:PHE:CZ	6:N:35:PHE:CZ	2.26	1.21
4:L:13:ILE:HD11	25:L:701:3PE:C2C	1.70	1.20
4:L:437:PHE:CE1	4:L:441:ILE:HG12	1.77	1.19
8:U:90:TYR:CE2	8:U:92:LYS:HB2	1.76	1.19
2:J:5:ILE:CG1	3:K:4:THR:HG21	1.72	1.19
6:N:200:LEU:HD21	6:N:265:ILE:HG12	1.24	1.18
16:h:183:PRO:O	16:h:184:LYS:HG2	1.44	1.17
6:N:29:MET:HE2	6:N:141:ILE:HG12	1.23	1.17
6:N:143:ILE:O	6:N:146:TYR:HD2	1.25	1.16
5:M:369:LEU:HD23	5:M:371:PRO:HD2	1.18	1.16
2:J:5:ILE:HG12	3:K:4:THR:HG21	1.23	1.16
4:L:141:PHE:CE2	5:M:375:LEU:HD21	1.81	1.15
1:D:47:PHE:HB3	6:N:227:ILE:HD11	1.20	1.15
4:L:247:LEU:CD1	4:L:248:HIS:CD2	2.30	1.14
5:M:162:ILE:HG23	6:N:271:MET:HE3	1.30	1.13
4:L:358:LYS:CG	22:n:80:TYR:CZ	2.30	1.13
2:J:3:ASN:ND2	2:J:120:LEU:HB2	1.63	1.12
26:L:706:CDL:H522	10:Y:107:THR:CG2	1.78	1.12
4:L:437:PHE:HE1	4:L:441:ILE:HG12	0.96	1.12
6:N:215:MET:CE	6:N:248:LEU:HD21	1.79	1.12
12:d:14:LEU:O	12:d:14:LEU:HD12	1.49	1.12
4:L:16:LEU:HD11	25:L:701:3PE:H2H1	1.30	1.11
8:U:90:TYR:OH	8:U:92:LYS:HD2	1.48	1.11
4:L:229:LEU:HD12	4:L:229:LEU:O	1.51	1.10
4:L:365:ILE:HD12	4:L:366:MET:HG3	1.32	1.10
8:U:105:MET:SD	8:U:139:MET:HE3	1.92	1.10
4:L:141:PHE:CE2	5:M:375:LEU:CD2	2.35	1.10
4:L:121:LEU:HD22	4:L:246:LEU:HD21	1.33	1.09
4:L:13:ILE:HD11	25:L:701:3PE:H2C2	1.33	1.09
17:i:11:ARG:HH22	22:n:154:LEU:HB2	0.99	1.08
19:k:34:PRO:HG2	19:k:59:TYR:CE1	1.88	1.08
4:L:141:PHE:CE2	5:M:370:PRO:HG3	1.87	1.07
4:L:141:PHE:HE2	5:M:375:LEU:CD2	1.67	1.07
4:L:569:LEU:HB2	10:Y:115:MET:HE1	1.36	1.06
26:L:705:CDL:HA62	16:h:68:LEU:HD13	1.37	1.06
5:M:143:LEU:HD21	6:N:303:THR:CG2	1.86	1.06
4:L:16:LEU:HD23	4:L:126:ILE:HD13	1.30	1.06

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:j:97:LEU:HB3	23:o:104:ARG:HB2	1.36	1.05
4:L:141:PHE:HE2	5:M:375:LEU:HD22	1.22	1.05
4:L:141:PHE:HB2	4:L:182:PHE:CE2	1.92	1.05
4:L:550:LEU:HD12	5:M:275:ILE:HB	1.32	1.05
7:O:227:MET:O	7:O:228:LYS:HG2	1.57	1.05
20:l:30:PHE:CZ	20:l:31:HIS:HE1	1.75	1.05
25:L:701:3PE:H122	17:i:89:HIS:ND1	1.71	1.04
6:N:233:LEU:HD23	6:N:241:LEU:HD12	1.36	1.04
5:M:249:ILE:O	5:M:250:LEU:HG	1.58	1.04
4:L:553:LEU:HD11	21:m:93:ALA:HB3	1.41	1.03
2:J:5:ILE:HG13	3:K:4:THR:CG2	1.88	1.03
5:M:127:ILE:CD1	6:N:256:PRO:HG3	1.89	1.03
4:L:173:LEU:HD23	25:L:703:3PE:H321	1.39	1.03
4:L:131:LEU:HD12	4:L:140:LEU:HD12	1.36	1.02
7:O:168:VAL:HG21	7:O:241:TYR:CE1	1.92	1.02
23:o:69:CYS:O	23:o:80:CYS:SG	2.17	1.02
26:L:706:CDL:H522	10:Y:107:THR:HG23	1.40	1.01
5:M:179:LEU:HB3	5:M:249:ILE:HD11	1.42	1.01
4:L:228:GLY:O	4:L:229:LEU:HG	1.61	1.01
4:L:222:GLY:HA2	4:L:229:LEU:HD11	1.40	1.01
25:M:502:3PE:H3A2	6:N:246:LEU:HD11	1.39	1.01
2:J:60:LEU:HD13	2:J:60:LEU:C	1.86	1.00
7:O:256:LEU:HD11	7:O:276:LEU:HD23	1.43	1.00
4:L:358:LYS:HG3	22:n:80:TYR:OH	1.61	1.00
5:M:143:LEU:HD21	6:N:303:THR:HG21	1.38	1.00
5:M:172:GLY:O	5:M:173:THR:HG23	1.61	1.00
7:O:209:VAL:HG12	7:O:260:SER:HB2	1.43	0.99
17:i:11:ARG:NH2	22:n:154:LEU:HB2	1.76	0.99
5:M:196:TRP:CD1	5:M:250:LEU:HD13	1.96	0.99
24:p:5:TRP:HZ3	24:p:10:TYR:O	1.45	0.99
7:O:168:VAL:HG11	7:O:241:TYR:CD1	1.97	0.99
17:i:105:PHE:CD2	23:o:68:LYS:HA	1.97	0.99
2:J:5:ILE:CG1	3:K:4:THR:CG2	2.41	0.99
6:N:143:ILE:O	6:N:146:TYR:CD2	2.15	0.99
6:N:164:MET:CE	25:Y:201:3PE:H271	1.93	0.99
1:D:36:GLN:HE22	5:M:135:ARG:NH1	1.60	0.98
2:J:3:ASN:HD22	2:J:120:LEU:HB2	1.20	0.98
6:N:179:MET:CG	6:N:216:PHE:HE1	1.75	0.98
4:L:141:PHE:HB2	4:L:182:PHE:HE2	1.27	0.98
5:M:173:THR:CG2	16:h:147:ALA:HB2	1.94	0.98
5:M:275:ILE:HD11	5:M:288:TYR:CG	1.98	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:307:THR:HB	7:O:319:ILE:CD1	1.94	0.98
3:K:40:LEU:HD13	6:N:71:LEU:HD23	1.46	0.97
4:L:316:THR:HG23	4:L:325:ALA:HB2	1.45	0.97
4:L:383:MET:HB3	4:L:386:LEU:HD12	1.43	0.97
2:J:9:SER:CB	3:K:7:ASN:HD22	1.77	0.96
4:L:174:TYR:HD2	4:L:232:TRP:CD1	1.82	0.96
4:L:511:LEU:HD21	19:k:38:VAL:HG22	1.47	0.96
4:L:13:ILE:HD11	25:L:701:3PE:H2C1	1.45	0.96
5:M:250:LEU:HD12	5:M:250:LEU:O	1.65	0.96
4:L:174:TYR:CD2	4:L:232:TRP:HD1	1.83	0.96
4:L:216:LEU:HD22	4:L:259:LEU:HD21	1.44	0.96
23:o:93:LEU:O	23:o:97:LYS:HG2	1.65	0.96
6:N:164:MET:HE1	25:Y:201:3PE:C26	1.96	0.96
8:U:90:TYR:HE2	8:U:92:LYS:HB2	1.25	0.96
4:L:363:THR:HG23	4:L:431:THR:HB	1.48	0.96
4:L:174:TYR:HD2	4:L:232:TRP:HD1	1.02	0.95
4:L:247:LEU:HD12	4:L:248:HIS:CD2	1.98	0.95
4:L:302:ILE:CG2	4:L:340:PHE:CZ	2.48	0.95
4:L:319:MET:HE1	4:L:399:ILE:HA	1.47	0.95
6:N:31:VAL:O	6:N:35:PHE:CD2	2.19	0.95
5:M:216:LEU:HG	5:M:220:HIS:CE1	2.01	0.94
5:M:4:ILE:HG22	5:M:107:ILE:HD13	1.47	0.94
13:e:96:PRO:HA	13:e:99:SER:HB2	1.50	0.94
5:M:369:LEU:CD2	5:M:371:PRO:HD2	1.97	0.94
3:K:66:PHE:HZ	6:N:35:PHE:HZ	1.14	0.94
4:L:246:LEU:HD12	4:L:247:LEU:N	1.81	0.94
4:L:466:PHE:HB2	18:j:68:TRP:HZ2	1.33	0.94
8:U:140:CYS:HB2	8:U:143:GLU:HG2	1.49	0.94
5:M:1:MET:HG3	5:M:4:ILE:HD13	1.50	0.94
20:l:91:GLN:HE21	22:n:2:ALA:HB1	1.30	0.94
4:L:247:LEU:HD11	4:L:248:HIS:NE2	1.83	0.94
4:L:274:LEU:HA	4:L:277:MET:HE3	1.49	0.93
2:J:12:PHE:CE2	3:K:42:ILE:CD1	2.51	0.93
2:J:12:PHE:CE2	3:K:42:ILE:HD13	2.03	0.93
5:M:453:LEU:CD1	5:M:454:ILE:HG23	1.99	0.93
25:L:702:3PE:H3C2	23:o:78:LEU:HD13	1.51	0.93
16:h:183:PRO:O	16:h:184:LYS:CG	2.17	0.93
4:L:41:LYS:HG3	4:L:98:TRP:CZ2	2.04	0.92
7:O:314:LEU:CD1	7:O:315:PRO:HD2	2.00	0.92
10:Y:19:GLN:HE21	10:Y:22:ARG:HG2	1.32	0.92
17:i:14:GLN:HB3	22:n:164:PRO:HG3	1.52	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:136:ASN:HD21	26:h:201:CDL:H273	1.33	0.92
5:M:106:LEU:HD13	5:M:234:ILE:CG2	2.00	0.91
4:L:466:PHE:HB2	18:j:68:TRP:CZ2	2.06	0.91
4:L:202:MET:HE3	4:L:265:PRO:HG3	1.53	0.91
4:L:245:ALA:O	4:L:249:SER:HB3	1.70	0.91
2:J:168:GLU:HA	2:J:171:ARG:HG2	1.52	0.91
4:L:362:ILE:HG23	4:L:366:MET:HE3	1.53	0.91
7:O:106:ILE:HG12	7:O:111:SER:HA	1.50	0.91
20:l:30:PHE:CE2	20:l:31:HIS:CE1	2.60	0.90
2:J:9:SER:HB3	3:K:7:ASN:HD22	1.35	0.90
20:l:38:PRO:HB2	21:m:75:ASN:HD22	1.36	0.90
25:L:702:3PE:H3B2	18:j:71:TRP:HH2	1.37	0.90
7:O:347:VAL:O	7:O:347:VAL:HG12	1.71	0.90
2:J:5:ILE:HG23	2:J:120:LEU:HD13	1.54	0.89
4:L:364:LYS:HE2	19:k:67:ILE:CD1	2.01	0.89
5:M:231:LEU:HD12	5:M:235:LEU:CD1	2.00	0.89
5:M:2:LEU:HA	5:M:5:ILE:HG12	1.53	0.89
5:M:453:LEU:HD12	5:M:454:ILE:N	1.87	0.89
1:D:36:GLN:HE22	5:M:135:ARG:HH12	1.19	0.89
2:J:5:ILE:HG13	3:K:4:THR:HG22	1.53	0.89
4:L:123:LEU:HD22	4:L:150:MET:SD	2.12	0.89
7:O:314:LEU:CG	7:O:315:PRO:HD2	2.02	0.89
15:g:145:ILE:HG23	24:p:160:LYS:HE2	1.53	0.89
26:L:706:CDL:H522	10:Y:107:THR:HG21	1.53	0.89
7:O:62:VAL:HG22	7:O:205:ILE:HB	1.52	0.89
4:L:9:LEU:HD11	25:L:701:3PE:H2B2	1.55	0.89
5:M:380:PHE:HA	5:M:383:MET:HE2	1.55	0.89
8:U:105:MET:SD	8:U:139:MET:CE	2.61	0.89
17:i:105:PHE:CE2	23:o:68:LYS:HA	2.08	0.89
5:M:8:SER:HA	5:M:11:LEU:HD13	1.54	0.88
5:M:173:THR:HG21	16:h:147:ALA:HB2	1.55	0.88
6:N:314:MET:HE2	6:N:319:LYS:HE2	1.54	0.88
4:L:428:TYR:HA	4:L:432:MET:HG2	1.56	0.87
5:M:368:ALA:HB1	5:M:375:LEU:HD13	1.56	0.87
5:M:447:LEU:HD11	5:M:454:ILE:HG21	1.54	0.87
6:N:307:THR:HB	7:O:319:ILE:HD11	1.56	0.87
13:e:17:HIS:CD2	13:e:18:PHE:HD1	1.92	0.87
4:L:496:LEU:HD12	4:L:497:GLY:N	1.90	0.87
4:L:41:LYS:HD3	25:L:702:3PE:H2A1	1.56	0.87
5:M:102:LEU:HD13	5:M:230:ILE:HG12	1.57	0.87
5:M:127:ILE:CD1	6:N:256:PRO:CG	2.53	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:358:LYS:HG2	22:n:80:TYR:CE1	2.10	0.87
5:M:142:ARG:HH21	6:N:303:THR:HG22	1.38	0.87
7:O:295:ARG:NH1	7:O:299:GLN:HB2	1.90	0.87
20:l:30:PHE:CZ	20:l:31:HIS:CE1	2.63	0.87
5:M:1:MET:HE1	5:M:111:SER:HB2	1.58	0.86
4:L:79:SER:HB2	4:L:135:ASN:HB2	1.55	0.86
6:N:211:LEU:HD23	6:N:333:SER:HB2	1.58	0.86
2:J:37:PHE:CE2	2:J:41:LEU:HD11	2.10	0.86
7:O:314:LEU:HG	7:O:315:PRO:HD2	1.58	0.85
6:N:200:LEU:HD21	6:N:265:ILE:CG1	2.06	0.85
6:N:323:ASN:OD1	6:N:324:LEU:N	2.08	0.85
20:l:167:TYR:HD2	20:l:168:LEU:HD12	1.41	0.85
5:M:127:ILE:HD12	6:N:256:PRO:HG3	1.56	0.85
16:h:182:SER:HB3	16:h:183:PRO:HD2	1.58	0.85
4:L:417:SER:HB3	4:L:493:ILE:HG13	1.58	0.85
7:O:176:GLN:HG3	7:O:177:GLY:H	1.41	0.85
8:U:105:MET:HE2	8:U:112:SER:HA	1.59	0.85
4:L:437:PHE:HE1	4:L:441:ILE:CG1	1.85	0.85
5:M:29:SER:HB3	15:g:91:PHE:CD2	2.12	0.85
4:L:302:ILE:HG22	4:L:340:PHE:CE2	2.11	0.85
4:L:247:LEU:HD11	4:L:248:HIS:CD2	2.11	0.84
5:M:115:LEU:HD21	5:M:176:LEU:HD21	1.59	0.84
4:L:128:MET:HG2	4:L:251:THR:HB	1.59	0.84
5:M:208:PRO:HD3	5:M:236:LEU:HD22	1.59	0.84
25:M:502:3PE:H261	25:O:401:3PE:H232	1.57	0.84
7:O:314:LEU:HD12	7:O:315:PRO:HD2	1.56	0.84
14:f:5:GLN:HB2	14:f:10:HIS:HD2	1.41	0.84
4:L:445:GLU:HB2	4:L:450:LEU:HD23	1.59	0.84
5:M:447:LEU:HD11	5:M:454:ILE:CG2	2.06	0.84
7:O:237:ILE:HG22	7:O:241:TYR:HE2	1.42	0.84
4:L:553:LEU:HD11	21:m:93:ALA:CB	2.06	0.84
6:N:215:MET:SD	6:N:248:LEU:HD21	2.18	0.84
20:l:167:TYR:CD2	20:l:168:LEU:HD12	2.13	0.84
1:D:67:ASN:HB2	7:O:193:LEU:CD2	2.07	0.84
5:M:191:SER:HB2	25:N:401:3PE:O12	1.77	0.84
7:O:238:GLU:HA	7:O:241:TYR:HD2	1.43	0.84
4:L:20:LEU:HD12	4:L:21:ILE:N	1.92	0.84
5:M:196:TRP:NE1	5:M:250:LEU:HD13	1.92	0.84
6:N:276:LEU:HD13	25:N:401:3PE:H2	1.60	0.84
6:N:99:LEU:HD11	6:N:154:ILE:CG2	2.08	0.83
6:N:175:MET:HG2	6:N:219:LEU:HD22	1.60	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:e:14:LEU:HD12	13:e:15:ASP:HB2	1.57	0.83
5:M:373:ILE:HG12	5:M:454:ILE:HD11	1.60	0.83
6:N:164:MET:HE1	25:Y:201:3PE:H262	1.58	0.83
7:O:256:LEU:HD11	7:O:276:LEU:CD2	2.07	0.83
8:U:100:VAL:HA	8:U:141:PRO:HG2	1.59	0.83
5:M:361:MET:HB3	5:M:441:MET:HE3	1.60	0.83
4:L:16:LEU:HD23	4:L:126:ILE:CD1	2.08	0.83
4:L:214:MET:HG3	25:L:704:3PE:H281	1.61	0.83
6:N:179:MET:HG3	6:N:216:PHE:CE1	2.14	0.83
2:J:33:ILE:HG23	2:J:60:LEU:CD2	2.09	0.83
5:M:269:MET:HE1	5:M:396:MET:HA	1.61	0.83
4:L:182:PHE:CE2	4:L:186:MET:HE3	2.14	0.82
5:M:162:ILE:HG23	6:N:271:MET:CE	2.08	0.82
10:Y:34:CYS:HB3	25:Y:201:3PE:H381	1.61	0.82
4:L:432:MET:HG3	4:L:432:MET:O	1.78	0.82
4:L:131:LEU:CD1	4:L:140:LEU:HD12	2.09	0.82
6:N:170:LEU:HD12	6:N:292:PHE:CD2	2.15	0.82
20:l:30:PHE:CE2	20:l:31:HIS:HE1	1.97	0.82
4:L:222:GLY:HA2	4:L:229:LEU:CD1	2.08	0.82
4:L:542:LEU:HD11	25:L:703:3PE:H261	1.60	0.82
26:L:706:CDL:H351	10:Y:114:ALA:HB1	1.60	0.82
25:M:501:3PE:H2A1	26:h:201:CDL:H202	1.62	0.82
12:d:109:TYR:HA	12:d:112:ILE:HG22	1.60	0.82
21:m:123:ARG:O	24:p:140:GLN:NE2	2.13	0.82
4:L:493:ILE:HD12	4:L:496:LEU:HD21	1.62	0.82
6:N:179:MET:CG	6:N:216:PHE:CE1	2.63	0.82
4:L:552:LEU:HD12	20:l:70:MET:HE1	1.60	0.82
25:L:703:3PE:H2G1	25:L:704:3PE:H3I1	1.61	0.81
3:K:22:PHE:HB2	4:L:585:LYS:HG2	1.59	0.81
15:g:139:TYR:HB2	24:p:142:ARG:CZ	2.10	0.81
19:k:34:PRO:HD2	19:k:59:TYR:CD1	2.16	0.81
4:L:16:LEU:CD2	4:L:126:ILE:HD13	2.10	0.81
8:U:105:MET:CG	8:U:139:MET:HE3	2.11	0.81
26:L:706:CDL:HB22	26:L:706:CDL:H512	1.62	0.81
19:k:30:ILE:HD11	19:k:39:GLN:HB2	1.61	0.81
5:M:336:ARG:NH2	5:M:429:SER:HA	1.95	0.81
19:k:38:VAL:HG13	22:n:39:TYR:HB2	1.62	0.81
24:p:5:TRP:CZ3	24:p:10:TYR:O	2.34	0.81
6:N:277:ILE:HG23	6:N:278:MET:N	1.96	0.81
2:J:22:LYS:HD2	3:K:23:ARG:HG2	1.62	0.81
4:L:229:LEU:O	4:L:229:LEU:CD1	2.28	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:458:THR:CG2	24:p:148:ALA:HB1	2.10	0.81
6:N:277:ILE:CG2	6:N:278:MET:H	1.93	0.81
6:N:338:PRO:HB3	26:X:201:CDL:H712	1.62	0.81
5:M:172:GLY:O	5:M:173:THR:CG2	2.28	0.80
1:D:47:PHE:CB	6:N:227:ILE:HD11	2.08	0.80
2:J:33:ILE:HG23	2:J:60:LEU:HD21	1.61	0.80
4:L:13:ILE:CD1	25:L:701:3PE:H2C2	2.11	0.80
4:L:424:MET:HE2	4:L:502:LEU:HB2	1.62	0.80
5:M:29:SER:HB3	15:g:91:PHE:HD2	1.46	0.80
4:L:364:LYS:HE2	19:k:67:ILE:HD11	1.64	0.80
5:M:453:LEU:HD12	5:M:454:ILE:HG23	1.63	0.80
7:O:227:MET:O	7:O:228:LYS:CG	2.30	0.80
5:M:173:THR:HG23	16:h:147:ALA:CB	2.11	0.80
4:L:358:LYS:HG2	22:n:80:TYR:CZ	2.16	0.80
5:M:216:LEU:HD12	5:M:236:LEU:HD21	1.60	0.80
4:L:466:PHE:CB	18:j:68:TRP:HZ2	1.94	0.80
7:O:117:PHE:CE1	7:O:173:MET:HE3	2.17	0.80
23:o:29:LEU:HD23	23:o:108:LEU:HD13	1.64	0.80
6:N:164:MET:CE	25:Y:201:3PE:C27	2.59	0.80
6:N:29:MET:CE	6:N:141:ILE:HG12	2.09	0.79
7:O:199:LEU:HD11	7:O:294:LEU:HD22	1.64	0.79
4:L:552:LEU:HD21	21:m:90:GLY:HA2	1.63	0.79
5:M:231:LEU:HA	5:M:235:LEU:HB2	1.62	0.79
1:D:47:PHE:HB3	6:N:227:ILE:CD1	2.10	0.79
5:M:151:PHE:CZ	6:N:291:PHE:HB2	2.17	0.79
6:N:99:LEU:HD11	6:N:154:ILE:HG23	1.65	0.79
5:M:122:PHE:CZ	5:M:206:LYS:HD3	2.18	0.79
7:O:305:LEU:HD12	7:O:305:LEU:O	1.82	0.79
22:n:20:TYR:CE2	22:n:24:LEU:HD11	2.18	0.79
4:L:123:LEU:HD21	26:L:705:CDL:H741	1.63	0.79
4:L:130:ILE:HG23	4:L:139:GLN:HE21	1.46	0.79
15:g:139:TYR:CD1	24:p:142:ARG:NH2	2.50	0.79
5:M:367:LEU:HD21	5:M:408:MET:HE2	1.64	0.79
6:N:164:MET:CE	25:Y:201:3PE:C26	2.60	0.79
17:i:22:TRP:CD2	22:n:172:THR:HG22	2.17	0.79
4:L:131:LEU:HD12	4:L:140:LEU:CD1	2.12	0.79
5:M:106:LEU:HD13	5:M:234:ILE:HG21	1.63	0.79
7:O:206:TYR:CD1	7:O:246:LEU:HD21	2.17	0.79
5:M:173:THR:HG23	16:h:147:ALA:HB2	1.65	0.78
7:O:206:TYR:HB3	7:O:257:VAL:HA	1.63	0.78
1:D:67:ASN:HB3	1:D:69:VAL:HG12	1.64	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:3:ILE:H	4:L:3:ILE:HD12	1.48	0.78
4:L:302:ILE:CG2	4:L:340:PHE:CE1	2.66	0.78
7:O:117:PHE:HE1	7:O:173:MET:CE	1.96	0.78
4:L:534:HIS:O	4:L:538:PRO:HG3	1.83	0.78
2:J:3:ASN:ND2	2:J:120:LEU:CB	2.46	0.78
5:M:9:LEU:HD23	5:M:104:ILE:HD13	1.65	0.78
5:M:248:ILE:HG13	5:M:249:ILE:HD12	1.64	0.78
7:O:314:LEU:HD12	7:O:315:PRO:CD	2.13	0.78
20:l:44:THR:OG1	20:l:45:PRO:HD2	1.83	0.78
4:L:136:ASN:HA	4:L:197:GLU:HA	1.66	0.78
5:M:388:TRP:CE2	21:m:109:ARG:HD2	2.19	0.78
5:M:231:LEU:HD12	5:M:235:LEU:HD13	1.64	0.78
5:M:370:PRO:HA	5:M:375:LEU:CD2	2.13	0.78
5:M:319:HIS:HA	5:M:322:THR:HG22	1.66	0.78
16:h:96:ALA:HB3	24:p:63:TYR:HD1	1.49	0.78
25:M:503:3PE:H2G2	21:m:97:PRO:HG3	1.65	0.78
6:N:120:GLN:HG3	6:N:177:LYS:CE	2.13	0.78
6:N:281:LEU:CD2	25:N:401:3PE:H281	2.13	0.78
6:N:215:MET:CE	6:N:248:LEU:CD2	2.62	0.78
2:J:67:PHE:CE2	3:K:75:LEU:HD21	2.19	0.77
2:J:3:ASN:HD22	2:J:120:LEU:CB	1.96	0.77
13:e:17:HIS:CD2	13:e:18:PHE:CD1	2.72	0.77
5:M:274:SER:O	5:M:277:LEU:HB2	1.85	0.77
6:N:45:ILE:O	6:N:45:ILE:HG13	1.83	0.77
6:N:254:LEU:HD12	6:N:255:PRO:CD	2.14	0.77
20:l:169:GLU:C	20:l:171:GLY:H	1.92	0.77
5:M:204:LEU:HD22	5:M:209:LEU:HD12	1.65	0.77
7:O:168:VAL:HG21	7:O:241:TYR:OH	1.82	0.77
1:D:67:ASN:HB2	7:O:193:LEU:HD23	1.65	0.77
5:M:453:LEU:HD11	5:M:454:ILE:HG23	1.65	0.77
19:k:55:GLU:CD	22:n:34:ARG:HD2	2.09	0.77
5:M:208:PRO:HG2	5:M:216:LEU:HD13	1.67	0.77
4:L:419:THR:HA	4:L:422:TYR:CE2	2.20	0.76
5:M:42:LEU:HG	5:M:67:ILE:HD11	1.67	0.76
5:M:98:MET:CE	5:M:128:PRO:HA	2.14	0.76
6:N:31:VAL:O	6:N:35:PHE:HD2	1.68	0.76
5:M:171:VAL:HG11	5:M:179:LEU:HD21	1.65	0.76
7:O:58:ARG:HG2	7:O:278:TYR:CE2	2.21	0.76
17:i:102:PRO:HB2	24:p:18:PRO:CD	2.15	0.76
4:L:302:ILE:HG22	4:L:340:PHE:CE1	2.20	0.76
4:L:542:LEU:HB3	5:M:278:ARG:HD2	1.66	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:123:GLU:HG2	8:U:130:ILE:HG12	1.67	0.76
23:o:116:ALA:O	23:o:119:GLU:HB2	1.83	0.76
3:K:95:LEU:HG	6:N:54:GLU:OE2	1.84	0.76
7:O:43:ALA:HA	7:O:46:GLY:O	1.86	0.76
5:M:60:PRO:O	5:M:64:PRO:HD3	1.85	0.76
6:N:314:MET:HB2	7:O:305:LEU:HD11	1.68	0.76
1:D:57:GLU:HA	1:D:60:HIS:CD2	2.21	0.76
4:L:496:LEU:HD12	4:L:496:LEU:C	2.09	0.76
6:N:179:MET:HG3	6:N:216:PHE:HE1	1.49	0.76
13:e:102:GLU:HG2	13:e:104:PRO:HD3	1.65	0.76
5:M:231:LEU:HD12	5:M:235:LEU:HD12	1.67	0.76
1:D:36:GLN:NE2	5:M:135:ARG:HH12	1.84	0.76
4:L:232:TRP:CZ3	4:L:233:LEU:CD2	2.69	0.76
15:g:147:LEU:HD11	24:p:163:MET:HB3	1.65	0.76
17:i:102:PRO:HG2	24:p:18:PRO:HD3	1.66	0.76
26:L:706:CDL:H801	26:L:706:CDL:H762	1.67	0.76
6:N:215:MET:HE2	6:N:248:LEU:HD21	1.67	0.76
17:i:22:TRP:CE2	22:n:172:THR:HG22	2.21	0.76
4:L:605:ASN:OD1	4:L:605:ASN:O	2.03	0.76
4:L:126:ILE:HG21	26:L:705:CDL:H582	1.68	0.75
4:L:506:ASN:HA	4:L:509:MET:HE2	1.66	0.75
7:O:121:PRO:O	7:O:122:LYS:HG2	1.85	0.75
7:O:168:VAL:HG11	7:O:241:TYR:CE1	2.19	0.75
22:n:20:TYR:CZ	22:n:24:LEU:HD11	2.21	0.75
4:L:358:LYS:HG3	22:n:80:TYR:CE2	2.20	0.75
5:M:458:THR:HG22	24:p:148:ALA:HB1	1.68	0.75
7:O:48:LYS:O	7:O:51:LYS:HG2	1.86	0.75
2:J:59:TYR:OH	3:K:34:GLU:HB3	1.86	0.75
2:J:60:LEU:C	2:J:60:LEU:CD1	2.59	0.75
4:L:387:THR:HG23	4:L:461:SER:O	1.85	0.75
6:N:170:LEU:HD12	6:N:292:PHE:HD2	1.49	0.75
16:h:57:VAL:HG22	22:n:104:LEU:HD11	1.69	0.75
6:N:227:ILE:HA	6:N:230:ILE:HG22	1.66	0.75
6:N:277:ILE:HG23	6:N:278:MET:H	1.50	0.75
4:L:393:ASP:OD1	4:L:394:LEU:N	2.19	0.75
4:L:482:MET:HE2	4:L:486:LEU:HB3	1.68	0.74
2:J:151:MET:HE2	6:N:28:LEU:HD13	1.69	0.74
4:L:475:THR:HA	23:o:55:GLN:NE2	2.01	0.74
17:i:11:ARG:HE	17:i:15:LEU:HD11	1.51	0.74
5:M:314:MET:HA	5:M:454:ILE:HD12	1.70	0.74
7:O:117:PHE:CE1	7:O:128:SER:HB2	2.22	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:333:GLU:O	7:O:333:GLU:CD	2.30	0.74
10:Y:71:MET:HG3	10:Y:102:THR:HG21	1.68	0.74
4:L:136:ASN:ND2	26:h:201:CDL:H273	2.01	0.74
6:N:43:MET:HB3	6:N:126:MET:SD	2.27	0.74
6:N:243:MET:HG2	12:d:44:MET:HE2	1.69	0.74
6:N:284:MET:HE2	25:N:401:3PE:H3B2	1.69	0.74
4:L:285:THR:HG22	4:L:415:ALA:HB1	1.70	0.74
7:O:59:VAL:HA	7:O:157:VAL:HG23	1.69	0.74
10:Y:76:THR:HG23	10:Y:95:GLY:HA3	1.70	0.74
16:h:57:VAL:HG12	22:n:99:VAL:HG21	1.69	0.74
20:l:91:GLN:NE2	22:n:2:ALA:HB1	2.03	0.74
5:M:1:MET:HB2	5:M:52:PHE:CD2	2.23	0.73
6:N:289:ASN:HA	6:N:292:PHE:CE2	2.23	0.73
17:i:103:ARG:O	17:i:105:PHE:CE1	2.41	0.73
25:L:702:3PE:H3B2	18:j:71:TRP:CH2	2.20	0.73
5:M:200:MET:HE1	5:M:247:SER:HB2	1.69	0.73
5:M:260:PRO:O	5:M:264:LEU:HG	1.88	0.73
4:L:232:TRP:CZ3	4:L:233:LEU:HD23	2.22	0.73
7:O:117:PHE:HE1	7:O:173:MET:HE3	1.53	0.73
17:i:102:PRO:CG	24:p:18:PRO:HD3	2.17	0.73
10:Y:143:VAL:HG23	16:h:157:ARG:HG2	1.69	0.73
5:M:143:LEU:HD21	6:N:303:THR:HG23	1.68	0.73
5:M:167:ILE:HD11	5:M:195:LEU:HD21	1.70	0.73
7:O:99:GLY:HA2	11:c:30:TYR:HD1	1.53	0.73
18:j:102:ASP:OD1	23:o:111:ARG:HG3	1.89	0.73
4:L:9:LEU:HD21	25:L:701:3PE:H2C1	1.69	0.73
4:L:20:LEU:HD12	4:L:20:LEU:C	2.13	0.73
5:M:73:LEU:HD22	5:M:103:GLN:CD	2.12	0.73
5:M:216:LEU:HG	5:M:220:HIS:HE1	1.48	0.73
25:M:502:3PE:H3D1	25:M:502:3PE:H2B2	1.71	0.73
14:f:38:ARG:HH12	14:f:54:VAL:HG21	1.54	0.73
4:L:579:ASN:OD1	4:L:579:ASN:O	2.06	0.73
9:X:151:ASN:HB2	9:X:152:PRO:HD2	1.70	0.73
4:L:556:ILE:HG21	21:m:80:PHE:CE1	2.24	0.73
6:N:211:LEU:CD2	6:N:333:SER:HB2	2.19	0.73
7:O:59:VAL:HA	7:O:157:VAL:CG2	2.19	0.73
7:O:254:GLU:HG2	7:O:276:LEU:HD13	1.71	0.73
5:M:122:PHE:CD1	5:M:238:LEU:HG	2.23	0.73
5:M:441:MET:SD	5:M:444:LEU:HD23	2.29	0.73
17:i:11:ARG:NE	17:i:15:LEU:HD11	2.04	0.72
2:J:165:ILE:HG23	6:N:42:PRO:HG3	1.69	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:155:LEU:HD12	10:Y:138:PHE:HA	1.71	0.72
15:g:106:TYR:CE2	16:h:86:ILE:HD12	2.24	0.72
24:p:7:LYS:O	24:p:11:PRO:HA	1.89	0.72
2:J:32:LEU:HG	2:J:64:LEU:HD21	1.71	0.72
4:L:9:LEU:HD22	17:i:82:VAL:HG13	1.71	0.72
4:L:141:PHE:HD2	5:M:370:PRO:HB3	1.54	0.72
4:L:316:THR:CG2	4:L:325:ALA:HB2	2.18	0.72
5:M:243:MET:HE1	5:M:302:MET:HE3	1.71	0.72
6:N:215:MET:SD	6:N:248:LEU:CD2	2.77	0.72
4:L:598:ILE:HD11	6:N:153:ILE:HG12	1.70	0.72
20:l:158:PRO:HD3	23:o:22:ILE:HB	1.71	0.72
4:L:102:GLN:HE21	4:L:449:ASP:HA	1.55	0.72
4:L:576:LEU:HD12	4:L:577:THR:N	2.05	0.72
19:k:34:PRO:HG2	19:k:59:TYR:HE1	1.55	0.72
6:N:59:TYR:CE2	6:N:63:GLN:HG3	2.23	0.72
17:i:95:TYR:CD1	24:p:112:ALA:CB	2.72	0.72
4:L:466:PHE:CZ	18:j:72:ARG:NH2	2.58	0.72
4:L:569:LEU:HB2	10:Y:115:MET:CE	2.17	0.72
5:M:127:ILE:HD11	6:N:256:PRO:CG	2.17	0.72
6:N:179:MET:SD	6:N:216:PHE:HE1	2.13	0.72
17:i:11:ARG:HH22	22:n:154:LEU:CB	1.92	0.72
23:o:94:ASP:HA	23:o:97:LYS:HG2	1.71	0.72
4:L:247:LEU:HD12	4:L:248:HIS:N	2.04	0.72
4:L:299:LYS:HB2	4:L:354:GLN:HE21	1.55	0.72
5:M:313:THR:HG21	5:M:456:GLY:HA3	1.72	0.72
5:M:373:ILE:CG1	5:M:454:ILE:HD11	2.19	0.72
6:N:232:LEU:HD23	6:N:307:THR:HG23	1.70	0.71
5:M:106:LEU:HD13	5:M:234:ILE:HG22	1.72	0.71
5:M:173:THR:HB	16:h:143:GLU:OE2	1.90	0.71
4:L:141:PHE:CD2	5:M:370:PRO:HB3	2.25	0.71
5:M:173:THR:CG2	16:h:147:ALA:CB	2.68	0.71
7:O:100:ASP:OD1	7:O:101:GLY:N	2.24	0.71
4:L:466:PHE:CE1	18:j:72:ARG:NH2	2.58	0.71
10:Y:34:CYS:HB3	25:Y:201:3PE:C38	2.20	0.71
20:l:106:HIS:CD2	20:l:107:TRP:H	2.08	0.71
7:O:336:GLY:H	7:O:344:ASN:ND2	1.89	0.71
21:m:9:ALA:HB1	21:m:10:PRO:HD2	1.71	0.71
5:M:220:HIS:CE1	5:M:231:LEU:HD23	2.26	0.71
5:M:370:PRO:HA	5:M:375:LEU:HD23	1.72	0.71
6:N:146:TYR:CG	6:N:147:PRO:HD3	2.25	0.71
4:L:368:PHE:HB3	4:L:445:GLU:CD	2.15	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:144:ILE:O	8:U:148:ILE:HG12	1.91	0.71
7:O:237:ILE:HG22	7:O:241:TYR:CE2	2.24	0.71
6:N:313:MET:CG	7:O:305:LEU:HD22	2.21	0.71
7:O:209:VAL:HG23	7:O:214:VAL:HG13	1.72	0.71
6:N:237:THR:HG23	6:N:237:THR:O	1.88	0.70
7:O:206:TYR:HD2	7:O:257:VAL:HG13	1.55	0.70
21:m:45:ARG:O	21:m:45:ARG:HG2	1.91	0.70
6:N:200:LEU:CD2	6:N:265:ILE:HG12	2.14	0.70
25:N:401:3PE:H3A2	25:N:401:3PE:H271	1.72	0.70
16:h:87:THR:HA	26:h:201:CDL:H512	1.73	0.70
4:L:73:SER:HB3	24:p:100:GLN:NE2	2.06	0.70
4:L:455:LYS:NZ	18:j:57:GLN:OE1	2.23	0.70
5:M:373:ILE:HG12	5:M:454:ILE:CD1	2.20	0.70
6:N:23:SER:HB2	13:e:15:ASP:OD2	1.91	0.70
17:i:102:PRO:CB	24:p:18:PRO:HD2	2.21	0.70
7:O:135:LEU:HB3	7:O:139:ARG:HH12	1.57	0.70
4:L:9:LEU:CD2	25:L:701:3PE:H2C1	2.21	0.70
4:L:428:TYR:OH	22:n:33:HIS:CE1	2.44	0.70
5:M:446:LEU:HD13	15:g:101:THR:HG21	1.73	0.70
4:L:428:TYR:HA	4:L:432:MET:CG	2.21	0.70
4:L:553:LEU:HD21	21:m:93:ALA:C	2.17	0.70
4:L:559:GLU:O	4:L:564:LYS:HB2	1.92	0.70
25:M:502:3PE:H3I3	26:X:201:CDL:H652	1.74	0.70
6:N:254:LEU:HD12	6:N:255:PRO:HD3	1.72	0.70
21:m:30:ARG:O	21:m:34:VAL:HG23	1.92	0.70
4:L:285:THR:HG22	4:L:415:ALA:CB	2.21	0.70
5:M:134:THR:O	5:M:142:ARG:HD2	1.92	0.70
7:O:206:TYR:CD2	7:O:257:VAL:HG13	2.27	0.70
4:L:73:SER:HB3	24:p:100:GLN:HE21	1.57	0.69
6:N:308:ASN:HB3	7:O:317:ILE:HG22	1.72	0.69
10:Y:19:GLN:HG3	10:Y:22:ARG:HB2	1.74	0.69
4:L:480:LEU:HD23	4:L:480:LEU:O	1.93	0.69
5:M:447:LEU:HD21	5:M:454:ILE:HD13	1.73	0.69
13:e:42:GLU:HG2	16:h:176:LYS:HG3	1.74	0.69
15:g:106:TYR:OH	16:h:86:ILE:HG23	1.92	0.69
6:N:342:GLN:HE21	12:d:30:ARG:HH11	1.36	0.69
11:c:34:PRO:HG2	11:c:37:ALA:HB2	1.74	0.69
14:f:56:TRP:CE3	16:h:131:LYS:HG3	2.26	0.69
5:M:216:LEU:HD11	5:M:236:LEU:HD11	1.72	0.69
5:M:369:LEU:HD23	5:M:371:PRO:CD	2.12	0.69
17:i:94:PRO:HG3	24:p:10:TYR:CE2	2.28	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:305:SER:HB2	4:L:422:TYR:HE1	1.57	0.69
6:N:220:MET:C	6:N:223:ASN:H	2.00	0.69
6:N:248:LEU:HD13	6:N:296:LEU:HD23	1.75	0.69
2:J:3:ASN:HD21	2:J:120:LEU:H	1.39	0.69
4:L:102:GLN:CD	4:L:453:PRO:HD3	2.18	0.69
7:O:40:LEU:HG	7:O:292:HIS:CE1	2.27	0.69
16:h:163:ARG:HG2	16:h:165:ASP:HB2	1.73	0.69
20:l:122:THR:HG21	20:l:129:MET:HE1	1.73	0.69
23:o:8:ARG:HB2	23:o:16:GLU:HG2	1.74	0.69
4:L:153:LEU:HD11	5:M:360:LEU:HD11	1.73	0.69
5:M:263:LEU:HD11	21:m:102:TYR:HD1	1.56	0.69
5:M:409:TYR:CD1	20:l:116:ARG:NH2	2.61	0.69
2:J:4:TYR:CZ	2:J:8:LEU:HD11	2.28	0.69
3:K:66:PHE:CZ	6:N:35:PHE:CE1	2.80	0.69
4:L:332:HIS:NE2	4:L:336:LYS:HG3	2.07	0.69
6:N:215:MET:HE2	6:N:248:LEU:CD2	2.23	0.69
8:U:74:LEU:HD23	8:U:79:ILE:HG12	1.75	0.68
4:L:18:PRO:O	4:L:21:ILE:HG22	1.92	0.68
5:M:127:ILE:HB	5:M:128:PRO:HD3	1.75	0.68
10:Y:77:CYS:SG	10:Y:78:VAL:N	2.66	0.68
23:o:20:GLU:O	23:o:21:LYS:HG2	1.93	0.68
4:L:312:LEU:HD21	4:L:395:ILE:HG21	1.76	0.68
7:O:140:LEU:HG	7:O:304:VAL:HG12	1.74	0.68
19:k:34:PRO:CD	19:k:59:TYR:CD1	2.75	0.68
20:l:78:LEU:HD11	20:l:104:PRO:HB2	1.74	0.68
5:M:311:GLY:HA2	5:M:314:MET:HE3	1.75	0.68
10:Y:143:VAL:CG2	16:h:157:ARG:HG2	2.23	0.68
13:e:8:LYS:HG2	13:e:16:ARG:HH12	1.58	0.68
10:Y:96:GLY:HA3	10:Y:121:GLY:HA2	1.75	0.68
17:i:102:PRO:HB2	24:p:18:PRO:HD2	1.74	0.68
4:L:211:ILE:N	4:L:212:PRO:HD2	2.08	0.68
5:M:379:LEU:O	5:M:383:MET:HG3	1.93	0.68
6:N:313:MET:HG3	7:O:305:LEU:HD22	1.75	0.68
17:i:99:SER:O	24:p:116:ARG:HA	1.93	0.68
5:M:39:LEU:HD23	5:M:67:ILE:HD13	1.74	0.68
5:M:344:MET:HE1	21:m:59:HIS:NE2	2.08	0.68
6:N:215:MET:HE1	6:N:248:LEU:HD21	1.71	0.68
21:m:48:LEU:HB3	22:n:166:LEU:HD23	1.74	0.68
4:L:383:MET:SD	4:L:384:PRO:HD2	2.33	0.68
4:L:556:ILE:HD11	21:m:76:ILE:HG22	1.76	0.68
5:M:446:LEU:HD13	15:g:101:THR:CG2	2.23	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:119:ILE:HD11	8:U:138:LEU:HB2	1.76	0.68
17:i:32:GLU:HG3	22:n:115:TYR:HA	1.76	0.68
4:L:228:GLY:C	4:L:229:LEU:HG	2.19	0.67
7:O:224:PRO:HA	7:O:227:MET:HE3	1.74	0.67
2:J:12:PHE:HE2	3:K:42:ILE:CD1	2.06	0.67
3:K:95:LEU:HG	6:N:54:GLU:CD	2.20	0.67
7:O:347:VAL:O	7:O:347:VAL:CG1	2.42	0.67
6:N:26:LEU:HD23	6:N:29:MET:SD	2.34	0.67
6:N:66:ALA:HB2	6:N:104:MET:SD	2.34	0.67
6:N:108:LEU:CD2	6:N:191:LEU:HD22	2.24	0.67
10:Y:34:CYS:HB3	25:Y:201:3PE:C39	2.24	0.67
20:l:122:THR:HG23	20:l:123:PRO:HD2	1.75	0.67
4:L:456:ARG:HG2	25:L:702:3PE:H221	1.77	0.67
5:M:19:SER:HB2	14:f:8:ARG:HD2	1.77	0.67
5:M:275:ILE:HD11	5:M:288:TYR:CD1	2.29	0.67
5:M:310:MET:HG2	5:M:314:MET:HE2	1.75	0.67
6:N:175:MET:HG2	6:N:219:LEU:CD2	2.23	0.67
12:d:14:LEU:O	12:d:14:LEU:CD1	2.37	0.67
4:L:80:PHE:C	4:L:135:ASN:ND2	2.53	0.67
5:M:11:LEU:HB3	5:M:100:ILE:HD13	1.76	0.67
5:M:142:ARG:NH2	6:N:303:THR:HG22	2.07	0.67
7:O:114:LEU:HA	7:O:131:LEU:CD2	2.25	0.67
2:J:102:LEU:O	2:J:106:LEU:HG	1.95	0.67
4:L:9:LEU:HD21	25:L:701:3PE:C2B	2.25	0.67
5:M:30:TYR:O	5:M:34:ILE:HG12	1.95	0.67
15:g:109:ASP:CB	15:g:114:GLU:HB3	2.24	0.67
20:l:106:HIS:HD2	20:l:107:TRP:H	1.43	0.67
5:M:98:MET:HE2	5:M:131:ILE:HB	1.77	0.67
5:M:282:LEU:HD21	5:M:359:TRP:HH2	1.60	0.67
5:M:285:LEU:HD13	5:M:342:MET:HE1	1.75	0.67
6:N:320:THR:HG23	6:N:320:THR:O	1.93	0.67
12:d:60:ARG:O	12:d:61:GLN:C	2.37	0.67
7:O:305:LEU:HD12	7:O:305:LEU:C	2.20	0.67
16:h:129:PRO:HG3	24:p:66:ARG:NH2	2.10	0.67
23:o:105:GLU:O	23:o:109:LEU:HD23	1.94	0.67
1:D:36:GLN:HE21	1:D:38:GLN:NE2	1.93	0.67
4:L:81:LYS:N	4:L:135:ASN:ND2	2.43	0.67
4:L:552:LEU:CD2	4:L:553:LEU:HD12	2.25	0.67
4:L:577:THR:HA	25:Y:201:3PE:H222	1.76	0.67
25:L:701:3PE:C12	17:i:89:HIS:ND1	2.55	0.67
5:M:270:ILE:HG22	5:M:271:MET:HE2	1.76	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:395:LEU:HD21	21:m:101:TRP:CE2	2.29	0.67
7:O:60:ILE:HD12	7:O:203:ALA:HB3	1.77	0.67
13:e:14:LEU:CD1	13:e:15:ASP:HB2	2.25	0.67
4:L:201:ILE:HG22	4:L:266:LEU:HD11	1.75	0.66
10:Y:71:MET:HG3	10:Y:102:THR:CG2	2.26	0.66
3:K:1:MET:HG3	3:K:50:ASN:HD22	1.61	0.66
4:L:428:TYR:OH	22:n:33:HIS:HE1	1.76	0.66
4:L:562:ILE:HB	4:L:563:PRO:HD3	1.78	0.66
5:M:123:GLU:HB3	6:N:255:PRO:HG2	1.77	0.66
5:M:361:MET:CB	5:M:441:MET:HE3	2.25	0.66
8:U:128:PHE:CZ	8:U:148:ILE:HD12	2.30	0.66
16:h:102:PRO:HD2	16:h:105:TYR:HB2	1.77	0.66
4:L:407:TRP:CE3	4:L:410:LEU:HD11	2.29	0.66
7:O:343:TYR:HD1	7:O:352:ILE:HG23	1.59	0.66
10:Y:76:THR:HG22	10:Y:92:TYR:HA	1.77	0.66
15:g:147:LEU:HD21	24:p:163:MET:HB2	1.77	0.66
2:J:55:VAL:HB	3:K:41:PHE:CE2	2.30	0.66
25:M:501:3PE:C2A	26:h:201:CDL:H202	2.25	0.66
6:N:273:ASN:ND2	10:Y:143:VAL:HA	2.11	0.66
20:l:38:PRO:HB2	21:m:75:ASN:ND2	2.10	0.66
4:L:174:TYR:CD2	4:L:232:TRP:CD1	2.68	0.66
5:M:255:LYS:NZ	12:d:117:HIS:HB3	2.11	0.66
3:K:12:PHE:CE1	6:N:72:LEU:HD22	2.31	0.66
4:L:518:PRO:HD2	4:L:520:SER:HB2	1.78	0.66
5:M:395:LEU:HD21	21:m:101:TRP:CZ2	2.30	0.66
6:N:197:ASN:CG	6:N:200:LEU:HD13	2.21	0.66
13:e:86:LEU:HB3	13:e:91:LYS:HB2	1.78	0.66
14:f:41:SER:O	14:f:45:GLN:HB2	1.96	0.66
16:h:57:VAL:HG12	22:n:99:VAL:CG2	2.26	0.66
23:o:25:PHE:HE2	23:o:109:LEU:HD22	1.60	0.66
7:O:200:PRO:HG3	7:O:282:PRO:HD2	1.77	0.66
16:h:183:PRO:C	16:h:184:LYS:HG2	2.17	0.66
2:J:56:PHE:O	2:J:60:LEU:HB3	1.96	0.66
4:L:116:ARG:HG2	4:L:120:TYR:CE2	2.31	0.66
4:L:141:PHE:CD2	5:M:375:LEU:HD21	2.31	0.66
4:L:552:LEU:HD23	4:L:553:LEU:HD12	1.77	0.66
2:J:9:SER:CB	3:K:7:ASN:ND2	2.54	0.66
4:L:25:ASN:OD1	4:L:25:ASN:O	2.14	0.66
5:M:318:ALA:HB2	5:M:373:ILE:HG23	1.76	0.66
6:N:25:ASN:ND2	13:e:18:PHE:CE2	2.64	0.66
7:O:249:MET:HB3	7:O:253:CYS:SG	2.36	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:k:34:PRO:CG	19:k:59:TYR:CE1	2.72	0.66
16:h:163:ARG:HG2	16:h:165:ASP:CB	2.26	0.66
8:U:134:ASP:OD2	22:n:2:ALA:N	2.29	0.65
21:m:49:LEU:HD12	21:m:49:LEU:O	1.95	0.65
4:L:141:PHE:CE2	5:M:375:LEU:HD22	2.12	0.65
4:L:142:ILE:HA	5:M:370:PRO:HB2	1.78	0.65
4:L:293:LEU:HD11	4:L:418:MET:SD	2.36	0.65
4:L:481:THR:HB	23:o:95:TYR:CD2	2.31	0.65
5:M:373:ILE:CD1	5:M:454:ILE:HD11	2.25	0.65
4:L:186:MET:SD	5:M:379:LEU:HD21	2.36	0.65
5:M:175:ASN:HD22	16:h:143:GLU:HG2	1.61	0.65
9:X:158:LEU:HB3	12:d:21:LEU:HD21	1.77	0.65
2:J:22:LYS:HB2	3:K:23:ARG:HD3	1.78	0.65
4:L:141:PHE:CE2	5:M:370:PRO:CG	2.73	0.65
5:M:367:LEU:CD2	5:M:408:MET:HE2	2.25	0.65
4:L:190:SER:HB2	4:L:196:TRP:HE1	1.60	0.65
4:L:214:MET:CG	25:L:704:3PE:H281	2.26	0.65
6:N:120:GLN:HG3	6:N:177:LYS:HE3	1.78	0.65
6:N:156:MET:HA	6:N:159:ILE:HG22	1.77	0.65
7:O:73:LEU:HD21	7:O:269:VAL:HG11	1.76	0.65
2:J:105:VAL:O	2:J:108:TYR:HB3	1.96	0.65
6:N:332:MET:SD	6:N:336:THR:HG21	2.37	0.65
8:U:74:LEU:HD23	8:U:79:ILE:CG1	2.27	0.65
2:J:12:PHE:CZ	3:K:42:ILE:CD1	2.80	0.65
4:L:88:LEU:HD23	4:L:326:PHE:CE2	2.32	0.65
2:J:33:ILE:CG2	2:J:60:LEU:HD21	2.26	0.65
2:J:39:GLY:HA2	2:J:42:MET:HE3	1.78	0.65
3:K:66:PHE:CE1	6:N:35:PHE:CZ	2.84	0.65
7:O:58:ARG:HA	7:O:202:HIS:ND1	2.11	0.65
15:g:106:TYR:OH	16:h:86:ILE:HD12	1.97	0.65
15:g:108:PRO:O	15:g:109:ASP:OD1	2.13	0.65
23:o:25:PHE:CE2	23:o:109:LEU:HD22	2.31	0.65
4:L:387:THR:HG22	4:L:465:GLY:H	1.61	0.65
26:L:705:CDL:HA62	16:h:68:LEU:CD1	2.21	0.65
5:M:388:TRP:NE1	21:m:109:ARG:HD2	2.12	0.65
14:f:38:ARG:NH1	14:f:54:VAL:HG21	2.11	0.65
3:K:96:LEU:O	3:K:97:GLN:C	2.40	0.65
5:M:122:PHE:HD1	5:M:238:LEU:HG	1.62	0.65
6:N:307:THR:O	7:O:319:ILE:N	2.30	0.65
7:O:168:VAL:CG2	7:O:241:TYR:CZ	2.62	0.65
7:O:343:TYR:CE1	7:O:355:LYS:HB2	2.32	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:h:127:ASP:OD1	16:h:127:ASP:O	2.15	0.65
17:i:123:PHE:CD2	23:o:40:VAL:HG11	2.32	0.65
4:L:385:PHE:CD1	18:j:72:ARG:HG3	2.32	0.64
23:o:71:ARG:HB3	23:o:71:ARG:HH11	1.61	0.64
24:p:24:THR:HG22	24:p:26:LEU:H	1.63	0.64
1:D:52:MET:O	1:D:54:PRO:HD3	1.98	0.64
4:L:368:PHE:HB3	4:L:445:GLU:OE2	1.97	0.64
5:M:119:TYR:CD1	5:M:160:LEU:HD22	2.33	0.64
7:O:58:ARG:HG2	7:O:278:TYR:CD2	2.33	0.64
18:j:100:PRO:HG3	23:o:29:LEU:O	1.97	0.64
5:M:167:ILE:O	5:M:171:VAL:HG12	1.98	0.64
25:M:503:3PE:H332	25:M:503:3PE:H372	1.78	0.64
7:O:117:PHE:CE1	7:O:173:MET:CE	2.77	0.64
7:O:194:THR:HG23	7:O:307:TYR:HB2	1.79	0.64
20:l:122:THR:CG2	20:l:123:PRO:HD2	2.27	0.64
2:J:99:GLU:O	2:J:103:ILE:HG12	1.98	0.64
4:L:81:LYS:N	4:L:135:ASN:HD21	1.96	0.64
4:L:366:MET:CG	4:L:443:ILE:HG21	2.28	0.64
4:L:385:PHE:CE1	18:j:72:ARG:HG3	2.33	0.64
6:N:254:LEU:HD12	6:N:255:PRO:HD2	1.78	0.64
10:Y:137:LEU:HD23	10:Y:138:PHE:CG	2.31	0.64
12:d:109:TYR:HA	12:d:112:ILE:CG2	2.28	0.64
20:l:158:PRO:HG3	23:o:23:PRO:HD3	1.79	0.64
4:L:40:ILE:HD13	4:L:97:THR:HG22	1.79	0.64
4:L:556:ILE:CG2	21:m:80:PHE:CZ	2.80	0.64
6:N:220:MET:HA	6:N:223:ASN:HA	1.78	0.64
6:N:275:CYS:SG	10:Y:139:PRO:HG2	2.37	0.64
4:L:556:ILE:HG23	21:m:80:PHE:CE2	2.33	0.64
5:M:300:SER:HB3	5:M:381:ILE:HG23	1.78	0.64
3:K:66:PHE:CE1	6:N:35:PHE:CE1	2.86	0.64
4:L:41:LYS:HG3	4:L:98:TRP:CE2	2.33	0.64
4:L:246:LEU:HD12	4:L:246:LEU:C	2.22	0.64
6:N:37:LEU:HD12	6:N:63:GLN:HB3	1.79	0.64
5:M:160:LEU:HD11	5:M:203:PHE:CZ	2.33	0.64
22:n:97:TYR:HB2	22:n:178:PRO:HG2	1.77	0.64
2:J:39:GLY:HA2	2:J:42:MET:CE	2.27	0.64
17:i:102:PRO:CB	24:p:18:PRO:CD	2.76	0.64
4:L:550:LEU:HB2	5:M:275:ILE:HG22	1.80	0.64
26:L:706:CDL:C52	10:Y:107:THR:CG2	2.68	0.64
5:M:196:TRP:HZ3	5:M:261:PHE:HE2	1.44	0.64
5:M:267:TRP:CZ2	5:M:271:MET:HE3	2.32	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Y:143:VAL:O	16:h:158:ARG:NH2	2.31	0.64
17:i:29:SER:HB2	17:i:32:GLU:OE1	1.96	0.64
20:l:106:HIS:CD2	20:l:107:TRP:N	2.66	0.64
4:L:305:SER:HB2	4:L:422:TYR:CE1	2.33	0.63
7:O:168:VAL:CG2	7:O:241:TYR:CE1	2.77	0.63
14:f:41:SER:OG	16:h:134:GLU:HG2	1.99	0.63
23:o:94:ASP:HA	23:o:97:LYS:CG	2.27	0.63
6:N:163:PHE:CD1	6:N:285:MET:HG3	2.33	0.63
9:X:167:PHE:HB3	9:X:170:TRP:CD1	2.33	0.63
23:o:17:PRO:HG3	23:o:106:ARG:HA	1.78	0.63
1:D:35:ARG:O	1:D:36:GLN:C	2.37	0.63
4:L:381:THR:HG21	4:L:498:PHE:CE2	2.33	0.63
5:M:250:LEU:O	5:M:250:LEU:CD1	2.44	0.63
6:N:193:ILE:HD13	6:N:200:LEU:CB	2.29	0.63
6:N:211:LEU:HD23	6:N:333:SER:CB	2.26	0.63
8:U:86:VAL:HB	8:U:122:MET:HE1	1.79	0.63
8:U:140:CYS:SG	8:U:143:GLU:OE2	2.52	0.63
17:i:102:PRO:CG	24:p:18:PRO:CD	2.77	0.63
22:n:94:TYR:CD2	22:n:177:ARG:HG3	2.34	0.63
4:L:100:ILE:HD13	4:L:341:MET:SD	2.39	0.63
4:L:410:LEU:HD12	4:L:411:ILE:N	2.13	0.63
4:L:433:THR:HG22	4:L:434:LYS:N	2.13	0.63
26:L:706:CDL:C52	10:Y:107:THR:HG21	2.28	0.63
5:M:220:HIS:NE2	5:M:231:LEU:HB3	2.13	0.63
5:M:231:LEU:HA	5:M:235:LEU:HD12	1.80	0.63
12:d:106:LYS:HB3	24:p:79:GLU:HB3	1.81	0.63
15:g:75:ASP:OD1	15:g:76:SER:N	2.32	0.63
3:K:70:GLU:HA	6:N:38:LEU:HD21	1.79	0.63
4:L:149:ILE:HG13	5:M:369:LEU:HD12	1.81	0.63
5:M:1:MET:HB2	5:M:52:PHE:HD2	1.60	0.63
5:M:105:LEU:O	5:M:109:THR:HG23	1.98	0.63
5:M:118:PHE:O	5:M:122:PHE:N	2.25	0.63
5:M:368:ALA:HB1	5:M:375:LEU:CD1	2.25	0.63
19:k:34:PRO:HG2	19:k:59:TYR:CD1	2.34	0.63
3:K:1:MET:HG3	3:K:50:ASN:ND2	2.14	0.63
4:L:80:PHE:C	4:L:135:ASN:HD21	2.06	0.63
10:Y:19:GLN:NE2	10:Y:22:ARG:HG2	2.09	0.63
14:f:38:ARG:NH1	14:f:54:VAL:CG2	2.62	0.63
2:J:5:ILE:CG2	2:J:120:LEU:HD13	2.28	0.63
4:L:202:MET:HE3	4:L:265:PRO:CG	2.25	0.63
8:U:88:LYS:HG2	8:U:98:LEU:HD21	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:h:96:ALA:HB3	24:p:63:TYR:CD1	2.33	0.63
25:L:701:3PE:H122	17:i:89:HIS:CG	2.34	0.63
25:M:502:3PE:H2D2	25:M:502:3PE:H3E2	1.79	0.63
7:O:227:MET:C	7:O:228:LYS:HG2	2.23	0.63
16:h:155:GLU:O	16:h:159:LEU:HD13	1.99	0.63
17:i:28:LEU:HD22	17:i:32:GLU:HG2	1.79	0.63
2:J:18:GLY:O	2:J:23:PRO:HD3	1.98	0.63
5:M:129:THR:HG21	5:M:235:LEU:HD13	1.80	0.63
6:N:172:GLN:OE1	6:N:177:LYS:HD3	1.98	0.63
6:N:193:ILE:HD11	6:N:200:LEU:HD22	1.81	0.63
4:L:361:ASN:OD1	4:L:361:ASN:O	2.17	0.62
20:l:30:PHE:CD2	20:l:31:HIS:ND1	2.67	0.62
4:L:437:PHE:CE1	4:L:441:ILE:CG1	2.69	0.62
4:L:445:GLU:HB2	4:L:450:LEU:CD2	2.29	0.62
5:M:73:LEU:CD2	5:M:103:GLN:NE2	2.61	0.62
25:M:503:3PE:H391	25:M:503:3PE:H232	1.80	0.62
5:M:264:LEU:HD23	21:m:98:LEU:HD11	1.82	0.62
5:M:307:TRP:CE3	5:M:383:MET:HE3	2.34	0.62
14:f:56:TRP:CZ3	16:h:131:LYS:HG3	2.35	0.62
2:J:169:ILE:HD13	6:N:45:ILE:HD11	1.81	0.62
5:M:318:ALA:CB	5:M:373:ILE:HG23	2.29	0.62
26:L:705:CDL:H581	26:L:705:CDL:H792	1.80	0.62
5:M:16:TRP:CE3	25:O:401:3PE:H12	2.35	0.62
7:O:121:PRO:O	7:O:122:LYS:CG	2.46	0.62
8:U:72:PRO:HG3	18:j:42:PRO:HG2	1.81	0.62
4:L:9:LEU:HD21	25:L:701:3PE:C2C	2.29	0.62
4:L:365:ILE:HD11	4:L:366:MET:HE2	1.82	0.62
5:M:129:THR:HG21	5:M:235:LEU:CD1	2.30	0.62
6:N:124:LEU:CD2	6:N:176:ARG:HG2	2.29	0.62
7:O:113:SER:HB3	7:O:116:LYS:HB2	1.80	0.62
22:n:168:TRP:O	22:n:172:THR:OG1	2.18	0.62
6:N:207:ILE:O	6:N:211:LEU:HG	2.00	0.62
7:O:117:PHE:HE1	7:O:128:SER:HB2	1.63	0.62
7:O:132:GLN:HE22	7:O:169:PHE:HB2	1.64	0.62
9:X:167:PHE:HD2	9:X:170:TRP:NE1	1.96	0.62
4:L:174:TYR:CE1	25:L:703:3PE:H331	2.34	0.62
4:L:187:VAL:HG22	5:M:383:MET:HG2	1.82	0.62
26:L:705:CDL:H321	16:h:71:MET:HE1	1.81	0.62
6:N:163:PHE:CE1	6:N:285:MET:HG3	2.34	0.62
7:O:323:GLN:HE22	15:g:54:GLN:HB3	1.64	0.62
8:U:104:PHE:HD1	8:U:108:LEU:HD12	1.65	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:56:PHE:HE1	5:M:108:MET:HG2	1.64	0.62
4:L:10:LEU:HD23	4:L:46:ILE:HG21	1.82	0.62
4:L:358:LYS:CG	22:n:80:TYR:CE2	2.78	0.62
6:N:108:LEU:HD21	6:N:191:LEU:HD23	1.82	0.62
8:U:128:PHE:CZ	8:U:148:ILE:HG23	2.35	0.61
15:g:139:TYR:HB2	24:p:142:ARG:NH2	2.15	0.61
20:l:57:MET:HG2	20:l:104:PRO:HG2	1.82	0.61
4:L:521:SER:O	4:L:522:PHE:C	2.41	0.61
5:M:73:LEU:CB	5:M:103:GLN:OE1	2.48	0.61
5:M:98:MET:HE3	5:M:128:PRO:HA	1.81	0.61
6:N:342:GLN:NE2	12:d:30:ARG:HH11	1.99	0.61
7:O:117:PHE:HD1	7:O:128:SER:HA	1.64	0.61
17:i:95:TYR:CD1	24:p:112:ALA:HB2	2.36	0.61
4:L:559:GLU:HA	4:L:563:PRO:HG2	1.82	0.61
5:M:81:GLN:O	5:M:85:LYS:HB2	2.01	0.61
15:g:106:TYR:CZ	16:h:86:ILE:HD12	2.35	0.61
17:i:123:PHE:HD2	23:o:40:VAL:HG11	1.65	0.61
23:o:69:CYS:C	23:o:80:CYS:SG	2.82	0.61
3:K:22:PHE:HZ	6:N:61:VAL:HG11	1.65	0.61
5:M:422:HIS:NE2	5:M:425:ASN:OD1	2.33	0.61
7:O:140:LEU:HD11	7:O:198:TYR:CZ	2.35	0.61
7:O:140:LEU:HD21	7:O:304:VAL:O	2.00	0.61
9:X:151:ASN:HB3	13:e:51:ARG:HH11	1.65	0.61
21:m:100:PHE:O	21:m:104:VAL:HG23	2.00	0.61
4:L:468:ILE:O	4:L:472:ILE:HG23	2.00	0.61
5:M:373:ILE:H	5:M:448:THR:HG22	1.65	0.61
6:N:218:ALA:HB1	6:N:240:MET:SD	2.40	0.61
8:U:138:LEU:HB3	8:U:144:ILE:HG12	1.83	0.61
11:c:66:VAL:CG1	11:c:70:LYS:HE3	2.31	0.61
5:M:98:MET:HE1	5:M:128:PRO:HA	1.83	0.61
5:M:109:THR:HG22	5:M:121:LEU:HB3	1.82	0.61
5:M:139:GLN:HB3	5:M:222:GLU:HG3	1.83	0.61
5:M:433:GLU:O	5:M:437:MET:HG2	2.01	0.61
6:N:240:MET:HE2	6:N:326:PHE:CZ	2.35	0.61
7:O:73:LEU:HD22	7:O:207:ILE:HD11	1.82	0.61
13:e:70:TYR:HA	13:e:73:MET:HG3	1.81	0.61
20:l:101:TRP:NE1	21:m:62:ASP:HA	2.14	0.61
2:J:169:ILE:CD1	6:N:45:ILE:HD11	2.31	0.61
5:M:318:ALA:HB2	5:M:373:ILE:CG2	2.30	0.61
6:N:179:MET:SD	6:N:216:PHE:CE1	2.94	0.61
7:O:72:LYS:O	7:O:75:LYS:HG2	2.01	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:l:62:TYR:CZ	20:l:64:PRO:HG3	2.36	0.61
24:p:6:ASP:HB3	24:p:9:VAL:HG22	1.83	0.61
4:L:180:ILE:HD11	5:M:400:ILE:HB	1.83	0.61
4:L:424:MET:HE2	4:L:502:LEU:CB	2.31	0.61
6:N:275:CYS:SG	10:Y:139:PRO:CG	2.88	0.61
14:f:38:ARG:HH12	14:f:54:VAL:CG2	2.14	0.61
18:j:97:LEU:HB3	23:o:104:ARG:CB	2.22	0.61
4:L:100:ILE:HG21	4:L:246:LEU:HD23	1.83	0.61
4:L:302:ILE:HB	4:L:340:PHE:CE1	2.36	0.61
25:L:702:3PE:H3C1	18:j:72:ARG:HH22	1.65	0.61
11:c:66:VAL:HG12	11:c:70:LYS:HE3	1.83	0.61
5:M:1:MET:CE	5:M:111:SER:HB2	2.29	0.61
5:M:423:MET:O	5:M:424:ILE:C	2.44	0.61
15:g:109:ASP:HB3	15:g:114:GLU:HB3	1.83	0.61
16:h:106:ILE:O	16:h:106:ILE:HG22	2.00	0.61
23:o:19:PRO:O	23:o:22:ILE:HG12	2.00	0.61
2:J:9:SER:HB2	3:K:7:ASN:HD22	1.63	0.60
2:J:61:GLY:O	2:J:65:VAL:HB	2.01	0.60
5:M:209:LEU:HD23	5:M:210:TYR:N	2.16	0.60
6:N:179:MET:HB3	6:N:216:PHE:CE1	2.36	0.60
4:L:40:ILE:HD12	4:L:101:MET:HG3	1.82	0.60
5:M:151:PHE:CE2	6:N:291:PHE:HB2	2.35	0.60
9:X:159:LYS:O	9:X:160:PRO:C	2.43	0.60
12:d:2:MET:HE2	16:h:169:TYR:H	1.66	0.60
4:L:466:PHE:CE1	18:j:72:ARG:CZ	2.84	0.60
4:L:482:MET:CE	4:L:486:LEU:HB3	2.31	0.60
5:M:178:ILE:HD12	16:h:143:GLU:HG3	1.83	0.60
6:N:59:TYR:CZ	6:N:63:GLN:HG3	2.36	0.60
6:N:108:LEU:HD21	6:N:191:LEU:CD2	2.31	0.60
20:l:108:ASP:HB3	20:l:111:MET:HE2	1.83	0.60
23:o:31:PHE:HD2	23:o:104:ARG:HH12	1.47	0.60
4:L:16:LEU:CD1	25:L:701:3PE:H2H1	2.18	0.60
7:O:57:SER:C	7:O:58:ARG:HD2	2.25	0.60
9:X:168:PHE:O	9:X:170:TRP:CD1	2.54	0.60
1:D:36:GLN:NE2	5:M:135:ARG:NH1	2.40	0.60
4:L:222:GLY:CA	4:L:229:LEU:HD11	2.26	0.60
6:N:281:LEU:HD23	25:N:401:3PE:C28	2.32	0.60
4:L:42:PHE:O	4:L:46:ILE:HG12	2.01	0.60
6:N:307:THR:HB	7:O:319:ILE:CG1	2.32	0.60
7:O:204:VAL:CG2	7:O:255:VAL:HG22	2.31	0.60
8:U:153:ASP:OD2	22:n:176:GLU:HB2	2.02	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:d:16:ASP:O	12:d:19:ARG:HG3	2.00	0.60
2:J:98:MET:O	2:J:101:PHE:HB3	2.02	0.60
4:L:204:SER:HA	4:L:207:ASN:HD22	1.67	0.60
5:M:263:LEU:CD1	21:m:102:TYR:HD1	2.15	0.60
5:M:452:LYS:HA	5:M:455:THR:HG23	1.82	0.60
6:N:308:ASN:CB	7:O:317:ILE:HG22	2.31	0.60
7:O:209:VAL:HG23	7:O:214:VAL:CG1	2.31	0.60
4:L:141:PHE:CD2	5:M:370:PRO:HG3	2.35	0.60
5:M:269:MET:HE3	5:M:399:ASN:CB	2.32	0.60
6:N:224:SER:HB2	6:N:229:SER:CB	2.32	0.60
16:h:73:PHE:HD2	16:h:74:TYR:CD1	2.20	0.60
2:J:55:VAL:HB	3:K:41:PHE:HE2	1.65	0.60
4:L:295:GLN:HE22	4:L:526:LEU:HD12	1.65	0.60
4:L:598:ILE:HD11	6:N:153:ILE:CG1	2.32	0.60
26:L:705:CDL:H762	5:M:369:LEU:HD21	1.83	0.60
5:M:77:LEU:HD23	5:M:99:LEU:HD12	1.83	0.60
5:M:207:MET:HG3	5:M:239:GLY:HA3	1.84	0.60
16:h:102:PRO:HD2	16:h:105:TYR:CB	2.32	0.60
22:n:143:GLU:OE1	22:n:155:PRO:HB3	2.02	0.60
22:n:176:GLU:O	22:n:178:PRO:HD3	2.02	0.60
2:J:9:SER:HB2	3:K:7:ASN:ND2	2.16	0.60
4:L:65:THR:HA	17:i:90:MET:HE2	1.84	0.60
4:L:436:ARG:HA	19:k:58:ARG:NH1	2.17	0.60
6:N:276:LEU:C	6:N:276:LEU:HD12	2.27	0.60
5:M:126:LEU:HD21	5:M:153:THR:HB	1.83	0.59
5:M:144:ASN:HA	5:M:147:ILE:HD12	1.82	0.59
5:M:329:LEU:HD23	5:M:437:MET:HE3	1.85	0.59
5:M:370:PRO:HA	5:M:375:LEU:HD22	1.83	0.59
6:N:307:THR:O	7:O:319:ILE:HG12	2.02	0.59
6:N:313:MET:O	6:N:317:GLN:OE1	2.19	0.59
8:U:90:TYR:CZ	8:U:92:LYS:HD2	2.35	0.59
8:U:97:LYS:O	8:U:98:LEU:C	2.43	0.59
16:h:73:PHE:CD2	16:h:74:TYR:CD1	2.90	0.59
1:D:36:GLN:HA	5:M:138:ASN:HA	1.84	0.59
4:L:247:LEU:HD12	4:L:248:HIS:CG	2.36	0.59
4:L:480:LEU:HD21	18:j:82:GLY:HA3	1.83	0.59
6:N:308:ASN:HB3	7:O:317:ILE:CG2	2.33	0.59
11:c:34:PRO:CG	11:c:37:ALA:HB2	2.32	0.59
15:g:147:LEU:HD11	24:p:163:MET:HE2	1.84	0.59
4:L:81:LYS:HB2	4:L:135:ASN:OD1	2.02	0.59
4:L:123:LEU:HD22	4:L:150:MET:CG	2.33	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:313:MET:HE2	4:L:328:HIS:CE1	2.38	0.59
5:M:115:LEU:O	5:M:118:PHE:HB3	2.02	0.59
5:M:294:MET:HE3	5:M:319:HIS:CD2	2.37	0.59
10:Y:137:LEU:CD2	10:Y:138:PHE:CD2	2.84	0.59
4:L:12:PHE:HB3	25:L:701:3PE:H2G2	1.84	0.59
6:N:281:LEU:HD21	25:N:401:3PE:H281	1.83	0.59
6:N:314:MET:CB	7:O:305:LEU:HD11	2.32	0.59
7:O:164:TYR:CE2	7:O:195:LEU:HD21	2.36	0.59
16:h:69:ARG:O	16:h:73:PHE:HB2	2.02	0.59
18:j:94:ASP:HB3	18:j:99:ILE:HB	1.83	0.59
3:K:73:VAL:HG21	6:N:38:LEU:HD22	1.85	0.59
5:M:350:MET:HG2	22:n:99:VAL:HG12	1.84	0.59
1:D:35:ARG:NH2	15:g:57:PRO:C	2.60	0.59
4:L:227:PHE:CD2	4:L:283:LEU:CD2	2.86	0.59
8:U:105:MET:HB2	8:U:139:MET:CE	2.32	0.59
1:D:35:ARG:HH22	15:g:56:ASP:C	2.11	0.59
4:L:149:ILE:HG21	5:M:364:LEU:HD21	1.84	0.59
4:L:214:MET:HG2	25:L:704:3PE:H261	1.84	0.59
4:L:302:ILE:CG2	4:L:340:PHE:CE2	2.80	0.59
4:L:562:ILE:HG23	25:L:707:3PE:H3B1	1.85	0.59
17:i:9:LYS:HG2	17:i:9:LYS:O	2.02	0.59
2:J:63:MET:SD	3:K:34:GLU:OE1	2.61	0.59
4:L:312:LEU:CD2	4:L:395:ILE:HG21	2.33	0.59
4:L:605:ASN:O	4:L:606:LEU:C	2.46	0.59
5:M:209:LEU:HD23	5:M:211:GLY:H	1.67	0.59
6:N:149:LEU:HD12	6:N:149:LEU:O	2.02	0.59
6:N:164:MET:HE1	25:Y:201:3PE:H271	1.85	0.59
7:O:343:TYR:HE1	7:O:355:LYS:HB2	1.67	0.59
4:L:570:HIS:O	4:L:571:THR:C	2.45	0.59
5:M:14:LEU:HD21	5:M:26:ASN:HB2	1.84	0.59
6:N:300:THR:HG23	6:N:301:SER:N	2.17	0.59
7:O:114:LEU:HA	7:O:131:LEU:HD21	1.84	0.59
13:e:69:ARG:HD2	13:e:72:THR:HG21	1.85	0.59
15:g:139:TYR:HD2	15:g:140:PHE:CD1	2.20	0.59
22:n:111:GLU:O	22:n:114:MET:HG2	2.03	0.59
3:K:51:SER:HA	13:e:32:ARG:HH11	1.67	0.59
4:L:23:MET:HE1	26:L:705:CDL:H162	1.85	0.59
4:L:466:PHE:CE1	4:L:470:TYR:HE2	2.21	0.59
5:M:275:ILE:HD11	5:M:288:TYR:CB	2.33	0.59
5:M:396:MET:HG3	5:M:396:MET:O	2.03	0.59
6:N:170:LEU:CD1	6:N:292:PHE:HD2	2.16	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:h:95:GLU:HB3	16:h:114:LYS:HG2	1.85	0.58
18:j:47:PHE:HA	19:k:63:PHE:CZ	2.38	0.58
4:L:9:LEU:HD21	25:L:701:3PE:H2A1	1.83	0.58
4:L:385:PHE:CD1	18:j:72:ARG:CG	2.86	0.58
4:L:560:LYS:NZ	26:L:706:CDL:H321	2.18	0.58
5:M:449:THR:OG1	25:M:501:3PE:H281	2.03	0.58
25:M:502:3PE:H11	6:N:238:PRO:HB2	1.85	0.58
6:N:77:ASN:OD1	6:N:81:LEU:HD12	2.04	0.58
14:f:5:GLN:HB3	14:f:9:GLU:OE1	2.03	0.58
21:m:45:ARG:CZ	22:n:140:LEU:HD11	2.33	0.58
24:p:37:TYR:CZ	24:p:41:VAL:HG11	2.38	0.58
4:L:52:LEU:HB2	24:p:30:ILE:HD11	1.85	0.58
4:L:161:ARG:HA	22:n:92:GLU:HB2	1.85	0.58
4:L:230:HIS:N	4:L:231:PRO:CD	2.66	0.58
4:L:417:SER:HB3	4:L:493:ILE:CG1	2.31	0.58
5:M:210:TYR:O	5:M:213:HIS:CD2	2.56	0.58
6:N:307:THR:CG2	6:N:311:SER:OG	2.51	0.58
4:L:25:ASN:HB2	16:h:72:LYS:HZ1	1.68	0.58
4:L:407:TRP:CZ3	4:L:410:LEU:HD11	2.38	0.58
4:L:427:ILE:CD1	19:k:69:PHE:HE1	2.16	0.58
4:L:404:THR:HG22	4:L:405:ASN:N	2.19	0.58
9:X:171:THR:O	9:X:172:VAL:C	2.47	0.58
1:D:37:TRP:CZ2	1:D:39:PRO:HA	2.38	0.58
5:M:196:TRP:HZ3	5:M:261:PHE:CE2	2.21	0.58
5:M:424:ILE:HG13	21:m:57:VAL:O	2.04	0.58
12:d:14:LEU:HD12	12:d:14:LEU:C	2.27	0.58
12:d:113:LEU:O	12:d:113:LEU:HG	2.02	0.58
21:m:75:ASN:O	21:m:75:ASN:OD1	2.20	0.58
4:L:15:LEU:O	4:L:18:PRO:HD2	2.03	0.58
6:N:26:LEU:O	6:N:27:MET:C	2.46	0.58
6:N:164:MET:HE3	25:Y:201:3PE:C27	2.33	0.58
6:N:179:MET:CB	6:N:216:PHE:HE1	2.16	0.58
6:N:193:ILE:HD13	6:N:200:LEU:HB3	1.86	0.58
7:O:326:ARG:HH21	15:g:56:ASP:CG	2.12	0.58
4:L:232:TRP:CZ3	4:L:233:LEU:HD21	2.37	0.58
4:L:514:ASN:HA	22:n:36:LYS:NZ	2.19	0.58
5:M:73:LEU:HB2	5:M:103:GLN:OE1	2.02	0.58
15:g:70:ASP:OD1	22:n:108:HIS:NE2	2.37	0.58
17:i:70:PHE:O	17:i:73:SER:HB3	2.04	0.58
17:i:103:ARG:CD	23:o:50:GLN:HB2	2.34	0.58
1:D:62:LYS:HB2	1:D:63:PRO:HD2	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:592:LEU:O	4:L:596:ILE:HG12	2.03	0.58
6:N:142:LEU:HB3	6:N:194:LEU:HD21	1.85	0.58
7:O:88:GLU:HB2	7:O:160:GLU:OE1	2.04	0.58
7:O:117:PHE:CD1	7:O:128:SER:CB	2.87	0.58
9:X:160:PRO:HG3	12:d:22:PRO:HD3	1.86	0.58
11:c:72:ARG:HH11	12:d:19:ARG:HD3	1.68	0.58
15:g:121:GLU:HA	15:g:124:VAL:HG22	1.86	0.58
17:i:111:LEU:HD11	24:p:20:PRO:HD3	1.85	0.58
4:L:425:ARG:HG3	4:L:429:PHE:CE2	2.39	0.58
26:L:706:CDL:H201	10:Y:119:TYR:HB3	1.86	0.58
13:e:14:LEU:HD12	13:e:15:ASP:CB	2.33	0.58
22:n:177:ARG:HG2	22:n:179:THR:OG1	2.04	0.58
2:J:164:PHE:HE2	6:N:4:ILE:HG12	1.68	0.57
4:L:598:ILE:HD11	6:N:153:ILE:CD1	2.34	0.57
5:M:109:THR:HG22	5:M:121:LEU:CB	2.34	0.57
21:m:125:PHE:CE1	24:p:133:THR:HG22	2.39	0.57
2:J:123:TRP:CZ2	13:e:73:MET:HG2	2.40	0.57
4:L:56:HIS:O	23:o:71:ARG:HG3	2.03	0.57
7:O:355:LYS:HE2	11:c:37:ALA:O	2.03	0.57
8:U:84:LEU:O	8:U:88:LYS:HG3	2.05	0.57
8:U:100:VAL:O	8:U:101:ASN:HB2	2.04	0.57
12:d:113:LEU:HD22	15:g:148:PRO:HG3	1.86	0.57
17:i:103:ARG:O	17:i:105:PHE:CD1	2.57	0.57
4:L:203:PHE:CZ	24:p:110:LEU:HD11	2.39	0.57
4:L:362:ILE:CG2	4:L:366:MET:HE3	2.32	0.57
5:M:73:LEU:HD22	5:M:103:GLN:NE2	2.18	0.57
5:M:296:LEU:HD22	5:M:396:MET:HE1	1.85	0.57
5:M:297:VAL:O	5:M:301:ILE:HG12	2.03	0.57
3:K:93:LEU:HA	6:N:54:GLU:OE2	2.03	0.57
4:L:145:GLU:HB3	5:M:370:PRO:CG	2.34	0.57
4:L:546:LEU:HD22	21:m:72:ARG:NH2	2.19	0.57
5:M:230:ILE:HG13	5:M:235:LEU:HG	1.87	0.57
6:N:273:ASN:O	6:N:274:ASN:HB2	2.05	0.57
6:N:284:MET:O	6:N:287:LEU:HB2	2.04	0.57
4:L:227:PHE:CD2	4:L:283:LEU:HD21	2.38	0.57
5:M:444:LEU:O	5:M:448:THR:HG23	2.04	0.57
6:N:253:GLY:N	6:N:290:LEU:HD11	2.19	0.57
6:N:314:MET:HB2	7:O:305:LEU:CD1	2.33	0.57
8:U:130:ILE:HG23	8:U:147:TYR:CE2	2.40	0.57
4:L:306:THR:HA	4:L:336:LYS:HZ2	1.67	0.57
4:L:425:ARG:HG3	4:L:429:PHE:HE2	1.68	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:158:ILE:HG21	6:N:283:ALA:HB1	1.86	0.57
5:M:172:GLY:C	5:M:173:THR:HG23	2.28	0.57
15:g:121:GLU:OE2	24:p:10:TYR:CE2	2.58	0.57
5:M:4:ILE:CG2	5:M:107:ILE:HD13	2.30	0.57
5:M:55:MET:HE1	26:X:201:CDL:CB5	2.34	0.57
5:M:447:LEU:HD21	5:M:454:ILE:CD1	2.33	0.57
6:N:109:ALA:HB2	6:N:161:SER:HB3	1.85	0.57
6:N:331:ILE:HG13	12:d:41:THR:HA	1.86	0.57
7:O:99:GLY:HA2	11:c:30:TYR:CD1	2.38	0.57
7:O:305:LEU:O	7:O:305:LEU:CD1	2.51	0.57
17:i:87:LYS:HG2	17:i:87:LYS:O	2.05	0.57
20:l:166:LEU:HB2	20:l:170:ARG:NH2	2.19	0.57
2:J:44:LEU:HA	2:J:48:GLY:O	2.05	0.57
4:L:247:LEU:CD1	4:L:248:HIS:NE2	2.52	0.57
5:M:14:LEU:HD11	5:M:26:ASN:HB3	1.87	0.57
5:M:42:LEU:HD11	5:M:67:ILE:CD1	2.34	0.57
7:O:295:ARG:HH12	7:O:299:GLN:HB2	1.67	0.57
17:i:110:ILE:HD13	24:p:16:ARG:HD2	1.87	0.57
4:L:246:LEU:HD12	4:L:247:LEU:CA	2.34	0.57
4:L:253:VAL:CG2	4:L:310:LEU:HD11	2.35	0.57
26:L:705:CDL:H381	16:h:75:LEU:HB3	1.87	0.57
5:M:12:LEU:HB2	5:M:13:PRO:HD3	1.85	0.57
5:M:269:MET:HE3	5:M:399:ASN:HB2	1.86	0.57
6:N:43:MET:HE3	6:N:126:MET:SD	2.44	0.57
7:O:206:TYR:CD2	7:O:257:VAL:HG22	2.40	0.57
16:h:57:VAL:CG1	22:n:99:VAL:CG2	2.83	0.57
18:j:101:PRO:O	18:j:102:ASP:C	2.46	0.57
3:K:12:PHE:CD1	6:N:72:LEU:HD22	2.40	0.56
4:L:88:LEU:HD23	4:L:326:PHE:HE2	1.69	0.56
6:N:120:GLN:HG3	6:N:177:LYS:HE2	1.86	0.56
13:e:42:GLU:HG2	16:h:176:LYS:HE2	1.87	0.56
16:h:57:VAL:CG1	22:n:99:VAL:HG23	2.35	0.56
21:m:45:ARG:NE	22:n:140:LEU:HD11	2.20	0.56
3:K:89:TYR:C	3:K:91:GLN:N	2.59	0.56
4:L:518:PRO:C	4:L:520:SER:H	2.13	0.56
6:N:226:THR:HG22	6:N:228:ASN:H	1.70	0.56
7:O:176:GLN:HG3	7:O:177:GLY:N	2.16	0.56
10:Y:68:ILE:CG2	10:Y:120:MET:HE1	2.35	0.56
10:Y:92:TYR:CE1	10:Y:128:LYS:HD3	2.40	0.56
2:J:12:PHE:CZ	3:K:42:ILE:HD12	2.40	0.56
2:J:33:ILE:HG23	2:J:60:LEU:HD22	1.85	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:229:LEU:HD12	4:L:229:LEU:C	2.28	0.56
4:L:264:HIS:O	4:L:265:PRO:C	2.49	0.56
4:L:466:PHE:CB	18:j:68:TRP:CZ2	2.79	0.56
5:M:118:PHE:O	5:M:122:PHE:CB	2.54	0.56
5:M:158:ILE:HG12	6:N:287:LEU:HD11	1.86	0.56
5:M:282:LEU:HD13	5:M:342:MET:HE2	1.87	0.56
6:N:164:MET:HE1	25:Y:201:3PE:C27	2.28	0.56
6:N:254:LEU:CD1	6:N:255:PRO:HD2	2.35	0.56
7:O:125:ASP:OD1	7:O:126:GLY:N	2.39	0.56
7:O:173:MET:HE2	7:O:179:ILE:HG23	1.87	0.56
9:X:160:PRO:HG3	12:d:22:PRO:CD	2.35	0.56
17:i:101:LYS:HB3	17:i:102:PRO:HD2	1.87	0.56
21:m:125:PHE:HE1	24:p:133:THR:HG22	1.70	0.56
24:p:39:LEU:O	24:p:44:PRO:HD3	2.05	0.56
3:K:89:TYR:C	3:K:91:GLN:H	2.13	0.56
5:M:78:MET:O	5:M:432:ARG:HD2	2.05	0.56
5:M:127:ILE:CG1	6:N:254:LEU:HD21	2.35	0.56
25:M:502:3PE:H3A2	6:N:246:LEU:CD1	2.27	0.56
6:N:193:ILE:HG21	6:N:266:ILE:HG12	1.88	0.56
7:O:77:ILE:HG23	7:O:81:LEU:HD12	1.86	0.56
16:h:165:ASP:OD1	16:h:165:ASP:O	2.22	0.56
17:i:80:TRP:HE1	24:p:44:PRO:HG2	1.68	0.56
18:j:99:ILE:HD12	23:o:107:ARG:HB2	1.88	0.56
22:n:50:GLU:HG2	22:n:51:HIS:N	2.20	0.56
5:M:57:SER:HB3	5:M:113:THR:HG22	1.87	0.56
9:X:151:ASN:ND2	16:h:170:GLN:NE2	2.54	0.56
13:e:14:LEU:HD12	13:e:14:LEU:C	2.31	0.56
14:f:38:ARG:NH1	14:f:56:TRP:O	2.39	0.56
3:K:36:MET:HE3	6:N:68:MET:HG3	1.87	0.56
3:K:45:SER:O	3:K:49:LEU:HG	2.06	0.56
6:N:108:LEU:CD2	6:N:191:LEU:CD2	2.83	0.56
7:O:114:LEU:O	7:O:117:PHE:HB3	2.06	0.56
8:U:87:LEU:HD21	8:U:118:ILE:HG23	1.86	0.56
17:i:95:TYR:HD1	24:p:112:ALA:CB	2.16	0.56
20:l:105:ILE:HG23	20:l:109:LEU:HD22	1.86	0.56
20:l:119:THR:HG22	21:m:13:THR:HG23	1.87	0.56
2:J:22:LYS:HE2	3:K:18:GLY:O	2.06	0.56
4:L:397:GLU:HB2	4:L:482:MET:SD	2.46	0.56
5:M:196:TRP:HE1	5:M:250:LEU:HD13	1.69	0.56
25:J:201:3PE:H2C1	6:N:11:PHE:HZ	1.70	0.56
4:L:14:LEU:HD21	17:i:74:HIS:O	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:355:ASP:HB3	4:L:357:ARG:HG2	1.88	0.56
4:L:390:TYR:CE2	18:j:68:TRP:HH2	2.23	0.56
5:M:370:PRO:CA	5:M:375:LEU:CD2	2.84	0.56
6:N:307:THR:C	7:O:319:ILE:HG12	2.31	0.56
15:g:123:LEU:HD12	24:p:98:VAL:CG1	2.36	0.56
18:j:97:LEU:O	23:o:104:ARG:NH1	2.38	0.56
22:n:57:MET:HE2	22:n:57:MET:HA	1.87	0.56
24:p:132:PHE:O	24:p:136:THR:OG1	2.17	0.56
4:L:353:GLU:OE1	22:n:80:TYR:OH	2.24	0.56
5:M:4:ILE:H	5:M:4:ILE:HD12	1.70	0.56
5:M:73:LEU:CD2	5:M:103:GLN:CD	2.79	0.56
5:M:422:HIS:HB3	21:m:51:TYR:CE2	2.41	0.56
6:N:253:GLY:H	6:N:290:LEU:HD11	1.71	0.56
13:e:75:ARG:O	13:e:79:ILE:HG13	2.06	0.56
17:i:14:GLN:HE22	22:n:157:ALA:HB3	1.71	0.56
7:O:61:THR:HB	7:O:160:GLU:O	2.06	0.55
10:Y:76:THR:CG2	10:Y:95:GLY:HA3	2.34	0.55
17:i:105:PHE:CD2	23:o:68:LYS:CA	2.84	0.55
18:j:45:ARG:HD3	19:k:57:TRP:CD1	2.41	0.55
23:o:39:MET:HE1	23:o:58:TYR:HA	1.86	0.55
4:L:102:GLN:HE22	4:L:452:ASN:HB2	1.72	0.55
4:L:538:PRO:O	4:L:542:LEU:HD13	2.06	0.55
26:L:705:CDL:H161	5:M:361:MET:HE1	1.88	0.55
7:O:62:VAL:HG22	7:O:205:ILE:CB	2.33	0.55
15:g:106:TYR:CE2	16:h:86:ILE:CD1	2.89	0.55
1:D:47:PHE:CE2	6:N:305:PHE:HZ	2.24	0.55
4:L:94:LEU:HD23	4:L:125:LEU:HD21	1.89	0.55
4:L:145:GLU:HG2	5:M:370:PRO:HD3	1.88	0.55
4:L:556:ILE:HG21	21:m:80:PHE:CZ	2.39	0.55
10:Y:71:MET:CG	10:Y:102:THR:HG21	2.37	0.55
12:d:106:LYS:CB	24:p:79:GLU:HB3	2.37	0.55
17:i:26:GLN:HA	22:n:118:TYR:HE1	1.71	0.55
17:i:127:HIS:O	17:i:128:HIS:C	2.47	0.55
23:o:69:CYS:O	23:o:69:CYS:SG	2.65	0.55
4:L:71:MET:HE2	4:L:74:MET:O	2.05	0.55
6:N:237:THR:O	6:N:237:THR:CG2	2.55	0.55
10:Y:137:LEU:HD23	10:Y:138:PHE:CD2	2.41	0.55
21:m:23:TYR:HB2	22:n:65:ARG:NH2	2.21	0.55
4:L:94:LEU:CD2	4:L:125:LEU:HD21	2.35	0.55
6:N:62:THR:HG21	6:N:114:TRP:CD1	2.41	0.55
7:O:170:LEU:HG	7:O:179:ILE:HD13	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:224:PRO:HA	7:O:227:MET:CE	2.36	0.55
7:O:230:THR:HG22	7:O:233:TYR:H	1.72	0.55
8:U:88:LYS:HG3	8:U:98:LEU:HD11	1.87	0.55
17:i:88:TYR:CE2	24:p:49:ARG:HB2	2.42	0.55
18:j:97:LEU:O	23:o:104:ARG:HG3	2.06	0.55
4:L:162:THR:O	4:L:166:THR:HG23	2.06	0.55
5:M:62:SER:C	5:M:64:PRO:HD2	2.32	0.55
5:M:127:ILE:HG12	6:N:254:LEU:HD21	1.88	0.55
6:N:224:SER:HB2	6:N:229:SER:HB3	1.89	0.55
7:O:238:GLU:HA	7:O:241:TYR:CD2	2.33	0.55
18:j:92:TRP:CZ3	23:o:100:LYS:HA	2.41	0.55
2:J:75:THR:CG2	3:K:25:HIS:HB3	2.37	0.55
4:L:230:HIS:N	4:L:231:PRO:HD3	2.22	0.55
4:L:336:LYS:O	4:L:340:PHE:HD2	1.90	0.55
4:L:561:THR:O	4:L:565:SER:HB2	2.07	0.55
5:M:231:LEU:CA	5:M:235:LEU:HD12	2.36	0.55
6:N:230:ILE:O	6:N:233:LEU:HB2	2.07	0.55
6:N:321:LYS:HB2	12:d:49:ARG:HE	1.71	0.55
13:e:14:LEU:HD12	13:e:15:ASP:N	2.21	0.55
14:f:49:ARG:HG3	14:f:52:GLU:HG2	1.89	0.55
17:i:11:ARG:NH2	22:n:154:LEU:CB	2.60	0.55
18:j:100:PRO:HG3	23:o:30:GLY:HA3	1.89	0.55
19:k:30:ILE:CD1	19:k:39:GLN:HB2	2.33	0.55
2:J:164:PHE:HD2	6:N:5:THR:HA	1.72	0.55
7:O:161:ARG:HH22	27:O:402:ADP:H5'1	1.72	0.55
8:U:110:LEU:HD22	8:U:118:ILE:HD11	1.87	0.55
17:i:83:HIS:CD2	24:p:37:TYR:CE2	2.95	0.55
20:l:109:LEU:HG	20:l:109:LEU:O	2.06	0.55
4:L:526:LEU:CD2	4:L:530:PRO:HG2	2.37	0.55
5:M:255:LYS:HZ3	12:d:117:HIS:HB3	1.72	0.55
14:f:46:ARG:HD2	16:h:106:ILE:HD13	1.87	0.55
16:h:73:PHE:CD2	16:h:74:TYR:CE1	2.94	0.55
2:J:168:GLU:HA	2:J:171:ARG:CG	2.32	0.55
4:L:182:PHE:CE2	4:L:186:MET:CE	2.88	0.55
4:L:258:PHE:HE1	4:L:262:ARG:HH21	1.55	0.55
5:M:6:LEU:HB3	5:M:7:PRO:HD3	1.88	0.55
5:M:453:LEU:HD12	5:M:454:ILE:CG2	2.34	0.55
25:M:502:3PE:H261	25:O:401:3PE:C23	2.32	0.55
17:i:83:HIS:HE1	17:i:87:LYS:HD2	1.71	0.55
4:L:381:THR:HG21	4:L:498:PHE:CZ	2.43	0.54
8:U:103:HIS:NE2	8:U:140:CYS:SG	2.81	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:e:32:ARG:O	13:e:33:CYS:HB2	2.06	0.54
13:e:42:GLU:CG	16:h:176:LYS:HE2	2.36	0.54
4:L:190:SER:HB2	4:L:196:TRP:NE1	2.22	0.54
5:M:409:TYR:CE1	20:l:116:ARG:NH2	2.75	0.54
7:O:319:ILE:HG13	7:O:320:GLY:H	1.72	0.54
17:i:16:ARG:O	17:i:20:ARG:HG2	2.08	0.54
20:l:152:SER:HA	23:o:5:LEU:HD21	1.88	0.54
1:D:61:TRP:HH2	4:L:579:ASN:HA	1.72	0.54
2:J:135:LEU:HA	3:K:54:MET:HE1	1.89	0.54
4:L:232:TRP:O	4:L:236:ALA:N	2.40	0.54
4:L:445:GLU:OE2	18:j:54:GLN:HG3	2.08	0.54
4:L:507:LEU:O	4:L:510:LYS:HG2	2.06	0.54
6:N:33:LEU:HD11	6:N:141:ILE:CD1	2.38	0.54
6:N:164:MET:HE2	25:Y:201:3PE:H271	1.86	0.54
6:N:179:MET:CB	6:N:216:PHE:CE1	2.89	0.54
6:N:314:MET:CE	6:N:319:LYS:HE2	2.34	0.54
8:U:85:TYR:HA	8:U:88:LYS:HD3	1.89	0.54
10:Y:68:ILE:HG12	10:Y:102:THR:OG1	2.07	0.54
15:g:106:TYR:HE2	16:h:86:ILE:CD1	2.20	0.54
23:o:103:GLU:OE2	23:o:106:ARG:HD2	2.07	0.54
4:L:66:TRP:HZ3	25:L:701:3PE:O14	1.90	0.54
4:L:174:TYR:HE1	25:L:703:3PE:H362	1.73	0.54
5:M:415:GLN:O	5:M:416:ARG:HG3	2.08	0.54
8:U:131:PRO:HG2	8:U:134:ASP:HB2	1.90	0.54
4:L:232:TRP:CH2	4:L:233:LEU:HD21	2.42	0.54
4:L:510:LYS:HE3	4:L:512:SER:HB2	1.90	0.54
4:L:551:THR:HA	4:L:555:LEU:HD12	1.90	0.54
5:M:336:ARG:HH22	5:M:429:SER:HA	1.73	0.54
5:M:373:ILE:HD11	5:M:454:ILE:HD11	1.88	0.54
15:g:117:ARG:NE	24:p:10:TYR:OH	2.41	0.54
4:L:362:ILE:HA	4:L:365:ILE:HG13	1.90	0.54
5:M:131:ILE:CD1	6:N:302:LEU:HD21	2.38	0.54
5:M:313:THR:HG21	5:M:456:GLY:CA	2.38	0.54
5:M:421:ASN:HB2	21:m:51:TYR:OH	2.08	0.54
18:j:98:GLY:O	18:j:100:PRO:HD3	2.06	0.54
22:n:20:TYR:CE2	22:n:24:LEU:CD1	2.91	0.54
2:J:9:SER:HB3	3:K:7:ASN:ND2	2.16	0.54
2:J:60:LEU:HD13	2:J:61:GLY:N	2.21	0.54
4:L:131:LEU:CD1	4:L:140:LEU:CD1	2.78	0.54
5:M:160:LEU:HD23	5:M:164:LEU:HD13	1.89	0.54
5:M:263:LEU:HD11	21:m:102:TYR:CD1	2.41	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:264:LEU:CD2	21:m:98:LEU:HD21	2.37	0.54
5:M:276:CYS:HB3	5:M:285:LEU:HG	1.89	0.54
6:N:33:LEU:HD11	6:N:141:ILE:HD12	1.90	0.54
7:O:170:LEU:HG	7:O:179:ILE:CD1	2.37	0.54
17:i:22:TRP:CE3	22:n:172:THR:HG22	2.43	0.54
1:D:35:ARG:HE	15:g:59:PRO:HD2	1.73	0.54
4:L:247:LEU:HD11	4:L:248:HIS:CE1	2.43	0.54
5:M:31:SER:HA	5:M:34:ILE:HG12	1.90	0.54
5:M:79:ALA:HB1	5:M:225:ILE:HD13	1.90	0.54
7:O:48:LYS:H	7:O:51:LYS:HE3	1.71	0.54
16:h:96:ALA:O	24:p:63:TYR:HE1	1.90	0.54
16:h:129:PRO:HG3	24:p:66:ARG:CZ	2.37	0.54
21:m:109:ARG:O	21:m:113:GLU:HG2	2.08	0.54
5:M:1:MET:HE2	5:M:52:PHE:CE2	2.42	0.54
5:M:283:LYS:HG3	5:M:327:PHE:CE1	2.43	0.54
6:N:108:LEU:HD22	6:N:191:LEU:HD22	1.90	0.54
6:N:164:MET:CE	25:Y:201:3PE:H261	2.37	0.54
21:m:8:PRO:HB3	21:m:14:LEU:N	2.23	0.54
4:L:174:TYR:HE1	25:L:703:3PE:H331	1.71	0.54
4:L:481:THR:HG22	23:o:95:TYR:CE2	2.42	0.54
4:L:512:SER:HA	22:n:40:PHE:HZ	1.73	0.54
4:L:550:LEU:HD11	5:M:279:GLN:NE2	2.23	0.54
5:M:231:LEU:O	5:M:236:LEU:HG	2.06	0.54
5:M:423:MET:SD	21:m:59:HIS:NE2	2.81	0.54
6:N:179:MET:HB3	6:N:216:PHE:CZ	2.43	0.54
6:N:321:LYS:HB2	12:d:49:ARG:NE	2.23	0.54
15:g:145:ILE:CG2	24:p:160:LYS:HE2	2.33	0.54
22:n:125:TRP:CE3	22:n:128:LEU:HD12	2.42	0.54
23:o:57:ASP:CG	23:o:59:CYS:H	2.16	0.54
24:p:31:THR:O	24:p:35:LYS:HG3	2.07	0.54
1:D:37:TRP:CE3	5:M:140:THR:HA	2.42	0.53
4:L:102:GLN:NE2	4:L:452:ASN:HB2	2.23	0.53
4:L:427:ILE:HD11	19:k:69:PHE:CE1	2.43	0.53
4:L:554:ASP:OD2	5:M:213:HIS:HE1	1.90	0.53
8:U:95:PRO:HG2	8:U:96:GLU:HG3	1.88	0.53
15:g:140:PHE:HZ	24:p:152:ALA:HB1	1.72	0.53
4:L:141:PHE:CD2	5:M:370:PRO:CG	2.91	0.53
4:L:407:TRP:HE1	20:l:140:MET:CE	2.21	0.53
4:L:559:GLU:HG2	4:L:564:LYS:HD3	1.90	0.53
4:L:578:THR:HG21	6:N:168:GLY:HA2	1.89	0.53
8:U:99:SER:O	8:U:100:VAL:C	2.51	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:201:3PE:H251	25:Y:201:3PE:H331	1.89	0.53
12:d:39:TYR:CE2	12:d:43:LEU:HD11	2.43	0.53
4:L:79:SER:CB	4:L:135:ASN:HB2	2.36	0.53
5:M:61:LEU:HD22	5:M:244:ILE:HG21	1.90	0.53
6:N:193:ILE:CD1	6:N:200:LEU:HD22	2.38	0.53
7:O:40:LEU:O	7:O:44:ILE:HG13	2.09	0.53
7:O:114:LEU:HA	7:O:131:LEU:HD22	1.91	0.53
23:o:93:LEU:C	23:o:96:VAL:HG12	2.33	0.53
24:p:103:MET:CE	24:p:135:VAL:HG12	2.38	0.53
4:L:9:LEU:HD21	25:L:701:3PE:C2A	2.38	0.53
4:L:226:GLN:OE1	4:L:284:THR:HG21	2.07	0.53
4:L:387:THR:HG22	4:L:465:GLY:N	2.24	0.53
4:L:400:ASN:HD21	4:L:413:LEU:HD11	1.73	0.53
7:O:140:LEU:HD11	7:O:198:TYR:OH	2.08	0.53
17:i:83:HIS:HD2	24:p:37:TYR:CE2	2.27	0.53
2:J:40:CYS:SG	2:J:56:PHE:HB2	2.49	0.53
3:K:22:PHE:CB	4:L:585:LYS:HG2	2.35	0.53
4:L:509:MET:HG2	22:n:33:HIS:CE1	2.43	0.53
4:L:518:PRO:C	4:L:520:SER:N	2.62	0.53
4:L:563:PRO:HG3	5:M:152:TYR:OH	2.08	0.53
7:O:80:GLN:HE22	7:O:267:THR:HG22	1.73	0.53
7:O:319:ILE:HG13	7:O:320:GLY:N	2.23	0.53
7:O:352:ILE:HG21	12:d:52:PRO:HG2	1.91	0.53
1:D:35:ARG:HE	15:g:59:PRO:CD	2.21	0.53
4:L:97:THR:HG21	4:L:125:LEU:HD22	1.90	0.53
6:N:99:LEU:HD11	6:N:154:ILE:HG22	1.90	0.53
6:N:328:THR:HG23	12:d:68:PHE:CZ	2.43	0.53
19:k:49:ASP:OD1	22:n:38:ARG:HG3	2.09	0.53
22:n:56:ASP:O	22:n:57:MET:C	2.50	0.53
4:L:358:LYS:CG	22:n:80:TYR:CE1	2.74	0.53
4:L:361:ASN:HA	4:L:431:THR:O	2.09	0.53
25:L:701:3PE:H2I1	26:L:705:CDL:C59	2.39	0.53
26:L:706:CDL:H822	25:Y:201:3PE:C39	2.38	0.53
5:M:55:MET:HG3	5:M:56:PHE:CD2	2.44	0.53
5:M:269:MET:CE	5:M:396:MET:HA	2.36	0.53
5:M:453:LEU:HD12	5:M:453:LEU:C	2.33	0.53
6:N:99:LEU:HD21	6:N:157:LEU:HD12	1.90	0.53
6:N:328:THR:HG23	12:d:68:PHE:HZ	1.74	0.53
9:X:158:LEU:HD13	12:d:17:GLU:HG3	1.91	0.53
12:d:109:TYR:O	12:d:110:ALA:C	2.50	0.53
22:n:39:TYR:CZ	22:n:43:LEU:HD11	2.44	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:12:PHE:HE2	3:K:42:ILE:HD11	1.74	0.53
4:L:124:PHE:HZ	4:L:252:MET:HB2	1.74	0.53
5:M:57:SER:CB	5:M:113:THR:HG22	2.39	0.53
5:M:59:ASP:O	5:M:60:PRO:C	2.49	0.53
5:M:73:LEU:HD23	5:M:103:GLN:NE2	2.23	0.53
6:N:203:LEU:HD13	6:N:344:ILE:HG22	1.90	0.53
7:O:73:LEU:CD2	7:O:207:ILE:HD11	2.38	0.53
7:O:170:LEU:HD13	7:O:187:TYR:CD2	2.44	0.53
10:Y:50:SER:HB3	10:Y:53:GLU:HG2	1.91	0.53
16:h:156:VAL:CG1	16:h:160:MET:HE3	2.39	0.53
19:k:38:VAL:CG1	22:n:39:TYR:HB2	2.34	0.53
1:D:36:GLN:OE1	5:M:136:TRP:HA	2.09	0.53
4:L:20:LEU:C	4:L:20:LEU:CD1	2.81	0.53
5:M:15:THR:HG21	5:M:100:ILE:HD12	1.90	0.53
5:M:188:ALA:H	5:M:253:LEU:HD11	1.74	0.53
5:M:348:LEU:HD12	5:M:415:GLN:NE2	2.24	0.53
6:N:193:ILE:HD12	6:N:266:ILE:HA	1.91	0.53
15:g:139:TYR:CD2	15:g:140:PHE:CD1	2.96	0.53
18:j:99:ILE:HA	23:o:108:LEU:HD21	1.90	0.53
20:l:55:TYR:O	20:l:104:PRO:HG3	2.09	0.53
22:n:136:GLU:OE2	22:n:167:TRP:NE1	2.42	0.53
3:K:5:PHE:HE1	3:K:47:THR:HG23	1.74	0.53
3:K:24:SER:O	3:K:90:VAL:HG13	2.10	0.53
4:L:450:LEU:HG	4:L:454:ILE:HD12	1.91	0.53
4:L:598:ILE:CD1	6:N:153:ILE:HG12	2.38	0.53
5:M:314:MET:HE1	5:M:380:PHE:CD2	2.44	0.53
6:N:81:LEU:HD23	13:e:60:PHE:HE1	1.74	0.53
6:N:155:LEU:HD13	6:N:278:MET:HG3	1.91	0.53
6:N:331:ILE:O	6:N:335:MET:HB2	2.09	0.53
7:O:77:ILE:HD13	7:O:273:ILE:HD11	1.90	0.53
16:h:184:LYS:HE3	16:h:186:THR:O	2.08	0.53
17:i:106:PRO:HD2	23:o:64:ILE:CG2	2.38	0.53
19:k:47:LEU:CD1	22:n:43:LEU:HD23	2.39	0.53
21:m:85:LYS:O	21:m:85:LYS:HG2	2.09	0.53
2:J:120:LEU:C	2:J:122:ASP:H	2.16	0.52
4:L:128:MET:CG	4:L:251:THR:HB	2.36	0.52
4:L:247:LEU:O	4:L:252:MET:HB3	2.09	0.52
5:M:73:LEU:HD21	5:M:100:ILE:HG12	1.90	0.52
6:N:313:MET:HG2	7:O:305:LEU:HD22	1.91	0.52
8:U:78:GLY:O	8:U:79:ILE:C	2.51	0.52
14:f:49:ARG:CG	14:f:52:GLU:HG3	2.39	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:51:VAL:HG21	1:D:58:THR:HG22	1.90	0.52
4:L:108:MET:HB2	4:L:114:ILE:HD13	1.90	0.52
4:L:228:GLY:O	4:L:229:LEU:CG	2.47	0.52
4:L:332:HIS:CD2	4:L:336:LYS:HG3	2.44	0.52
5:M:160:LEU:CD2	5:M:164:LEU:HD13	2.39	0.52
5:M:354:LEU:O	5:M:357:THR:N	2.41	0.52
5:M:447:LEU:HD11	5:M:454:ILE:HG23	1.90	0.52
6:N:227:ILE:HA	6:N:230:ILE:CG2	2.39	0.52
7:O:350:LYS:O	7:O:351:TRP:HB2	2.09	0.52
13:e:41:ILE:HD13	16:h:174:PRO:HD2	1.92	0.52
19:k:20:MET:HE3	19:k:22:LEU:HD21	1.91	0.52
22:n:163:LEU:O	22:n:164:PRO:C	2.51	0.52
5:M:196:TRP:HE1	5:M:254:THR:HB	1.75	0.52
5:M:213:HIS:O	5:M:217:PRO:HD3	2.09	0.52
5:M:313:THR:HA	5:M:316:MET:HE3	1.89	0.52
5:M:388:TRP:CD1	21:m:109:ARG:HD2	2.44	0.52
7:O:121:PRO:C	7:O:122:LYS:HG2	2.33	0.52
4:L:536:ILE:HG23	4:L:537:THR:N	2.25	0.52
5:M:403:THR:HA	5:M:406:TYR:CE2	2.44	0.52
6:N:10:TYR:O	6:N:13:ILE:HG22	2.09	0.52
6:N:220:MET:O	6:N:221:LEU:C	2.51	0.52
7:O:310:ILE:HG13	7:O:311:PRO:HD2	1.91	0.52
8:U:74:LEU:HD23	8:U:79:ILE:HD11	1.91	0.52
17:i:19:ARG:HH11	22:n:173:ARG:HH21	1.56	0.52
20:l:119:THR:HG23	21:m:11:LEU:HA	1.91	0.52
3:K:38:LEU:HG	3:K:42:ILE:CD1	2.39	0.52
4:L:297:ASP:HB3	4:L:300:LYS:CG	2.39	0.52
4:L:324:LEU:HB3	4:L:395:ILE:HD11	1.90	0.52
25:L:707:3PE:H3C1	5:M:155:ILE:HD11	1.91	0.52
5:M:171:VAL:HG11	5:M:179:LEU:CD2	2.35	0.52
5:M:278:ARG:HH22	20:l:108:ASP:CG	2.18	0.52
6:N:320:THR:O	6:N:320:THR:CG2	2.58	0.52
7:O:336:GLY:N	7:O:344:ASN:ND2	2.57	0.52
17:i:31:ARG:O	17:i:32:GLU:C	2.51	0.52
21:m:49:LEU:HA	22:n:133:TRP:HH2	1.74	0.52
3:K:57:MET:N	3:K:58:PRO:HD2	2.24	0.52
7:O:168:VAL:CG2	7:O:241:TYR:OH	2.56	0.52
10:Y:68:ILE:CD1	10:Y:103:LEU:HB2	2.39	0.52
12:d:62:LEU:O	12:d:66:THR:OG1	2.22	0.52
16:h:87:THR:HG22	26:h:201:CDL:H512	1.90	0.52
16:h:111:GLU:O	24:p:63:TYR:HA	2.08	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:h:201:CDL:H721	17:i:84:TYR:CD2	2.44	0.52
2:J:121:GLY:C	2:J:123:TRP:N	2.64	0.52
4:L:123:LEU:HD22	4:L:150:MET:HG3	1.91	0.52
4:L:481:THR:CG2	23:o:95:TYR:CD2	2.93	0.52
4:L:496:LEU:C	4:L:496:LEU:CD1	2.79	0.52
7:O:170:LEU:HD13	7:O:187:TYR:CG	2.44	0.52
24:p:50:GLU:HG3	24:p:54:ARG:HH21	1.75	0.52
1:D:67:ASN:HB2	7:O:193:LEU:HD22	1.89	0.52
4:L:108:MET:HB2	4:L:114:ILE:CD1	2.39	0.52
4:L:145:GLU:HB3	5:M:370:PRO:HG2	1.90	0.52
4:L:427:ILE:HD11	19:k:69:PHE:HE1	1.73	0.52
25:L:707:3PE:H121	6:N:295:ARG:HG3	1.92	0.52
5:M:68:LEU:HG	5:M:234:ILE:HD11	1.92	0.52
5:M:84:LEU:HD21	5:M:95:TYR:HB3	1.90	0.52
5:M:346:ARG:O	5:M:419:LEU:HA	2.09	0.52
15:g:121:GLU:OE2	24:p:10:TYR:CZ	2.63	0.52
18:j:81:LEU:O	18:j:82:GLY:C	2.51	0.52
4:L:49:LEU:HD12	24:p:33:LEU:HD23	1.92	0.52
4:L:533:ILE:HG23	4:L:534:HIS:HD2	1.74	0.52
5:M:72:LEU:HD11	5:M:233:ALA:HB1	1.91	0.52
8:U:128:PHE:CE1	8:U:148:ILE:HG23	2.45	0.52
4:L:483:PRO:HG2	4:L:486:LEU:HD13	1.91	0.52
6:N:200:LEU:HD22	6:N:269:GLU:HG3	1.92	0.52
20:l:169:GLU:C	20:l:171:GLY:N	2.55	0.52
22:n:168:TRP:HD1	22:n:169:HIS:CE1	2.27	0.52
2:J:60:LEU:CD1	2:J:61:GLY:N	2.72	0.51
4:L:286:LEU:HG	4:L:290:ILE:CD1	2.40	0.51
5:M:103:GLN:O	5:M:107:ILE:HB	2.10	0.51
5:M:139:GLN:HB3	5:M:222:GLU:CG	2.40	0.51
7:O:121:PRO:HB3	7:O:178:TYR:CE1	2.45	0.51
8:U:133:ILE:HG23	8:U:134:ASP:N	2.26	0.51
13:e:44:ALA:HA	13:e:47:ILE:HG12	1.92	0.51
19:k:47:LEU:HD12	22:n:43:LEU:HD23	1.91	0.51
22:n:143:GLU:O	22:n:143:GLU:HG2	2.10	0.51
24:p:164:LEU:O	24:p:168:LYS:N	2.42	0.51
2:J:63:MET:O	2:J:64:LEU:C	2.53	0.51
2:J:150:TRP:CD1	6:N:28:LEU:HD21	2.44	0.51
4:L:556:ILE:HD11	21:m:76:ILE:CG2	2.40	0.51
5:M:115:LEU:HD21	5:M:176:LEU:CD2	2.37	0.51
13:e:50:THR:O	13:e:54:LYS:NZ	2.44	0.51
14:f:37:PHE:HA	14:f:40:LYS:HB2	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:49:LEU:HB3	4:L:50:PRO:HD3	1.91	0.51
4:L:202:MET:CE	4:L:265:PRO:HG3	2.33	0.51
4:L:539:MET:SD	21:m:11:LEU:HD21	2.50	0.51
4:L:569:LEU:O	4:L:573:MET:HG2	2.11	0.51
13:e:8:LYS:HG2	13:e:16:ARG:NH1	2.23	0.51
17:i:85:TYR:CE2	17:i:90:MET:HE3	2.46	0.51
3:K:59:ILE:O	3:K:60:PRO:C	2.49	0.51
17:i:77:ILE:HD13	17:i:80:TRP:CZ3	2.46	0.51
24:p:5:TRP:CE3	24:p:10:TYR:HB2	2.45	0.51
4:L:261:VAL:O	4:L:264:HIS:HD2	1.93	0.51
5:M:20:PRO:HB3	5:M:89:ASN:ND2	2.25	0.51
5:M:275:ILE:CD1	5:M:288:TYR:CG	2.84	0.51
6:N:174:GLN:HB2	6:N:177:LYS:HD2	1.92	0.51
6:N:307:THR:HB	7:O:319:ILE:HG12	1.91	0.51
7:O:332:ARG:NH1	12:d:50:MET:HE1	2.26	0.51
12:d:28:ASP:O	12:d:29:PRO:C	2.53	0.51
12:d:87:ASP:O	12:d:88:HIS:C	2.51	0.51
17:i:101:LYS:HB3	17:i:102:PRO:CD	2.41	0.51
17:i:106:PRO:HD2	23:o:64:ILE:HG21	1.93	0.51
4:L:530:PRO:O	4:L:534:HIS:HB2	2.11	0.51
5:M:11:LEU:O	5:M:15:THR:HG23	2.09	0.51
5:M:31:SER:HA	5:M:34:ILE:CG1	2.41	0.51
5:M:129:THR:CG2	5:M:235:LEU:HD11	2.40	0.51
5:M:251:ASP:N	5:M:252:PRO:HD2	2.26	0.51
6:N:149:LEU:HD12	6:N:149:LEU:C	2.34	0.51
14:f:49:ARG:CG	14:f:52:GLU:CG	2.88	0.51
17:i:83:HIS:CD2	24:p:37:TYR:HE2	2.28	0.51
17:i:83:HIS:CE1	17:i:87:LYS:HD2	2.46	0.51
19:k:34:PRO:HD2	19:k:59:TYR:CG	2.46	0.51
19:k:39:GLN:HE22	19:k:49:ASP:HB3	1.75	0.51
7:O:60:ILE:HG12	7:O:83:MET:HE1	1.93	0.51
16:h:159:LEU:HD23	16:h:163:ARG:HH12	1.75	0.51
2:J:84:SER:OG	2:J:87:LEU:HB3	2.10	0.51
4:L:161:ARG:NE	4:L:163:ASP:HB2	2.26	0.51
4:L:595:ILE:O	4:L:599:ILE:HG13	2.11	0.51
5:M:304:GLN:HA	5:M:309:PHE:CE1	2.45	0.51
6:N:239:ALA:HB1	12:d:47:MET:HG2	1.93	0.51
6:N:333:SER:O	6:N:334:THR:OG1	2.26	0.51
8:U:74:LEU:HD23	8:U:79:ILE:CD1	2.40	0.51
18:j:67:PHE:CE1	19:k:84:PHE:HA	2.46	0.51
21:m:23:TYR:HB2	22:n:65:ARG:HH21	1.76	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:404:THR:HG22	4:L:405:ASN:H	1.75	0.51
4:L:414:ILE:O	4:L:418:MET:HG2	2.10	0.51
5:M:166:LEU:HD11	25:N:401:3PE:O14	2.11	0.51
5:M:249:ILE:HG22	5:M:250:LEU:N	2.26	0.51
13:e:70:TYR:OH	13:e:74:ARG:HD3	2.11	0.51
20:l:155:PRO:HG3	23:o:4:HIS:CG	2.46	0.51
4:L:451:MET:O	4:L:452:ASN:C	2.53	0.51
5:M:4:ILE:HD11	5:M:41:LEU:HD21	1.92	0.51
6:N:45:ILE:HA	6:N:52:SER:OG	2.11	0.51
6:N:183:SER:O	6:N:187:MET:HE2	2.11	0.51
7:O:289:TRP:HA	7:O:289:TRP:CE3	2.46	0.51
8:U:122:MET:HA	8:U:122:MET:HE2	1.91	0.51
8:U:134:ASP:OD2	22:n:3:PHE:N	2.41	0.51
2:J:22:LYS:CE	3:K:18:GLY:O	2.59	0.50
25:J:201:3PE:H2C1	6:N:11:PHE:CZ	2.46	0.50
4:L:21:ILE:HG12	4:L:27:ILE:HG23	1.93	0.50
5:M:123:GLU:CG	6:N:255:PRO:HG2	2.41	0.50
6:N:159:ILE:HG12	6:N:163:PHE:CE2	2.46	0.50
7:O:182:GLN:O	7:O:183:CYS:C	2.54	0.50
8:U:119:ILE:CD1	8:U:138:LEU:HB2	2.40	0.50
11:c:46:LEU:O	11:c:50:ALA:HB2	2.12	0.50
16:h:73:PHE:CE2	16:h:74:TYR:CE1	2.98	0.50
24:p:49:ARG:O	24:p:52:ILE:HB	2.10	0.50
24:p:113:CYS:O	24:p:113:CYS:SG	2.69	0.50
2:J:96:VAL:O	2:J:99:GLU:HG2	2.11	0.50
4:L:395:ILE:O	4:L:399:ILE:HG13	2.11	0.50
25:L:704:3PE:H2	25:L:704:3PE:H112	1.93	0.50
6:N:104:MET:HE3	6:N:111:PHE:CE1	2.47	0.50
6:N:189:TRP:HB2	6:N:204:ASN:HD21	1.76	0.50
6:N:313:MET:HG3	7:O:305:LEU:CD2	2.40	0.50
15:g:115:TRP:HA	15:g:118:ARG:HH11	1.75	0.50
17:i:19:ARG:HA	22:n:171:VAL:HG13	1.94	0.50
20:l:87:ASP:OD1	20:l:88:PRO:HD2	2.11	0.50
21:m:22:GLU:OE2	22:n:15:LYS:HD3	2.11	0.50
4:L:117:PHE:HE1	4:L:243:VAL:CG2	2.23	0.50
4:L:264:HIS:O	4:L:267:THR:N	2.43	0.50
4:L:349:SER:HB2	4:L:443:ILE:HG23	1.93	0.50
4:L:365:ILE:CD1	4:L:366:MET:HE2	2.42	0.50
5:M:154:LEU:HD13	6:N:287:LEU:CD2	2.41	0.50
5:M:294:MET:HE3	5:M:319:HIS:HD2	1.76	0.50
5:M:354:LEU:O	5:M:355:MET:C	2.52	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:248:LEU:CD1	6:N:296:LEU:HD23	2.41	0.50
7:O:40:LEU:H	7:O:40:LEU:HD12	1.76	0.50
7:O:326:ARG:NH2	15:g:56:ASP:OD1	2.45	0.50
20:l:38:PRO:HG2	21:m:71:ALA:HB2	1.93	0.50
4:L:70:THR:HG21	24:p:101:GLU:OE2	2.12	0.50
4:L:109:HIS:O	4:L:110:SER:HB2	2.11	0.50
4:L:383:MET:CB	4:L:386:LEU:HD12	2.30	0.50
5:M:63:THR:N	5:M:64:PRO:HD2	2.26	0.50
7:O:211:VAL:HB	7:O:212:PRO:HD3	1.91	0.50
25:O:401:3PE:O22	25:O:401:3PE:H322	2.12	0.50
8:U:93:ILE:HD11	8:U:118:ILE:HD11	1.92	0.50
10:Y:90:LEU:O	10:Y:94:ILE:HG12	2.11	0.50
15:g:63:ASN:OD1	22:n:106:TYR:HE1	1.95	0.50
15:g:74:TYR:CE2	15:g:85:MET:HB3	2.47	0.50
26:h:201:CDL:H132	26:h:201:CDL:H172	1.92	0.50
17:i:108:ASP:OD2	24:p:18:PRO:HB2	2.11	0.50
22:n:114:MET:O	22:n:115:TYR:C	2.52	0.50
4:L:424:MET:HE2	4:L:502:LEU:HA	1.93	0.50
5:M:118:PHE:O	5:M:122:PHE:HB2	2.11	0.50
19:k:34:PRO:CG	19:k:59:TYR:CD1	2.94	0.50
5:M:248:ILE:HG13	5:M:249:ILE:N	2.25	0.50
6:N:326:PHE:CE2	12:d:48:LEU:HD13	2.46	0.50
9:X:151:ASN:HB3	13:e:51:ARG:NH1	2.26	0.50
15:g:139:TYR:HD1	24:p:142:ARG:HH22	1.52	0.50
20:l:49:ALA:HA	20:l:59:VAL:HG13	1.93	0.50
2:J:52:GLY:O	2:J:55:VAL:HG12	2.12	0.50
2:J:68:GLY:O	2:J:69:TYR:C	2.54	0.50
4:L:515:LYS:HD2	22:n:74:ASN:HB3	1.94	0.50
5:M:19:SER:HB2	14:f:8:ARG:CD	2.42	0.50
5:M:122:PHE:CE1	5:M:238:LEU:HG	2.46	0.50
5:M:328:CYS:SG	5:M:436:LEU:HD21	2.51	0.50
5:M:370:PRO:CA	5:M:375:LEU:HD22	2.40	0.50
20:l:34:LYS:HG3	20:l:35:ASP:OD1	2.12	0.50
21:m:124:LYS:HE2	21:m:125:PHE:CE2	2.47	0.50
4:L:149:ILE:HG21	5:M:364:LEU:CD2	2.42	0.50
4:L:306:THR:HA	4:L:336:LYS:NZ	2.27	0.50
4:L:336:LYS:O	4:L:340:PHE:CD2	2.65	0.50
4:L:354:GLN:O	4:L:354:GLN:HG2	2.12	0.50
4:L:514:ASN:HA	22:n:36:LYS:HZ1	1.77	0.50
5:M:432:ARG:HA	5:M:435:THR:HG22	1.94	0.50
8:U:86:VAL:HG13	19:k:54:ASN:ND2	2.27	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:90:TYR:HD2	8:U:93:ILE:H	1.60	0.50
10:Y:12:HIS:NE2	10:Y:127:PHE:HZ	2.09	0.50
4:L:302:ILE:CB	4:L:340:PHE:CE1	2.95	0.50
4:L:560:LYS:HZ2	26:L:706:CDL:H321	1.75	0.50
7:O:136:TYR:OH	7:O:191:LYS:HA	2.11	0.50
8:U:142:GLN:O	8:U:145:VAL:N	2.43	0.50
21:m:35:GLU:O	21:m:38:SER:N	2.43	0.50
4:L:123:LEU:CD2	4:L:150:MET:HG3	2.43	0.49
4:L:141:PHE:CD2	5:M:370:PRO:CB	2.94	0.49
5:M:388:TRP:NE1	21:m:109:ARG:CD	2.74	0.49
5:M:441:MET:HG3	5:M:445:ILE:HD12	1.94	0.49
6:N:336:THR:CG2	12:d:37:LEU:HD11	2.42	0.49
7:O:60:ILE:O	7:O:158:VAL:HA	2.12	0.49
7:O:237:ILE:CG2	7:O:241:TYR:CE2	2.95	0.49
7:O:276:LEU:HD11	7:O:278:TYR:CE2	2.47	0.49
7:O:319:ILE:HD12	7:O:324:GLY:HA3	1.94	0.49
4:L:203:PHE:CE1	24:p:114:GLN:HG3	2.47	0.49
7:O:170:LEU:HD21	7:O:184:VAL:HG22	1.95	0.49
15:g:139:TYR:CG	24:p:142:ARG:NH2	2.80	0.49
17:i:95:TYR:HE2	24:p:10:TYR:HB3	1.77	0.49
20:l:159:LYS:HA	23:o:98:ARG:HE	1.76	0.49
3:K:38:LEU:HG	3:K:42:ILE:HD11	1.94	0.49
4:L:434:LYS:NZ	19:k:66:ASN:HA	2.27	0.49
4:L:445:GLU:CB	4:L:450:LEU:HD23	2.37	0.49
26:L:706:CDL:H362	10:Y:118:VAL:HG21	1.95	0.49
5:M:88:ASN:O	5:M:89:ASN:HB3	2.12	0.49
5:M:184:HIS:CD2	5:M:249:ILE:HG23	2.47	0.49
5:M:207:MET:SD	5:M:240:SER:HA	2.52	0.49
6:N:317:GLN:HE21	7:O:141:LEU:HD13	1.76	0.49
17:i:95:TYR:CE2	24:p:10:TYR:HB3	2.47	0.49
21:m:124:LYS:C	21:m:126:ASN:N	2.70	0.49
4:L:217:LEU:HD13	4:L:273:ILE:HG23	1.94	0.49
4:L:296:ASN:HB3	4:L:357:ARG:HH11	1.77	0.49
4:L:393:ASP:OD1	4:L:393:ASP:C	2.56	0.49
4:L:399:ILE:HG22	4:L:409:LEU:HD13	1.93	0.49
5:M:311:GLY:HA2	5:M:314:MET:CE	2.40	0.49
7:O:114:LEU:CD2	27:O:402:ADP:H1'	2.43	0.49
17:i:90:MET:O	17:i:91:ALA:C	2.53	0.49
20:l:81:ARG:HD3	20:l:85:GLU:OE2	2.13	0.49
2:J:127:GLU:CD	13:e:32:ARG:HG2	2.36	0.49
2:J:131:VAL:HG23	2:J:131:VAL:O	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:316:THR:CG2	4:L:325:ALA:CB	2.89	0.49
4:L:390:TYR:HE2	18:j:68:TRP:CH2	2.31	0.49
5:M:391:PHE:HE2	25:M:503:3PE:H232	1.77	0.49
5:M:420:THR:HG21	5:M:423:MET:HG2	1.93	0.49
6:N:164:MET:HE3	25:Y:201:3PE:H271	1.85	0.49
6:N:243:MET:CG	12:d:44:MET:HE2	2.40	0.49
18:j:92:TRP:O	23:o:107:ARG:NH2	2.46	0.49
20:l:167:TYR:OH	20:l:176:LYS:O	2.14	0.49
2:J:16:CYS:SG	3:K:11:ALA:HB1	2.53	0.49
2:J:66:VAL:O	2:J:69:TYR:HB3	2.12	0.49
4:L:67:HIS:HE2	4:L:69:VAL:C	2.21	0.49
5:M:5:ILE:HG13	5:M:6:LEU:N	2.28	0.49
7:O:146:ALA:HB2	7:O:159:LEU:HD21	1.95	0.49
11:c:68:GLU:HG3	12:d:19:ARG:HH21	1.76	0.49
15:g:53:TRP:CD1	15:g:53:TRP:H	2.30	0.49
2:J:54:MET:HE1	2:J:58:ILE:HG13	1.94	0.49
25:J:201:3PE:H242	25:J:201:3PE:H3A2	1.93	0.49
5:M:285:LEU:HD22	5:M:410:MET:SD	2.53	0.49
6:N:149:LEU:HD11	6:N:195:PRO:HG3	1.95	0.49
6:N:230:ILE:HG21	6:N:296:LEU:HD11	1.94	0.49
6:N:240:MET:HE2	6:N:326:PHE:CE2	2.47	0.49
7:O:260:SER:O	7:O:263:ALA:HB3	2.13	0.49
7:O:351:TRP:HB3	11:c:39:PRO:HG3	1.95	0.49
8:U:88:LYS:CG	8:U:98:LEU:HD11	2.43	0.49
11:c:62:HIS:O	11:c:66:VAL:HG23	2.12	0.49
14:f:25:TYR:OH	14:f:29:LYS:HE3	2.13	0.49
22:n:20:TYR:OH	22:n:45:ARG:HB2	2.11	0.49
4:L:227:PHE:CD2	4:L:283:LEU:HD23	2.48	0.49
4:L:566:THR:HG21	25:L:707:3PE:H381	1.95	0.49
5:M:139:GLN:HG3	5:M:140:THR:N	2.27	0.49
5:M:248:ILE:CG1	5:M:249:ILE:HD12	2.39	0.49
5:M:348:LEU:HD12	5:M:415:GLN:HE22	1.78	0.49
6:N:231:SER:HA	6:N:300:THR:HA	1.93	0.49
8:U:94:ASP:OD1	8:U:95:PRO:HD2	2.12	0.49
13:e:36:PHE:O	13:e:39:GLU:N	2.45	0.49
13:e:102:GLU:CG	13:e:104:PRO:HD3	2.41	0.49
17:i:92:THR:O	24:p:5:TRP:HD1	1.95	0.49
21:m:75:ASN:OD1	21:m:79:ASN:ND2	2.46	0.49
4:L:68:TRP:CE3	4:L:76:LEU:HD21	2.47	0.49
4:L:403:ASN:OD1	20:l:153:TYR:HB3	2.11	0.49
4:L:496:LEU:HA	4:L:499:LEU:HB2	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:1:MET:HB2	5:M:52:PHE:CE2	2.47	0.49
5:M:123:GLU:CD	6:N:255:PRO:HG2	2.37	0.49
7:O:306:ASN:O	7:O:309:THR:HG22	2.13	0.49
17:i:69:LEU:HG	17:i:71:ALA:HB3	1.94	0.49
1:D:55:SER:HB3	4:L:575:THR:HG21	1.95	0.49
5:M:134:THR:O	5:M:142:ARG:CD	2.59	0.49
5:M:158:ILE:CG1	6:N:287:LEU:HD11	2.43	0.49
5:M:348:LEU:HB2	5:M:415:GLN:OE1	2.13	0.49
6:N:124:LEU:CD2	6:N:176:ARG:CG	2.91	0.49
6:N:220:MET:O	6:N:223:ASN:N	2.45	0.49
17:i:103:ARG:NE	23:o:49:ALA:O	2.45	0.49
20:l:153:TYR:CD2	23:o:19:PRO:HB3	2.48	0.49
22:n:114:MET:HG3	22:n:115:TYR:HD2	1.78	0.49
1:D:36:GLN:HG3	1:D:38:GLN:HE21	1.78	0.48
4:L:390:TYR:HE2	18:j:68:TRP:HH2	1.61	0.48
5:M:193:ASN:HA	5:M:253:LEU:HD23	1.94	0.48
5:M:227:GLY:HA2	5:M:230:ILE:HG22	1.95	0.48
6:N:200:LEU:HD23	6:N:265:ILE:HG23	1.95	0.48
6:N:317:GLN:HG2	7:O:301:LYS:HB3	1.95	0.48
6:N:321:LYS:HB2	12:d:49:ARG:HD3	1.94	0.48
9:X:158:LEU:HD13	12:d:17:GLU:CG	2.43	0.48
10:Y:60:ARG:CZ	10:Y:60:ARG:HB2	2.41	0.48
10:Y:143:VAL:HG23	16:h:157:ARG:O	2.13	0.48
17:i:7:ASP:OD1	17:i:8:GLU:N	2.46	0.48
2:J:121:GLY:O	2:J:122:ASP:C	2.52	0.48
4:L:390:TYR:CE2	18:j:68:TRP:CH2	3.01	0.48
4:L:521:SER:O	4:L:524:THR:N	2.46	0.48
5:M:4:ILE:HG22	5:M:107:ILE:CD1	2.32	0.48
5:M:190:TRP:CE2	10:Y:89:PRO:HG2	2.48	0.48
5:M:216:LEU:HD12	5:M:236:LEU:CD2	2.39	0.48
5:M:309:PHE:HB2	5:M:458:THR:HG21	1.95	0.48
5:M:351:VAL:HA	16:h:59:PRO:HB3	1.96	0.48
8:U:133:ILE:HD13	22:n:7:PRO:HD3	1.95	0.48
15:g:109:ASP:HB2	15:g:114:GLU:HB3	1.94	0.48
2:J:22:LYS:CD	3:K:23:ARG:HG2	2.39	0.48
4:L:144:TRP:HH2	4:L:256:GLY:HA2	1.78	0.48
4:L:350:LEU:HD23	4:L:443:ILE:HD11	1.96	0.48
4:L:357:ARG:HD3	22:n:80:TYR:HB2	1.95	0.48
4:L:402:CYS:SG	4:L:403:ASN:N	2.87	0.48
5:M:16:TRP:HE3	25:O:401:3PE:H12	1.78	0.48
5:M:59:ASP:OD1	5:M:245:ARG:NH2	2.47	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:313:THR:HA	5:M:316:MET:CE	2.43	0.48
6:N:321:LYS:HB2	12:d:49:ARG:CD	2.43	0.48
1:D:42:GLU:HA	1:D:45:GLU:HG2	1.96	0.48
4:L:41:LYS:HG3	4:L:98:TRP:CH2	2.45	0.48
4:L:101:MET:HE1	4:L:121:LEU:CB	2.43	0.48
4:L:152:PHE:HE1	5:M:412:ILE:HD11	1.79	0.48
4:L:316:THR:HG21	4:L:325:ALA:HA	1.95	0.48
4:L:361:ASN:O	4:L:361:ASN:CG	2.54	0.48
4:L:424:MET:HE2	4:L:502:LEU:CA	2.43	0.48
6:N:31:VAL:HB	6:N:35:PHE:CE2	2.48	0.48
6:N:243:MET:HE2	6:N:330:ALA:HB1	1.95	0.48
16:h:73:PHE:O	16:h:77:LEU:N	2.46	0.48
17:i:14:GLN:CB	22:n:164:PRO:HG3	2.35	0.48
17:i:69:LEU:O	17:i:72:VAL:HG22	2.12	0.48
22:n:51:HIS:HB3	22:n:63:LEU:HD13	1.95	0.48
23:o:4:HIS:ND1	23:o:102:PHE:HE2	2.11	0.48
4:L:372:CYS:SG	4:L:454:ILE:HG22	2.54	0.48
6:N:4:ILE:HG23	6:N:5:THR:N	2.29	0.48
6:N:172:GLN:OE1	6:N:177:LYS:CD	2.59	0.48
9:X:170:TRP:CZ3	26:X:201:CDL:H521	2.48	0.48
14:f:4:PHE:O	14:f:5:GLN:C	2.57	0.48
14:f:5:GLN:HB2	14:f:10:HIS:CD2	2.33	0.48
15:g:106:TYR:HE2	16:h:86:ILE:HD12	1.78	0.48
15:g:117:ARG:NH2	24:p:10:TYR:OH	2.45	0.48
2:J:28:GLY:O	2:J:31:GLY:N	2.46	0.48
4:L:141:PHE:HD1	4:L:182:PHE:CD2	2.31	0.48
4:L:433:THR:HG21	4:L:436:ARG:NH2	2.29	0.48
5:M:154:LEU:HD13	6:N:287:LEU:HD22	1.95	0.48
5:M:166:LEU:HD21	5:M:170:HIS:CE1	2.48	0.48
5:M:307:TRP:CE3	5:M:383:MET:CE	2.97	0.48
12:d:109:TYR:HE2	24:p:85:ILE:HD12	1.79	0.48
13:e:47:ILE:HG13	13:e:47:ILE:O	2.12	0.48
16:h:73:PHE:HE2	16:h:74:TYR:HE1	1.62	0.48
17:i:69:LEU:HD23	17:i:72:VAL:HG13	1.95	0.48
19:k:69:PHE:CE1	19:k:73:ILE:HD11	2.48	0.48
20:l:167:TYR:HD2	20:l:168:LEU:CD1	2.19	0.48
3:K:6:PHE:CZ	3:K:10:MET:HE3	2.49	0.48
4:L:496:LEU:HD12	4:L:497:GLY:CA	2.44	0.48
6:N:281:LEU:HD23	25:N:401:3PE:C29	2.44	0.48
7:O:314:LEU:HD12	7:O:315:PRO:HD3	1.93	0.48
17:i:103:ARG:HD2	23:o:50:GLN:HB2	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:274:LEU:O	4:L:277:MET:HG2	2.14	0.48
5:M:42:LEU:HG	5:M:67:ILE:CD1	2.42	0.48
6:N:227:ILE:CA	6:N:230:ILE:HG22	2.38	0.48
7:O:114:LEU:HD21	27:O:402:ADP:H1'	1.94	0.48
9:X:153:VAL:O	9:X:155:GLU:HG3	2.14	0.48
26:X:201:CDL:HB32	12:d:29:PRO:HB2	1.95	0.48
17:i:102:PRO:HG3	24:p:16:ARG:O	2.14	0.48
20:l:162:PRO:HG3	23:o:39:MET:HE3	1.94	0.48
2:J:20:ALA:C	2:J:22:LYS:H	2.21	0.48
4:L:57:ASN:OD1	4:L:59:MET:HG3	2.14	0.48
4:L:319:MET:O	4:L:319:MET:HG2	2.13	0.48
5:M:269:MET:HE3	5:M:399:ASN:HB3	1.96	0.48
5:M:422:HIS:CE1	5:M:425:ASN:OD1	2.66	0.48
7:O:63:ASP:OD1	7:O:64:GLY:N	2.43	0.48
11:c:72:ARG:HD2	12:d:20:SER:HA	1.96	0.48
12:d:119:VAL:O	12:d:120:ARG:C	2.55	0.48
15:g:58:GLU:HB2	20:l:30:PHE:HE1	1.79	0.48
3:K:73:VAL:HG21	6:N:38:LEU:CD2	2.44	0.48
5:M:176:LEU:HD13	5:M:245:ARG:HH11	1.79	0.48
8:U:90:TYR:CD1	19:k:51:TRP:CE2	3.02	0.48
8:U:128:PHE:HZ	8:U:148:ILE:HD12	1.76	0.48
10:Y:83:ARG:HH11	10:Y:91:ASN:HD21	1.61	0.48
12:d:8:HIS:O	12:d:10:PRO:HD3	2.14	0.48
19:k:84:PHE:CZ	19:k:88:LEU:HD22	2.49	0.48
20:l:111:MET:HE3	20:l:112:TYR:CZ	2.49	0.48
21:m:25:VAL:HB	21:m:29:THR:HB	1.96	0.48
3:K:29:THR:O	3:K:32:CYS:N	2.47	0.47
3:K:66:PHE:HE1	6:N:35:PHE:CE1	2.31	0.47
4:L:3:ILE:HG22	4:L:49:LEU:HD21	1.96	0.47
4:L:588:PHE:CZ	6:N:61:VAL:HG12	2.48	0.47
5:M:7:PRO:HG3	14:f:20:PHE:HA	1.94	0.47
5:M:127:ILE:CD1	6:N:256:PRO:HG2	2.43	0.47
5:M:336:ARG:HH21	5:M:429:SER:HA	1.78	0.47
7:O:60:ILE:CG1	7:O:83:MET:HE1	2.43	0.47
20:l:89:TRP:CZ2	22:n:86:PRO:HD3	2.49	0.47
21:m:125:PHE:CD1	24:p:132:PHE:CE2	3.03	0.47
4:L:542:LEU:HD21	20:l:116:ARG:HD3	1.96	0.47
5:M:192:ASN:C	5:M:194:LEU:N	2.72	0.47
9:X:168:PHE:O	9:X:169:PHE:CG	2.67	0.47
17:i:90:MET:SD	17:i:97:ILE:HD11	2.54	0.47
21:m:124:LYS:C	21:m:126:ASN:H	2.21	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:3:ASN:HD22	2:J:120:LEU:CG	2.27	0.47
4:L:31:ASN:HD22	4:L:34:LEU:HB2	1.79	0.47
26:L:706:CDL:H551	26:L:706:CDL:H582	1.66	0.47
5:M:94:LEU:O	5:M:98:MET:HG2	2.14	0.47
5:M:309:PHE:O	5:M:313:THR:HG23	2.14	0.47
6:N:173:THR:O	6:N:227:ILE:HG23	2.14	0.47
26:X:201:CDL:H522	26:X:201:CDL:HB62	1.96	0.47
20:l:48:ARG:HH22	20:l:64:PRO:HD2	1.80	0.47
1:D:43:TRP:CZ2	5:M:143:LEU:CD1	2.97	0.47
1:D:55:SER:HB3	4:L:575:THR:CG2	2.44	0.47
2:J:95:GLY:HA2	2:J:98:MET:HB2	1.95	0.47
4:L:54:PHE:CZ	4:L:84:PHE:HB2	2.49	0.47
4:L:296:ASN:ND2	4:L:357:ARG:HE	2.12	0.47
4:L:362:ILE:HG12	4:L:430:VAL:O	2.13	0.47
4:L:433:THR:CG2	4:L:434:LYS:N	2.78	0.47
26:L:705:CDL:H152	5:M:358:TRP:CH2	2.49	0.47
5:M:458:THR:HG21	24:p:148:ALA:HB1	1.93	0.47
7:O:70:LYS:HG3	7:O:71:ASN:N	2.30	0.47
12:d:73:TYR:O	12:d:77:LYS:HB2	2.14	0.47
13:e:42:GLU:CD	16:h:176:LYS:HE2	2.39	0.47
14:f:37:PHE:O	14:f:38:ARG:C	2.57	0.47
17:i:95:TYR:CE1	24:p:112:ALA:CB	2.97	0.47
17:i:102:PRO:HG3	24:p:17:THR:HA	1.96	0.47
22:n:44:MET:HE2	22:n:44:MET:HB2	1.74	0.47
22:n:156:PRO:HD2	22:n:158:ARG:NH1	2.29	0.47
1:D:43:TRP:CZ2	5:M:143:LEU:HD12	2.50	0.47
4:L:63:ILE:HG23	17:i:97:ILE:CD1	2.45	0.47
4:L:277:MET:SD	4:L:318:GLY:HA2	2.54	0.47
5:M:78:MET:HG2	5:M:432:ARG:HG3	1.97	0.47
5:M:177:MET:HE1	24:p:86:TYR:CE1	2.49	0.47
5:M:370:PRO:CA	5:M:375:LEU:HD23	2.42	0.47
6:N:1:MET:HE1	6:N:43:MET:SD	2.54	0.47
6:N:89:GLN:H	6:N:89:GLN:CD	2.22	0.47
7:O:343:TYR:CE1	7:O:355:LYS:CB	2.96	0.47
17:i:79:MET:O	17:i:80:TRP:C	2.57	0.47
3:K:69:CYS:O	3:K:70:GLU:C	2.57	0.47
5:M:430:HIS:HB3	15:g:73:GLY:HA3	1.97	0.47
6:N:1:MET:O	6:N:2:ASN:C	2.54	0.47
6:N:26:LEU:O	6:N:29:MET:N	2.47	0.47
7:O:99:GLY:O	11:c:30:TYR:HA	2.14	0.47
8:U:90:TYR:CE2	8:U:110:LEU:HD21	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:e:41:ILE:CD1	16:h:174:PRO:HD2	2.45	0.47
17:i:108:ASP:OD2	24:p:18:PRO:CB	2.62	0.47
20:l:42:PRO:HB2	20:l:48:ARG:HG2	1.97	0.47
1:D:58:THR:HG23	1:D:61:TRP:CZ3	2.49	0.47
3:K:57:MET:C	3:K:60:PRO:HD2	2.39	0.47
4:L:102:GLN:NE2	4:L:449:ASP:HA	2.27	0.47
4:L:264:HIS:HA	4:L:267:THR:OG1	2.14	0.47
4:L:439:PRO:HA	19:k:57:TRP:CZ2	2.49	0.47
4:L:552:LEU:HD22	4:L:553:LEU:HD12	1.97	0.47
4:L:576:LEU:HA	4:L:579:ASN:ND2	2.29	0.47
5:M:51:ASN:O	16:h:135:LYS:HD2	2.13	0.47
5:M:57:SER:OG	5:M:113:THR:HG22	2.15	0.47
5:M:122:PHE:HZ	5:M:206:LYS:HD3	1.75	0.47
5:M:196:TRP:HD1	5:M:250:LEU:HB2	1.80	0.47
5:M:231:LEU:CD1	5:M:235:LEU:HD12	2.42	0.47
5:M:263:LEU:HD21	21:m:105:PHE:HD2	1.80	0.47
6:N:89:GLN:HG2	13:e:60:PHE:CD2	2.50	0.47
7:O:62:VAL:CG1	7:O:207:ILE:HG12	2.44	0.47
7:O:116:LYS:HA	7:O:119:ASP:OD1	2.14	0.47
7:O:135:LEU:HB3	7:O:139:ARG:NH1	2.26	0.47
8:U:128:PHE:CE2	8:U:151:LYS:HG2	2.50	0.47
10:Y:64:THR:O	10:Y:68:ILE:HG13	2.15	0.47
10:Y:142:LYS:O	10:Y:143:VAL:C	2.57	0.47
11:c:46:LEU:O	11:c:50:ALA:CB	2.63	0.47
12:d:51:ARG:O	12:d:52:PRO:C	2.55	0.47
13:e:28:LYS:HB3	16:h:184:LYS:HA	1.96	0.47
14:f:38:ARG:HD3	14:f:56:TRP:NE1	2.30	0.47
17:i:26:GLN:CD	22:n:118:TYR:HH	2.16	0.47
20:l:48:ARG:NH2	20:l:64:PRO:HD2	2.30	0.47
2:J:6:PHE:HB2	2:J:120:LEU:HD11	1.96	0.47
3:K:29:THR:O	3:K:30:LEU:C	2.56	0.47
3:K:75:LEU:O	3:K:79:VAL:HG23	2.15	0.47
4:L:121:LEU:HD22	4:L:246:LEU:CD2	2.24	0.47
4:L:296:ASN:HD22	4:L:357:ARG:NH1	2.13	0.47
4:L:420:ALA:HB1	4:L:498:PHE:CD2	2.50	0.47
5:M:305:THR:O	5:M:306:PRO:C	2.58	0.47
6:N:146:TYR:CD1	6:N:147:PRO:HD3	2.49	0.47
7:O:48:LYS:HE2	7:O:289:TRP:CH2	2.50	0.47
7:O:341:PRO:HB2	11:c:34:PRO:HB3	1.96	0.47
18:j:44:TYR:HD2	19:k:23:PRO:HD2	1.80	0.47
20:l:44:THR:CG2	20:l:47:GLU:HG3	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:n:50:GLU:O	22:n:51:HIS:C	2.55	0.47
24:p:29:PRO:O	24:p:33:LEU:HD13	2.14	0.47
4:L:183:ILE:HD13	5:M:400:ILE:HD13	1.96	0.47
4:L:237:MET:HE1	4:L:248:HIS:HB2	1.97	0.47
6:N:307:THR:HG22	6:N:308:ASN:N	2.29	0.47
10:Y:116:GLY:O	10:Y:120:MET:HB2	2.15	0.47
24:p:93:ARG:NH2	24:p:150:TYR:CE1	2.83	0.47
2:J:157:TRP:HE1	6:N:11:PHE:HD2	1.62	0.47
4:L:474:PRO:HD2	23:o:67:LEU:HD21	1.96	0.47
7:O:129:TYR:CE2	7:O:183:CYS:HB3	2.50	0.47
15:g:151:ASP:C	24:p:171:ARG:HH22	2.23	0.47
16:h:55:PHE:HB2	17:i:28:LEU:HD21	1.95	0.47
20:l:127:ASP:O	20:l:128:VAL:C	2.58	0.47
22:n:57:MET:O	22:n:58:MET:C	2.58	0.47
24:p:43:TRP:O	24:p:44:PRO:C	2.58	0.47
2:J:75:THR:HG21	3:K:25:HIS:HB3	1.96	0.46
5:M:232:ALA:HA	5:M:236:LEU:HD12	1.98	0.46
6:N:3:PRO:HG2	7:O:289:TRP:CH2	2.51	0.46
6:N:101:ALA:O	6:N:104:MET:HB3	2.14	0.46
6:N:217:MET:HA	6:N:220:MET:HG2	1.97	0.46
14:f:38:ARG:O	14:f:56:TRP:NE1	2.48	0.46
18:j:51:THR:O	18:j:52:ARG:C	2.53	0.46
21:m:14:LEU:HD12	21:m:15:PRO:HD2	1.96	0.46
3:K:13:SER:O	3:K:17:LEU:HG	2.15	0.46
4:L:86:SER:OG	4:L:133:SER:HB3	2.15	0.46
4:L:172:ILE:O	4:L:176:ARG:HG2	2.16	0.46
4:L:305:SER:C	4:L:336:LYS:HZ3	2.24	0.46
6:N:159:ILE:HB	6:N:278:MET:HE1	1.98	0.46
12:d:59:HIS:CE1	12:d:60:ARG:HG3	2.50	0.46
14:f:37:PHE:O	16:h:134:GLU:HB3	2.15	0.46
18:j:99:ILE:CD1	23:o:107:ARG:HB2	2.45	0.46
20:l:153:TYR:CZ	23:o:19:PRO:HD3	2.50	0.46
4:L:277:MET:CG	4:L:318:GLY:HA2	2.45	0.46
4:L:373:LEU:CD2	4:L:427:ILE:HG22	2.45	0.46
4:L:427:ILE:CD1	19:k:69:PHE:CE1	2.99	0.46
5:M:4:ILE:HD12	5:M:4:ILE:N	2.30	0.46
5:M:300:SER:HB2	5:M:308:SER:HB3	1.97	0.46
5:M:380:PHE:HD1	5:M:380:PHE:N	2.13	0.46
25:M:501:3PE:O22	26:h:201:CDL:H122	2.15	0.46
6:N:250:SER:HB2	6:N:334:THR:HG22	1.98	0.46
6:N:336:THR:HG23	12:d:37:LEU:HD11	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:130:ILE:HG21	8:U:138:LEU:HD11	1.97	0.46
9:X:167:PHE:HD2	9:X:170:TRP:HE1	1.62	0.46
12:d:78:ARG:O	12:d:81:TYR:N	2.49	0.46
14:f:16:VAL:O	14:f:17:PRO:C	2.57	0.46
18:j:40:ILE:HG13	18:j:41:GLN:H	1.80	0.46
22:n:35:ASP:OD1	22:n:36:LYS:N	2.47	0.46
23:o:31:PHE:CG	23:o:34:ARG:HD2	2.51	0.46
3:K:57:MET:N	3:K:58:PRO:CD	2.78	0.46
3:K:61:ILE:O	3:K:62:THR:C	2.58	0.46
4:L:21:ILE:HG12	4:L:27:ILE:CG2	2.45	0.46
4:L:74:MET:HE3	5:M:307:TRP:HH2	1.80	0.46
5:M:213:HIS:O	5:M:217:PRO:CD	2.63	0.46
5:M:380:PHE:N	5:M:380:PHE:CD1	2.82	0.46
25:M:503:3PE:H2G2	21:m:97:PRO:CG	2.41	0.46
6:N:120:GLN:HG3	6:N:177:LYS:CG	2.45	0.46
6:N:175:MET:HE1	6:N:227:ILE:HG22	1.97	0.46
7:O:204:VAL:HG22	7:O:255:VAL:HG22	1.97	0.46
7:O:232:ALA:O	7:O:235:GLN:HB3	2.14	0.46
8:U:114:ASP:O	8:U:117:GLU:N	2.48	0.46
4:L:225:ALA:CB	4:L:233:LEU:HD12	2.45	0.46
5:M:348:LEU:O	5:M:351:VAL:N	2.38	0.46
21:m:17:THR:HB	22:n:68:GLU:OE1	2.15	0.46
22:n:133:TRP:O	22:n:137:VAL:HG22	2.15	0.46
2:J:164:PHE:HB3	6:N:5:THR:HG23	1.97	0.46
5:M:10:MET:C	5:M:13:PRO:HD2	2.41	0.46
5:M:139:GLN:HG3	5:M:141:GLU:H	1.80	0.46
7:O:50:THR:OG1	7:O:288:ASP:HB3	2.16	0.46
18:j:71:TRP:HA	19:k:84:PHE:CE1	2.50	0.46
22:n:136:GLU:O	22:n:139:GLN:N	2.49	0.46
24:p:50:GLU:CG	24:p:54:ARG:HH21	2.28	0.46
4:L:52:LEU:CB	24:p:30:ILE:HD11	2.46	0.46
4:L:407:TRP:HE1	20:l:140:MET:HE1	1.81	0.46
4:L:434:LYS:HZ2	19:k:66:ASN:HA	1.80	0.46
4:L:581:LYS:HB2	4:L:586:LEU:HD22	1.97	0.46
5:M:116:ILE:HD12	5:M:119:TYR:HB3	1.97	0.46
5:M:303:ILE:HG22	5:M:305:THR:HG23	1.98	0.46
6:N:321:LYS:HG3	6:N:321:LYS:O	2.15	0.46
7:O:246:LEU:O	7:O:247:PRO:C	2.57	0.46
7:O:343:TYR:HB3	12:d:52:PRO:HD3	1.98	0.46
11:c:67:LEU:O	11:c:68:GLU:C	2.59	0.46
16:h:69:ARG:O	16:h:73:PHE:CB	2.63	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:m:9:ALA:O	21:m:10:PRO:C	2.56	0.46
4:L:31:ASN:ND2	4:L:34:LEU:HB2	2.31	0.46
4:L:529:PHE:CZ	4:L:533:ILE:HG21	2.50	0.46
4:L:560:LYS:HZ3	26:L:706:CDL:C32	2.28	0.46
26:L:706:CDL:H732	26:L:706:CDL:OB8	2.16	0.46
5:M:15:THR:HG21	5:M:100:ILE:CD1	2.46	0.46
5:M:173:THR:HG22	16:h:150:ARG:NH1	2.31	0.46
5:M:319:HIS:CA	5:M:322:THR:HG22	2.41	0.46
5:M:435:THR:O	5:M:436:LEU:C	2.59	0.46
5:M:453:LEU:CD1	5:M:454:ILE:CG2	2.84	0.46
6:N:37:LEU:HD21	6:N:60:PHE:CD1	2.51	0.46
6:N:104:MET:CE	6:N:111:PHE:CE1	2.99	0.46
6:N:197:ASN:ND2	6:N:200:LEU:HD13	2.30	0.46
6:N:277:ILE:HG22	6:N:278:MET:H	1.79	0.46
6:N:319:LYS:HA	7:O:302:THR:HG21	1.98	0.46
10:Y:74:LEU:HD23	10:Y:74:LEU:C	2.41	0.46
23:o:71:ARG:HB3	23:o:71:ARG:NH1	2.27	0.46
23:o:93:LEU:O	23:o:96:VAL:CG1	2.64	0.46
2:J:29:GLY:O	2:J:30:LEU:C	2.58	0.46
2:J:103:ILE:HG22	2:J:107:ASN:HD21	1.81	0.46
4:L:12:PHE:O	4:L:16:LEU:HG	2.15	0.46
4:L:101:MET:HE1	4:L:121:LEU:HB2	1.98	0.46
5:M:6:LEU:HD21	14:f:22:PHE:HD2	1.81	0.46
5:M:186:LEU:HD22	5:M:250:LEU:HA	1.97	0.46
6:N:243:MET:CE	6:N:330:ALA:HB1	2.46	0.46
6:N:276:LEU:HD13	25:N:401:3PE:C2	2.38	0.46
11:c:38:LYS:HA	11:c:39:PRO:HD3	1.58	0.46
15:g:77:ASP:HA	15:g:78:PRO:HD3	1.70	0.46
16:h:82:VAL:O	16:h:85:GLY:N	2.49	0.46
3:K:26:LEU:O	3:K:29:THR:N	2.48	0.46
4:L:324:LEU:HA	4:L:327:LEU:HD12	1.97	0.46
4:L:339:LEU:HD11	4:L:376:GLY:HA3	1.98	0.46
4:L:475:THR:O	4:L:476:SER:HB2	2.16	0.46
4:L:590:SER:HB2	10:Y:45:LEU:HD11	1.98	0.46
6:N:119:THR:O	6:N:122:ILE:HG13	2.16	0.46
6:N:241:LEU:O	6:N:244:ILE:HG22	2.15	0.46
7:O:59:VAL:HA	7:O:157:VAL:HG22	1.97	0.46
7:O:71:ASN:C	7:O:75:LYS:HE3	2.40	0.46
7:O:344:ASN:OD1	7:O:346:GLU:HG2	2.15	0.46
8:U:118:ILE:O	8:U:122:MET:HG2	2.16	0.46
10:Y:19:GLN:HE21	10:Y:22:ARG:CG	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:d:13:PHE:O	12:d:78:ARG:NE	2.43	0.46
12:d:107:LYS:HB3	12:d:111:GLU:HB3	1.98	0.46
16:h:95:GLU:OE1	16:h:114:LYS:HD3	2.15	0.46
16:h:96:ALA:CB	24:p:63:TYR:HD1	2.25	0.46
18:j:92:TRP:O	18:j:93:THR:C	2.59	0.46
19:k:39:GLN:NE2	19:k:49:ASP:HB3	2.31	0.46
19:k:69:PHE:CZ	19:k:73:ILE:HG13	2.51	0.46
20:l:166:LEU:HD12	20:l:170:ARG:HH22	1.81	0.46
3:K:57:MET:O	3:K:58:PRO:C	2.58	0.45
4:L:161:ARG:HA	22:n:92:GLU:CB	2.45	0.45
4:L:277:MET:HG3	4:L:318:GLY:CA	2.46	0.45
4:L:550:LEU:O	4:L:554:ASP:HB3	2.16	0.45
5:M:122:PHE:CZ	5:M:206:LYS:CD	2.95	0.45
5:M:158:ILE:CG2	6:N:283:ALA:HB1	2.45	0.45
5:M:282:LEU:HD11	5:M:410:MET:HE3	1.96	0.45
6:N:300:THR:CG2	6:N:301:SER:N	2.79	0.45
6:N:326:PHE:HE2	12:d:48:LEU:HD13	1.81	0.45
7:O:140:LEU:HD11	7:O:198:TYR:CE2	2.51	0.45
14:f:49:ARG:HG2	14:f:52:GLU:HG3	1.98	0.45
17:i:15:LEU:HD21	22:n:167:TRP:HB3	1.97	0.45
17:i:18:LEU:CD2	22:n:125:TRP:HH2	2.29	0.45
22:n:37:TYR:O	22:n:38:ARG:C	2.58	0.45
4:L:55:PHE:CB	23:o:74:PHE:HE1	2.29	0.45
4:L:142:ILE:HA	5:M:370:PRO:CB	2.45	0.45
4:L:204:SER:HA	4:L:207:ASN:ND2	2.31	0.45
4:L:357:ARG:NH2	22:n:29:SER:HA	2.31	0.45
26:L:705:CDL:H341	16:h:71:MET:SD	2.57	0.45
5:M:22:LYS:HG2	5:M:22:LYS:O	2.17	0.45
5:M:56:PHE:CE1	5:M:108:MET:HG2	2.47	0.45
5:M:61:LEU:C	5:M:64:PRO:HD2	2.42	0.45
5:M:207:MET:O	5:M:208:PRO:C	2.59	0.45
6:N:148:LEU:H	6:N:148:LEU:HD12	1.82	0.45
6:N:154:ILE:HB	6:N:191:LEU:HG	1.98	0.45
6:N:281:LEU:HD23	25:N:401:3PE:H292	1.98	0.45
7:O:63:ASP:O	7:O:161:ARG:HG2	2.16	0.45
14:f:12:VAL:HG23	14:f:13:HIS:N	2.31	0.45
19:k:47:LEU:HD13	22:n:42:CYS:O	2.16	0.45
22:n:44:MET:O	22:n:45:ARG:C	2.54	0.45
3:K:59:ILE:HD12	6:N:27:MET:HG2	1.98	0.45
4:L:135:ASN:O	4:L:198:LEU:HD13	2.16	0.45
4:L:210:LEU:HD23	4:L:210:LEU:C	2.41	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:19:SER:H	14:f:8:ARG:HD2	1.82	0.45
5:M:42:LEU:HD21	5:M:67:ILE:HD12	1.97	0.45
5:M:393:ILE:O	5:M:397:GLY:N	2.49	0.45
6:N:130:LEU:O	6:N:134:GLN:HB2	2.16	0.45
7:O:265:ASP:O	7:O:266:PRO:C	2.58	0.45
10:Y:75:THR:HB	10:Y:95:GLY:HA2	1.98	0.45
13:e:18:PHE:O	13:e:18:PHE:CD2	2.69	0.45
19:k:48:ARG:HG3	19:k:48:ARG:O	2.15	0.45
20:l:101:TRP:HE1	21:m:62:ASP:HA	1.80	0.45
22:n:45:ARG:O	22:n:49:GLU:N	2.37	0.45
23:o:63:LEU:O	23:o:64:ILE:C	2.59	0.45
23:o:73:SER:HA	24:p:24:THR:OG1	2.17	0.45
24:p:173:GLU:O	24:p:174:ALA:C	2.59	0.45
4:L:23:MET:O	26:L:705:CDL:HA61	2.16	0.45
6:N:26:LEU:HG	6:N:85:MET:SD	2.56	0.45
6:N:124:LEU:HD21	6:N:176:ARG:CG	2.46	0.45
6:N:215:MET:SD	6:N:244:ILE:HD11	2.56	0.45
7:O:112:CYS:HB3	7:O:131:LEU:HA	1.97	0.45
7:O:246:LEU:O	7:O:250:SER:N	2.48	0.45
7:O:342:GLY:O	7:O:355:LYS:NZ	2.50	0.45
10:Y:39:SER:HB2	10:Y:58:VAL:HA	1.98	0.45
13:e:19:MET:HE2	13:e:19:MET:HB3	1.85	0.45
17:i:5:THR:HG22	17:i:6:PRO:HD2	1.98	0.45
20:l:57:MET:HE2	20:l:57:MET:HB3	1.75	0.45
23:o:118:LYS:HD2	23:o:118:LYS:HA	1.85	0.45
24:p:24:THR:HG22	24:p:26:LEU:N	2.31	0.45
2:J:28:GLY:O	2:J:29:GLY:C	2.59	0.45
4:L:74:MET:HE3	4:L:74:MET:HB2	1.76	0.45
4:L:145:GLU:CG	5:M:370:PRO:HD3	2.47	0.45
4:L:195:SER:O	4:L:201:ILE:HD11	2.16	0.45
4:L:310:LEU:HA	4:L:313:MET:HB2	1.99	0.45
4:L:366:MET:SD	4:L:443:ILE:HG21	2.57	0.45
4:L:403:ASN:HA	20:l:152:SER:O	2.17	0.45
5:M:42:LEU:HD11	5:M:67:ILE:HD12	1.99	0.45
5:M:42:LEU:CG	5:M:67:ILE:HD11	2.43	0.45
5:M:208:PRO:CD	5:M:236:LEU:HD22	2.38	0.45
5:M:283:LYS:HG3	5:M:327:PHE:HE1	1.78	0.45
7:O:249:MET:HE3	7:O:253:CYS:SG	2.56	0.45
8:U:133:ILE:CD1	22:n:7:PRO:HD3	2.46	0.45
26:X:201:CDL:OA4	14:f:29:LYS:HD2	2.16	0.45
15:g:67:LYS:O	15:g:68:ASN:C	2.60	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:h:73:PHE:HD2	16:h:74:TYR:CE1	2.33	0.45
19:k:26:ARG:O	19:k:27:GLN:C	2.57	0.45
19:k:42:LEU:HG	22:n:39:TYR:HD1	1.82	0.45
23:o:13:ALA:C	23:o:15:VAL:N	2.74	0.45
24:p:107:GLN:O	24:p:111:LYS:HG3	2.15	0.45
3:K:85:TYR:OH	3:K:95:LEU:HD11	2.17	0.45
4:L:246:LEU:C	4:L:246:LEU:CD1	2.90	0.45
4:L:247:LEU:HD12	4:L:247:LEU:C	2.41	0.45
4:L:446:ASN:ND2	18:j:51:THR:HG21	2.32	0.45
4:L:446:ASN:HD21	18:j:51:THR:HG21	1.82	0.45
4:L:508:THR:HG22	22:n:33:HIS:CD2	2.51	0.45
4:L:589:MET:O	4:L:592:LEU:HB3	2.16	0.45
5:M:65:LEU:O	5:M:66:ILE:C	2.59	0.45
7:O:351:TRP:HB2	7:O:355:LYS:HE3	1.98	0.45
8:U:102:SER:O	8:U:141:PRO:HD3	2.16	0.45
17:i:7:ASP:HB2	22:n:156:PRO:HD3	1.99	0.45
23:o:93:LEU:O	23:o:96:VAL:HG12	2.16	0.45
4:L:47:SER:O	4:L:50:PRO:HD2	2.17	0.45
4:L:241:THR:N	4:L:242:PRO:HD2	2.31	0.45
4:L:560:LYS:NZ	26:L:706:CDL:C32	2.80	0.45
25:L:704:3PE:C3B	25:L:704:3PE:H271	2.47	0.45
5:M:25:THR:HG22	15:g:84:ASN:CG	2.42	0.45
6:N:293:TYR:O	6:N:297:ILE:HG12	2.16	0.45
7:O:60:ILE:CD1	7:O:203:ALA:HB3	2.45	0.45
11:c:65:ASP:O	11:c:66:VAL:C	2.56	0.45
17:i:95:TYR:HD1	24:p:112:ALA:HB2	1.77	0.45
18:j:59:GLU:HG2	19:k:75:LYS:HZ1	1.82	0.45
19:k:57:TRP:O	19:k:58:ARG:C	2.59	0.45
23:o:44:GLN:O	23:o:45:GLU:C	2.59	0.45
2:J:17:LEU:O	2:J:21:LEU:HG	2.16	0.45
4:L:387:THR:HA	4:L:465:GLY:HA3	1.98	0.45
4:L:532:ILE:HG23	4:L:533:ILE:N	2.31	0.45
4:L:591:PHE:N	4:L:591:PHE:CD1	2.83	0.45
4:L:591:PHE:N	4:L:591:PHE:HD1	2.15	0.45
25:L:701:3PE:H221	17:i:89:HIS:NE2	2.32	0.45
5:M:3:LYS:HA	5:M:7:PRO:HD2	1.99	0.45
5:M:42:LEU:CG	5:M:67:ILE:CD1	2.94	0.45
5:M:129:THR:CG2	5:M:235:LEU:CD1	2.95	0.45
5:M:272:THR:O	5:M:275:ILE:HG13	2.17	0.45
6:N:82:GLY:HA3	13:e:21:LEU:HG	1.98	0.45
6:N:176:ARG:CZ	6:N:225:MET:SD	3.05	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:103:HIS:CD2	8:U:140:CYS:SG	3.10	0.45
12:d:2:MET:HE3	12:d:2:MET:HB3	1.88	0.45
12:d:13:PHE:CE2	12:d:14:LEU:HD23	2.52	0.45
18:j:87:PRO:HG3	23:o:96:VAL:HG23	1.99	0.45
20:l:30:PHE:CE1	20:l:31:HIS:CE1	3.05	0.45
23:o:4:HIS:HD1	23:o:102:PHE:HE2	1.64	0.45
24:p:110:LEU:O	24:p:111:LYS:C	2.58	0.45
2:J:126:TYR:CD2	3:K:50:ASN:HB2	2.52	0.45
4:L:81:LYS:CA	4:L:135:ASN:HD21	2.29	0.45
4:L:100:ILE:O	4:L:104:SER:N	2.42	0.45
4:L:226:GLN:HG3	4:L:314:MET:HE2	1.98	0.45
4:L:231:PRO:CG	4:L:529:PHE:HD2	2.30	0.45
4:L:287:PHE:CZ	4:L:527:GLY:HA3	2.52	0.45
4:L:508:THR:HG22	22:n:33:HIS:HD2	1.82	0.45
4:L:578:THR:CG2	6:N:168:GLY:HA2	2.47	0.45
5:M:73:LEU:HB3	5:M:103:GLN:OE1	2.15	0.45
5:M:87:ASP:HB3	5:M:91:LEU:HB2	1.99	0.45
5:M:151:PHE:HZ	6:N:291:PHE:CA	2.30	0.45
5:M:209:LEU:HD11	5:M:261:PHE:HD1	1.81	0.45
8:U:110:LEU:CD2	8:U:118:ILE:HD11	2.46	0.45
12:d:3:ASN:C	12:d:5:ARG:H	2.25	0.45
26:h:201:CDL:H162	26:h:201:CDL:H191	1.75	0.45
21:m:40:ARG:NH1	22:n:152:GLU:OE1	2.49	0.45
24:p:49:ARG:O	24:p:50:GLU:C	2.57	0.45
4:L:149:ILE:CG2	5:M:364:LEU:HD21	2.47	0.45
5:M:249:ILE:O	5:M:250:LEU:CG	2.47	0.45
6:N:214:PRO:HB2	6:N:247:MET:SD	2.56	0.45
7:O:60:ILE:HB	7:O:83:MET:HE1	1.99	0.45
7:O:129:TYR:CD2	7:O:183:CYS:HB3	2.52	0.45
8:U:118:ILE:HA	19:k:51:TRP:CH2	2.52	0.45
13:e:70:TYR:O	13:e:71:LYS:C	2.60	0.45
15:g:64:VAL:HG11	15:g:71:PHE:CE1	2.52	0.45
5:M:187:ASP:H	5:M:192:ASN:ND2	2.15	0.44
6:N:109:ALA:HB3	6:N:110:PRO:HD3	1.99	0.44
7:O:39:GLY:O	7:O:40:LEU:C	2.60	0.44
7:O:230:THR:HG22	7:O:232:ALA:N	2.32	0.44
7:O:245:PHE:CE1	7:O:249:MET:HG3	2.52	0.44
7:O:336:GLY:HA2	7:O:344:ASN:HB3	1.99	0.44
10:Y:68:ILE:HD13	10:Y:103:LEU:HB2	1.98	0.44
12:d:11:LEU:HD12	12:d:11:LEU:HA	1.69	0.44
12:d:78:ARG:O	12:d:79:GLN:C	2.59	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:h:56:VAL:O	16:h:58:LYS:HG3	2.16	0.44
16:h:73:PHE:CE2	16:h:74:TYR:HE1	2.35	0.44
16:h:120:TRP:NE1	16:h:124:ASN:ND2	2.64	0.44
17:i:92:THR:O	24:p:5:TRP:CD1	2.69	0.44
2:J:54:MET:HE3	2:J:54:MET:HB3	1.70	0.44
4:L:117:PHE:CE1	4:L:243:VAL:CG2	3.00	0.44
4:L:155:ILE:HG12	4:L:248:HIS:CE1	2.53	0.44
4:L:231:PRO:C	4:L:234:PRO:HD2	2.41	0.44
4:L:437:PHE:CZ	4:L:441:ILE:HG12	2.43	0.44
25:L:707:3PE:H261	25:L:707:3PE:H322	1.98	0.44
5:M:43:TRP:HZ2	16:h:122:ALA:HB2	1.82	0.44
6:N:164:MET:HE3	25:Y:201:3PE:C26	2.44	0.44
6:N:239:ALA:CB	12:d:47:MET:HG2	2.48	0.44
7:O:70:LYS:HE3	27:O:402:ADP:O2A	2.17	0.44
7:O:350:LYS:HD3	7:O:351:TRP:N	2.32	0.44
8:U:137:LYS:O	17:i:4:TYR:CE2	2.70	0.44
12:d:108:THR:O	12:d:109:TYR:C	2.60	0.44
16:h:182:SER:HB3	16:h:183:PRO:CD	2.39	0.44
23:o:49:ALA:O	23:o:50:GLN:C	2.60	0.44
4:L:2:ASN:O	4:L:3:ILE:C	2.59	0.44
4:L:54:PHE:CB	4:L:87:ILE:HD11	2.47	0.44
4:L:366:MET:SD	4:L:443:ILE:CG2	3.06	0.44
4:L:526:LEU:CB	4:L:530:PRO:HG2	2.47	0.44
5:M:98:MET:SD	25:M:502:3PE:H3C1	2.57	0.44
5:M:321:LEU:HD23	5:M:321:LEU:HA	1.81	0.44
5:M:415:GLN:O	5:M:416:ARG:CG	2.64	0.44
6:N:208:TYR:O	6:N:212:THR:HG22	2.18	0.44
6:N:250:SER:O	6:N:259:GLY:HA3	2.17	0.44
7:O:342:GLY:HA3	11:c:36:ASN:OD1	2.18	0.44
7:O:351:TRP:O	7:O:355:LYS:HG2	2.16	0.44
8:U:106:LYS:HE2	8:U:106:LYS:HB3	1.79	0.44
10:Y:88:ASP:H	10:Y:128:LYS:HZ3	1.64	0.44
14:f:3:LEU:O	14:f:4:PHE:C	2.60	0.44
16:h:55:PHE:C	16:h:55:PHE:CD1	2.94	0.44
16:h:87:THR:HG22	26:h:201:CDL:C51	2.46	0.44
23:o:110:GLN:O	23:o:111:ARG:C	2.59	0.44
2:J:3:ASN:HD22	2:J:120:LEU:HD12	1.83	0.44
2:J:150:TRP:CZ3	25:J:201:3PE:H251	2.52	0.44
4:L:537:THR:N	4:L:538:PRO:HD2	2.32	0.44
5:M:154:LEU:HD22	6:N:287:LEU:HD21	2.00	0.44
5:M:177:MET:HB3	16:h:140:LEU:HD21	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:200:MET:HE2	5:M:250:LEU:HD21	2.00	0.44
25:M:502:3PE:H242	12:d:47:MET:HE1	1.99	0.44
6:N:193:ILE:HD13	6:N:200:LEU:HB2	1.99	0.44
7:O:211:VAL:N	7:O:212:PRO:CD	2.80	0.44
10:Y:120:MET:HE2	10:Y:120:MET:HB3	1.90	0.44
17:i:19:ARG:HH11	22:n:173:ARG:NH2	2.16	0.44
20:l:30:PHE:CD2	20:l:31:HIS:CE1	3.00	0.44
21:m:32:ALA:O	21:m:35:GLU:N	2.48	0.44
3:K:33:LEU:HA	3:K:36:MET:HE2	2.00	0.44
3:K:73:VAL:CG2	6:N:38:LEU:HD22	2.47	0.44
4:L:152:PHE:HD2	4:L:153:LEU:HD12	1.83	0.44
4:L:482:MET:HE2	4:L:486:LEU:CB	2.45	0.44
26:L:705:CDL:H531	26:L:705:CDL:H212	2.00	0.44
5:M:22:LYS:HG2	5:M:26:ASN:ND2	2.33	0.44
5:M:24:TRP:CE3	5:M:81:GLN:HG2	2.52	0.44
5:M:424:ILE:O	5:M:424:ILE:CG2	2.65	0.44
6:N:87:GLN:O	6:N:88:GLN:C	2.59	0.44
6:N:175:MET:HE1	6:N:296:LEU:HD13	1.98	0.44
6:N:309:ASN:N	7:O:317:ILE:O	2.48	0.44
7:O:200:PRO:HG3	7:O:282:PRO:CD	2.47	0.44
7:O:262:GLU:HB3	7:O:268:LYS:NZ	2.33	0.44
13:e:96:PRO:C	13:e:99:SER:H	2.25	0.44
23:o:13:ALA:C	23:o:15:VAL:H	2.25	0.44
2:J:104:CYS:O	2:J:108:TYR:N	2.46	0.44
4:L:526:LEU:HD12	4:L:526:LEU:N	2.32	0.44
4:L:529:PHE:HB3	4:L:530:PRO:HD3	1.99	0.44
5:M:18:SER:OG	5:M:26:ASN:ND2	2.51	0.44
5:M:42:LEU:CD1	5:M:67:ILE:CD1	2.96	0.44
5:M:123:GLU:CB	6:N:255:PRO:HG2	2.44	0.44
5:M:263:LEU:CD2	21:m:105:PHE:HD2	2.31	0.44
6:N:122:ILE:HD11	6:N:127:GLY:HA2	1.99	0.44
6:N:239:ALA:HA	12:d:47:MET:HE2	1.99	0.44
7:O:238:GLU:HG3	7:O:242:LYS:HD3	1.99	0.44
7:O:272:ASP:O	7:O:275:TYR:HB2	2.18	0.44
8:U:104:PHE:O	8:U:108:LEU:HB2	2.18	0.44
10:Y:7:PHE:CZ	10:Y:26:ILE:HG12	2.52	0.44
10:Y:141:PRO:HB2	16:h:161:ARG:NH1	2.33	0.44
25:Y:201:3PE:H31	25:Y:201:3PE:H112	1.98	0.44
12:d:27:ASN:O	12:d:28:ASP:C	2.61	0.44
12:d:93:TYR:CD2	16:h:156:VAL:HG13	2.53	0.44
13:e:91:LYS:NZ	13:e:91:LYS:HB3	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:h:179:ILE:HB	16:h:181:HIS:CE1	2.52	0.44
4:L:231:PRO:CG	4:L:529:PHE:CD2	3.00	0.44
4:L:231:PRO:HG2	4:L:529:PHE:CD2	2.52	0.44
5:M:29:SER:HB3	15:g:91:PHE:CE2	2.50	0.44
5:M:446:LEU:CD1	15:g:97:LEU:HD12	2.47	0.44
5:M:450:SER:HB3	25:M:501:3PE:H32	2.00	0.44
6:N:227:ILE:HG13	6:N:228:ASN:N	2.32	0.44
6:N:281:LEU:HD23	25:N:401:3PE:H281	1.84	0.44
10:Y:12:HIS:CD2	10:Y:131:LYS:HE2	2.53	0.44
11:c:33:GLU:CD	11:c:33:GLU:H	2.26	0.44
11:c:61:THR:HG22	11:c:65:ASP:OD2	2.18	0.44
12:d:57:GLY:O	12:d:60:ARG:N	2.51	0.44
24:p:140:GLN:HG2	24:p:144:LEU:CD1	2.47	0.44
4:L:529:PHE:O	4:L:533:ILE:HG22	2.17	0.44
25:L:703:3PE:H331	25:L:703:3PE:H362	1.64	0.44
5:M:8:SER:O	5:M:11:LEU:HB2	2.18	0.44
5:M:186:LEU:HD13	5:M:250:LEU:HA	2.00	0.44
5:M:264:LEU:HD23	21:m:98:LEU:CD1	2.47	0.44
5:M:344:MET:HE3	5:M:423:MET:CE	2.48	0.44
6:N:31:VAL:C	6:N:35:PHE:CD2	2.91	0.44
7:O:132:GLN:HE22	27:O:402:ADP:HN62	1.66	0.44
10:Y:7:PHE:O	10:Y:8:PHE:C	2.61	0.44
12:d:101:PHE:CZ	16:h:156:VAL:HG22	2.53	0.44
12:d:101:PHE:CZ	16:h:159:LEU:HD22	2.52	0.44
13:e:50:THR:HB	16:h:164:GLY:HA3	1.99	0.44
22:n:150:MET:HE2	22:n:150:MET:HB3	1.87	0.44
2:J:84:SER:HG	2:J:87:LEU:HB3	1.83	0.44
3:K:57:MET:O	3:K:60:PRO:HD2	2.18	0.44
4:L:55:PHE:HB2	23:o:74:PHE:HE1	1.82	0.44
4:L:68:TRP:HE3	4:L:76:LEU:HD21	1.83	0.44
4:L:556:ILE:CG2	21:m:80:PHE:CE2	3.00	0.44
5:M:126:LEU:HD11	5:M:153:THR:HG21	2.00	0.44
5:M:165:ILE:HD11	6:N:264:TRP:HE1	1.83	0.44
7:O:148:GLU:HG3	7:O:295:ARG:NH1	2.33	0.44
10:Y:89:PRO:HG3	10:Y:129:ILE:HG12	1.99	0.44
16:h:83:ILE:HG12	26:h:201:CDL:H561	2.00	0.44
17:i:5:THR:O	17:i:6:PRO:C	2.57	0.44
17:i:95:TYR:HE1	24:p:116:ARG:HH22	1.66	0.44
20:l:41:TYR:HD2	20:l:43:ARG:HD3	1.82	0.44
20:l:142:PHE:O	20:l:145:TRP:N	2.51	0.44
23:o:39:MET:HE1	23:o:57:ASP:O	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:30:LEU:O	2:J:34:VAL:HG23	2.17	0.43
4:L:305:SER:OG	4:L:336:LYS:HE2	2.18	0.43
4:L:537:THR:HG21	25:L:703:3PE:H352	2.00	0.43
5:M:46:ASP:OD1	5:M:47:GLU:N	2.50	0.43
6:N:164:MET:HE3	25:Y:201:3PE:H261	2.00	0.43
6:N:193:ILE:CD1	6:N:200:LEU:CD2	2.96	0.43
25:N:401:3PE:H231	25:N:401:3PE:H262	1.87	0.43
10:Y:26:ILE:O	10:Y:30:LEU:HG	2.17	0.43
10:Y:83:ARG:O	10:Y:84:GLU:HB3	2.18	0.43
24:p:165:GLU:C	24:p:167:ARG:H	2.26	0.43
1:D:41:ILE:HD11	15:g:53:TRP:HB3	2.00	0.43
3:K:26:LEU:HG	3:K:30:LEU:HD13	1.98	0.43
3:K:66:PHE:CZ	6:N:35:PHE:CE2	2.97	0.43
4:L:226:GLN:OE1	4:L:284:THR:CG2	2.66	0.43
25:L:703:3PE:C2G	25:L:704:3PE:H3I1	2.40	0.43
5:M:1:MET:HB3	5:M:1:MET:HE3	1.73	0.43
5:M:49:TYR:CZ	5:M:457:LEU:HD11	2.52	0.43
6:N:12:THR:CG2	6:N:39:ALA:HB2	2.48	0.43
6:N:166:ALA:HB1	6:N:288:LEU:HB3	1.99	0.43
6:N:265:ILE:HD12	6:N:344:ILE:HG21	2.00	0.43
11:c:40:ASN:O	11:c:43:ALA:N	2.50	0.43
13:e:87:MET:HE3	13:e:94:PRO:HD3	2.00	0.43
4:L:22:SER:HA	4:L:27:ILE:HG21	2.00	0.43
4:L:136:ASN:HD21	26:h:201:CDL:C27	2.18	0.43
4:L:309:GLN:HB2	4:L:336:LYS:HZ1	1.83	0.43
5:M:307:TRP:HB2	21:m:129:TYR:O	2.19	0.43
5:M:423:MET:C	5:M:424:ILE:O	2.56	0.43
5:M:452:LYS:HA	5:M:455:THR:CG2	2.48	0.43
10:Y:19:GLN:OE1	10:Y:19:GLN:HA	2.17	0.43
12:d:72:GLY:O	12:d:73:TYR:C	2.60	0.43
17:i:95:TYR:OH	24:p:11:PRO:O	2.34	0.43
3:K:32:CYS:O	3:K:33:LEU:C	2.59	0.43
4:L:53:MET:HE2	4:L:53:MET:HB3	1.78	0.43
4:L:92:VAL:HG21	4:L:330:CYS:HB3	2.00	0.43
4:L:283:LEU:CD1	20:l:140:MET:HE2	2.48	0.43
4:L:296:ASN:ND2	4:L:357:ARG:NE	2.67	0.43
5:M:348:LEU:O	5:M:349:GLN:C	2.60	0.43
5:M:353:PRO:HG3	16:h:61:LEU:CD2	2.48	0.43
6:N:29:MET:HE1	6:N:141:ILE:HA	2.01	0.43
7:O:214:VAL:O	7:O:218:ILE:HG13	2.18	0.43
10:Y:19:GLN:O	10:Y:23:LYS:HG2	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:g:58:GLU:CD	15:g:59:PRO:HD2	2.44	0.43
15:g:89:PHE:HB3	16:h:74:TYR:HD2	1.84	0.43
22:n:131:GLU:O	22:n:131:GLU:HG2	2.17	0.43
22:n:163:LEU:HA	22:n:164:PRO:HD2	1.75	0.43
24:p:103:MET:HE1	24:p:135:VAL:HG12	1.98	0.43
3:K:93:LEU:CD2	6:N:57:THR:HG21	2.47	0.43
4:L:70:THR:O	4:L:75:GLU:HA	2.17	0.43
4:L:81:LYS:HD3	4:L:262:ARG:NH1	2.34	0.43
5:M:63:THR:N	5:M:64:PRO:CD	2.81	0.43
5:M:304:GLN:HA	5:M:309:PHE:HE1	1.83	0.43
6:N:120:GLN:CG	6:N:177:LYS:HE3	2.47	0.43
6:N:240:MET:O	6:N:240:MET:HG2	2.18	0.43
6:N:254:LEU:HA	6:N:255:PRO:HD3	1.60	0.43
6:N:279:ALA:HA	6:N:282:MET:HE2	2.00	0.43
7:O:239:ASN:HA	7:O:242:LYS:HE2	2.01	0.43
7:O:332:ARG:O	7:O:338:LYS:HA	2.19	0.43
8:U:105:MET:HG3	8:U:139:MET:HE3	1.98	0.43
9:X:151:ASN:CB	9:X:152:PRO:HD2	2.39	0.43
12:d:93:TYR:OH	16:h:163:ARG:HD2	2.18	0.43
23:o:59:CYS:SG	23:o:90:CYS:C	3.01	0.43
1:D:36:GLN:NE2	1:D:38:GLN:NE2	2.62	0.43
4:L:246:LEU:HD12	4:L:247:LEU:CB	2.49	0.43
4:L:327:LEU:HD21	4:L:472:ILE:HD13	2.00	0.43
4:L:427:ILE:HG13	4:L:428:TYR:N	2.33	0.43
25:L:707:3PE:H251	6:N:288:LEU:CD1	2.48	0.43
5:M:95:TYR:OH	5:M:226:ALA:HB3	2.19	0.43
5:M:207:MET:SD	5:M:240:SER:CA	3.06	0.43
6:N:120:GLN:CG	6:N:177:LYS:HG3	2.48	0.43
6:N:150:ASN:ND2	6:N:152:THR:OG1	2.50	0.43
7:O:203:ALA:CB	7:O:254:GLU:HB3	2.48	0.43
8:U:72:PRO:HD3	18:j:42:PRO:HG3	1.99	0.43
8:U:113:LEU:HD11	22:n:20:TYR:CD1	2.53	0.43
12:d:78:ARG:HG2	12:d:82:LEU:HD23	2.00	0.43
12:d:94:ILE:HD13	16:h:152:LYS:HE3	2.01	0.43
13:e:72:THR:O	13:e:73:MET:C	2.60	0.43
16:h:127:ASP:OD1	16:h:127:ASP:C	2.60	0.43
17:i:18:LEU:HD22	22:n:125:TRP:CH2	2.54	0.43
22:n:94:TYR:HB3	22:n:178:PRO:HD2	2.01	0.43
23:o:17:PRO:HG3	23:o:106:ARG:CA	2.45	0.43
2:J:67:PHE:O	2:J:68:GLY:C	2.59	0.43
2:J:128:VAL:O	2:J:129:ASP:C	2.60	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:135:LEU:HG	2:J:135:LEU:O	2.18	0.43
3:K:5:PHE:CE1	3:K:47:THR:HG23	2.53	0.43
4:L:193:MET:HE1	21:m:125:PHE:CD2	2.54	0.43
4:L:446:ASN:O	4:L:447:ASP:C	2.57	0.43
4:L:532:ILE:HG13	20:l:126:TRP:CH2	2.54	0.43
4:L:569:LEU:CD1	26:L:706:CDL:H131	2.49	0.43
25:L:703:3PE:H2G1	25:L:704:3PE:C3I	2.41	0.43
5:M:73:LEU:HD23	5:M:103:GLN:HE22	1.84	0.43
5:M:119:TYR:HD1	5:M:160:LEU:HD22	1.80	0.43
6:N:11:PHE:O	6:N:15:LEU:N	2.49	0.43
7:O:303:GLU:O	7:O:304:VAL:C	2.59	0.43
8:U:87:LEU:HB2	8:U:98:LEU:CD1	2.49	0.43
20:l:97:LEU:O	20:l:98:ARG:C	2.60	0.43
21:m:17:THR:O	21:m:18:LEU:HB3	2.17	0.43
21:m:45:ARG:O	21:m:45:ARG:CG	2.61	0.43
4:L:496:LEU:CD1	4:L:497:GLY:N	2.73	0.43
4:L:569:LEU:CB	10:Y:115:MET:HE1	2.27	0.43
5:M:231:LEU:CD1	5:M:235:LEU:CD1	2.85	0.43
5:M:263:LEU:CD1	21:m:102:TYR:CD1	2.99	0.43
6:N:12:THR:HG22	6:N:39:ALA:HB2	2.00	0.43
6:N:39:ALA:O	6:N:42:PRO:HD2	2.18	0.43
6:N:219:LEU:CD2	6:N:230:ILE:HD12	2.49	0.43
8:U:142:GLN:O	8:U:143:GLU:C	2.60	0.43
12:d:120:ARG:O	21:m:109:ARG:NH2	2.52	0.43
13:e:49:GLY:O	13:e:50:THR:C	2.61	0.43
16:h:90:ASN:OD1	16:h:115:HIS:NE2	2.52	0.43
2:J:72:ALA:O	2:J:76:GLU:HG2	2.18	0.43
3:K:22:PHE:O	4:L:585:LYS:HE3	2.19	0.43
3:K:33:LEU:HD11	6:N:64:ALA:HB1	2.01	0.43
4:L:172:ILE:HD13	4:L:172:ILE:HA	1.89	0.43
4:L:493:ILE:O	4:L:496:LEU:HG	2.19	0.43
5:M:51:ASN:ND2	16:h:136:THR:HG23	2.34	0.43
5:M:100:ILE:O	5:M:103:GLN:HG2	2.19	0.43
5:M:154:LEU:HA	5:M:154:LEU:HD23	1.84	0.43
5:M:367:LEU:C	5:M:367:LEU:HD12	2.44	0.43
5:M:369:LEU:CD2	5:M:371:PRO:CD	2.84	0.43
6:N:43:MET:CE	6:N:126:MET:SD	3.07	0.43
6:N:109:ALA:O	6:N:112:HIS:HB3	2.19	0.43
6:N:189:TRP:CB	6:N:204:ASN:HD21	2.32	0.43
7:O:96:THR:O	11:c:31:VAL:HG21	2.18	0.43
10:Y:115:MET:O	10:Y:119:TYR:HD2	2.02	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:e:102:GLU:HG2	13:e:103:GLU:N	2.33	0.43
22:n:45:ARG:O	22:n:46:ALA:C	2.61	0.43
24:p:118:GLY:O	24:p:119:GLU:HB2	2.19	0.43
1:D:51:VAL:HB	6:N:171:ASN:OD1	2.19	0.43
2:J:55:VAL:HG13	2:J:56:PHE:N	2.33	0.43
3:K:50:ASN:C	3:K:50:ASN:OD1	2.62	0.43
4:L:38:THR:O	4:L:41:LYS:HB3	2.19	0.43
4:L:141:PHE:CB	4:L:182:PHE:CE2	2.81	0.43
4:L:217:LEU:CD1	4:L:273:ILE:HG23	2.49	0.43
4:L:253:VAL:HG21	4:L:310:LEU:HD11	1.99	0.43
4:L:296:ASN:CB	4:L:357:ARG:HH11	2.32	0.43
4:L:357:ARG:HG3	22:n:80:TYR:CD1	2.54	0.43
4:L:441:ILE:HD12	18:j:46:GLU:O	2.19	0.43
5:M:208:PRO:HG2	5:M:216:LEU:CD1	2.44	0.43
6:N:106:LEU:HD21	6:N:139:LEU:HG	2.00	0.43
6:N:108:LEU:HD12	6:N:187:MET:HB3	2.01	0.43
6:N:308:ASN:C	7:O:319:ILE:HG23	2.43	0.43
7:O:121:PRO:HB3	7:O:178:TYR:HE1	1.83	0.43
13:e:30:ALA:HB3	16:h:186:THR:HG21	2.00	0.43
17:i:22:TRP:CZ2	22:n:172:THR:HG22	2.53	0.43
23:o:57:ASP:OD2	23:o:59:CYS:HB2	2.19	0.43
4:L:138:PHE:CD1	26:h:201:CDL:H271	2.54	0.42
4:L:246:LEU:CD1	4:L:247:LEU:N	2.68	0.42
4:L:275:THR:HG23	4:L:276:THR:N	2.34	0.42
5:M:131:ILE:HD13	6:N:302:LEU:HD21	2.01	0.42
6:N:28:LEU:HD22	13:e:15:ASP:CG	2.44	0.42
6:N:219:LEU:HD23	6:N:230:ILE:HD12	2.01	0.42
7:O:117:PHE:HD1	7:O:128:SER:CA	2.31	0.42
7:O:224:PRO:O	7:O:228:LYS:NZ	2.52	0.42
16:h:59:PRO:O	16:h:61:LEU:HG	2.19	0.42
21:m:5:LYS:HB2	21:m:5:LYS:HE3	1.73	0.42
23:o:46:MET:HE2	23:o:60:ALA:HB3	2.00	0.42
2:J:100:VAL:HG12	2:J:104:CYS:SG	2.59	0.42
4:L:34:LEU:HD12	4:L:34:LEU:HA	1.88	0.42
4:L:521:SER:C	4:L:523:SER:N	2.75	0.42
26:L:706:CDL:H512	26:L:706:CDL:HB4	1.71	0.42
7:O:77:ILE:CG2	7:O:81:LEU:HD12	2.49	0.42
7:O:310:ILE:HG23	7:O:312:VAL:HG23	2.01	0.42
7:O:323:GLN:HB2	15:g:56:ASP:OD1	2.18	0.42
10:Y:8:PHE:CD1	10:Y:30:LEU:HD21	2.53	0.42
17:i:93:LYS:HE3	17:i:96:THR:HG21	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:k:28:TRP:CE3	19:k:60:MET:HG2	2.54	0.42
20:l:36:MET:O	20:l:36:MET:HG2	2.19	0.42
24:p:36:ALA:O	24:p:37:TYR:C	2.60	0.42
4:L:5:THR:O	4:L:6:THR:C	2.62	0.42
4:L:272:PHE:O	4:L:275:THR:HG22	2.19	0.42
4:L:489:THR:HG23	4:L:490:ALA:N	2.33	0.42
5:M:14:LEU:HD21	5:M:26:ASN:CB	2.50	0.42
5:M:68:LEU:HD23	5:M:234:ILE:CD1	2.50	0.42
5:M:72:LEU:HD12	5:M:234:ILE:HG12	2.01	0.42
5:M:214:LEU:C	5:M:217:PRO:HD2	2.45	0.42
5:M:306:PRO:HA	5:M:458:THR:HG21	2.01	0.42
25:M:502:3PE:O22	6:N:242:THR:OG1	2.36	0.42
6:N:80:GLN:O	6:N:80:GLN:HG2	2.19	0.42
6:N:89:GLN:HB3	13:e:60:PHE:CZ	2.53	0.42
10:Y:68:ILE:HG21	10:Y:120:MET:HE1	2.01	0.42
13:e:82:GLN:O	13:e:86:LEU:HG	2.19	0.42
13:e:89:GLU:HB2	13:e:91:LYS:HG2	2.00	0.42
16:h:129:PRO:HD2	16:h:130:GLU:OE1	2.19	0.42
17:i:4:TYR:O	17:i:5:THR:C	2.62	0.42
17:i:22:TRP:O	17:i:26:GLN:HG2	2.19	0.42
17:i:81:PHE:O	17:i:82:VAL:C	2.60	0.42
18:j:44:TYR:CE2	18:j:45:ARG:HG3	2.54	0.42
4:L:9:LEU:HG	25:L:701:3PE:H2D2	2.01	0.42
4:L:309:GLN:CG	4:L:336:LYS:HZ1	2.32	0.42
4:L:335:PHE:O	4:L:339:LEU:HD13	2.18	0.42
4:L:357:ARG:HG2	4:L:357:ARG:H	1.59	0.42
4:L:358:LYS:CG	22:n:80:TYR:OH	2.47	0.42
5:M:47:GLU:O	5:M:48:ASN:C	2.62	0.42
6:N:80:GLN:O	6:N:81:LEU:HG	2.19	0.42
6:N:241:LEU:HG	6:N:301:SER:OG	2.19	0.42
6:N:272:LYS:HE3	16:h:154:GLN:HG2	2.00	0.42
7:O:170:LEU:HD21	7:O:184:VAL:HG13	2.00	0.42
7:O:242:LYS:HE2	7:O:242:LYS:HB2	1.92	0.42
7:O:297:LEU:C	7:O:297:LEU:HD23	2.44	0.42
7:O:339:TYR:CE1	12:d:52:PRO:HA	2.54	0.42
8:U:125:GLU:OE2	18:j:44:TYR:CE1	2.73	0.42
17:i:103:ARG:NH2	23:o:67:LEU:HD13	2.33	0.42
19:k:58:ARG:HH12	22:n:34:ARG:HH11	1.68	0.42
22:n:110:SER:O	22:n:113:ALA:HB3	2.20	0.42
22:n:139:GLN:HA	22:n:142:GLU:HG2	2.01	0.42
24:p:6:ASP:OD1	24:p:8:ASP:HB2	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:p:43:TRP:NE1	24:p:47:LEU:HD11	2.33	0.42
4:L:591:PHE:O	4:L:595:ILE:HG13	2.20	0.42
25:L:707:3PE:H3B2	25:L:707:3PE:H3E1	1.72	0.42
5:M:29:SER:CB	15:g:91:PHE:HD2	2.24	0.42
5:M:44:GLN:HG2	5:M:46:ASP:O	2.18	0.42
5:M:77:LEU:O	5:M:81:GLN:HG3	2.19	0.42
5:M:118:PHE:HE2	5:M:203:PHE:CE1	2.37	0.42
5:M:131:ILE:HD12	6:N:302:LEU:HD21	2.01	0.42
5:M:206:LYS:HA	5:M:215:TRP:CZ2	2.54	0.42
5:M:293:HIS:O	5:M:294:MET:HE2	2.20	0.42
5:M:347:GLY:O	5:M:348:LEU:C	2.63	0.42
7:O:209:VAL:HA	7:O:210:PRO:HD3	1.80	0.42
7:O:350:LYS:HD3	7:O:351:TRP:CD1	2.54	0.42
8:U:124:ASP:CG	22:n:25:ARG:HH12	2.27	0.42
12:d:87:ASP:HB3	12:d:91:PHE:CE2	2.54	0.42
12:d:114:GLU:O	12:d:114:GLU:HG2	2.18	0.42
20:l:57:MET:HG2	20:l:104:PRO:CG	2.49	0.42
4:L:220:ALA:HB2	4:L:260:LEU:CD1	2.49	0.42
4:L:396:ILE:HD13	4:L:396:ILE:HA	1.89	0.42
5:M:181:PHE:CZ	24:p:86:TYR:HD1	2.37	0.42
5:M:200:MET:CE	5:M:247:SER:HB2	2.46	0.42
5:M:207:MET:HE3	5:M:240:SER:HB2	2.02	0.42
5:M:210:TYR:O	5:M:213:HIS:HD2	2.01	0.42
5:M:230:ILE:HG23	5:M:235:LEU:HD11	2.01	0.42
6:N:226:THR:HG22	6:N:228:ASN:N	2.34	0.42
10:Y:45:LEU:O	10:Y:46:ASN:C	2.62	0.42
10:Y:76:THR:CG2	10:Y:92:TYR:HA	2.48	0.42
10:Y:141:PRO:HB2	16:h:161:ARG:NE	2.35	0.42
15:g:119:GLU:OE1	15:g:122:ARG:NH1	2.53	0.42
15:g:147:LEU:O	15:g:148:PRO:C	2.62	0.42
19:k:42:LEU:HD11	22:n:39:TYR:HA	2.02	0.42
20:l:62:TYR:CE2	20:l:64:PRO:HG3	2.55	0.42
21:m:26:SER:HB2	21:m:27:PRO:HD2	2.00	0.42
4:L:21:ILE:HG23	4:L:27:ILE:CG2	2.50	0.42
4:L:81:LYS:HD3	4:L:262:ARG:HH11	1.83	0.42
4:L:189:PHE:CZ	4:L:212:PRO:HB2	2.55	0.42
4:L:277:MET:CG	4:L:318:GLY:CA	2.98	0.42
4:L:365:ILE:CD1	4:L:366:MET:HG3	2.24	0.42
4:L:405:ASN:HB2	4:L:408:ALA:HB3	2.01	0.42
5:M:16:TRP:HZ2	25:M:502:3PE:H282	1.84	0.42
5:M:123:GLU:OE2	5:M:154:LEU:HD21	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:191:SER:O	5:M:194:LEU:HB2	2.20	0.42
5:M:216:LEU:HD23	5:M:287:ALA:HB1	2.02	0.42
7:O:272:ASP:HA	7:O:275:TYR:HD2	1.85	0.42
8:U:84:LEU:HD11	8:U:98:LEU:HG	2.02	0.42
11:c:55:TRP:CZ2	12:d:66:THR:HG22	2.55	0.42
18:j:96:GLU:HG2	18:j:97:LEU:HD23	2.01	0.42
20:l:120:SER:O	20:l:121:PRO:C	2.60	0.42
1:D:37:TRP:CE3	1:D:37:TRP:O	2.73	0.42
4:L:112:PRO:HD2	22:n:97:TYR:CE2	2.55	0.42
4:L:264:HIS:HA	4:L:267:THR:HG23	2.02	0.42
4:L:552:LEU:HD12	20:l:70:MET:CE	2.42	0.42
5:M:445:ILE:HG23	25:M:501:3PE:H292	2.02	0.42
6:N:154:ILE:CG2	6:N:191:LEU:HD11	2.49	0.42
6:N:281:LEU:CD2	25:N:401:3PE:C28	2.88	0.42
8:U:125:GLU:OE2	18:j:44:TYR:HE1	2.02	0.42
12:d:87:ASP:HB3	12:d:91:PHE:CD2	2.55	0.42
15:g:123:LEU:CD1	24:p:98:VAL:HG11	2.49	0.42
16:h:144:SER:HB2	24:p:82:VAL:HG21	2.02	0.42
20:l:167:TYR:CG	20:l:178:PRO:HG3	2.55	0.42
23:o:104:ARG:O	23:o:108:LEU:HG	2.20	0.42
2:J:120:LEU:C	2:J:122:ASP:N	2.78	0.42
4:L:23:MET:SD	26:L:705:CDL:H112	2.60	0.42
4:L:226:GLN:OE1	4:L:281:GLY:HA2	2.20	0.42
4:L:534:HIS:O	4:L:538:PRO:CG	2.60	0.42
6:N:215:MET:SD	6:N:244:ILE:CD1	3.08	0.42
7:O:66:ILE:HG23	27:O:402:ADP:O3'	2.19	0.42
7:O:195:LEU:N	7:O:196:PRO:HD2	2.34	0.42
12:d:100:ASP:HB3	16:h:159:LEU:HD21	2.01	0.42
14:f:6:LEU:O	14:f:7:LEU:HB2	2.19	0.42
16:h:55:PHE:HE1	16:h:57:VAL:HA	1.84	0.42
20:l:84:HIS:NE2	20:l:114:ARG:HA	2.34	0.42
22:n:100:PRO:HB2	22:n:102:TRP:NE1	2.35	0.42
23:o:22:ILE:N	23:o:23:PRO:HD2	2.35	0.42
23:o:31:PHE:CD1	23:o:34:ARG:HD2	2.55	0.42
2:J:20:ALA:C	2:J:22:LYS:N	2.77	0.42
3:K:59:ILE:HB	3:K:60:PRO:HD3	2.01	0.42
4:L:51:LEU:HA	4:L:87:ILE:HD12	2.02	0.42
4:L:193:MET:CE	21:m:125:PHE:CD2	3.03	0.42
4:L:293:LEU:O	4:L:425:ARG:HD2	2.20	0.42
4:L:568:THR:O	4:L:569:LEU:C	2.61	0.42
4:L:597:LEU:HD21	10:Y:37:ILE:HD12	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:263:LEU:HD13	21:m:102:TYR:HB2	2.01	0.42
6:N:25:ASN:HB3	13:e:15:ASP:CG	2.45	0.42
6:N:324:LEU:HD11	12:d:64:PHE:HZ	1.85	0.42
7:O:209:VAL:CG1	7:O:260:SER:HB2	2.31	0.42
8:U:103:HIS:HB2	8:U:106:LYS:HG2	2.02	0.42
12:d:24:PRO:HD2	12:d:73:TYR:CE2	2.55	0.42
13:e:44:ALA:HA	13:e:47:ILE:CG1	2.49	0.42
13:e:81:LYS:O	13:e:85:LYS:HG3	2.19	0.42
13:e:83:ARG:HG2	13:e:87:MET:SD	2.60	0.42
17:i:9:LYS:O	17:i:13:GLN:HB2	2.20	0.42
20:l:159:LYS:HE3	20:l:161:TYR:HE1	1.85	0.42
21:m:8:PRO:HD3	21:m:14:LEU:HD13	2.02	0.42
2:J:84:SER:O	2:J:88:ILE:HG12	2.19	0.41
4:L:117:PHE:HZ	4:L:242:PRO:HG2	1.85	0.41
4:L:407:TRP:CE3	4:L:410:LEU:HD21	2.54	0.41
5:M:108:MET:HB3	5:M:121:LEU:HD13	2.02	0.41
5:M:158:ILE:HG21	6:N:283:ALA:CB	2.48	0.41
5:M:258:ALA:O	5:M:259:TYR:C	2.62	0.41
7:O:58:ARG:HB3	7:O:202:HIS:HB2	2.01	0.41
26:X:201:CDL:OB7	26:X:201:CDL:HB61	2.20	0.41
10:Y:10:SER:O	10:Y:11:TYR:C	2.62	0.41
13:e:36:PHE:O	13:e:37:GLU:C	2.62	0.41
13:e:96:PRO:HA	13:e:99:SER:CB	2.33	0.41
16:h:90:ASN:HD21	26:h:201:CDL:PA1	2.43	0.41
20:l:59:VAL:O	20:l:59:VAL:HG12	2.20	0.41
22:n:132:SER:O	22:n:133:TRP:C	2.62	0.41
22:n:164:PRO:HA	22:n:165:PRO:HD3	1.94	0.41
23:o:42:THR:O	23:o:43:GLN:C	2.62	0.41
24:p:9:VAL:O	24:p:109:ARG:NH2	2.51	0.41
1:D:35:ARG:HH21	15:g:59:PRO:HD3	1.84	0.41
2:J:39:GLY:HA2	2:J:42:MET:HE2	1.99	0.41
4:L:16:LEU:HD11	25:L:701:3PE:C2H	2.23	0.41
4:L:355:ASP:O	4:L:359:MET:HG3	2.20	0.41
4:L:489:THR:O	4:L:492:ILE:HG13	2.20	0.41
4:L:553:LEU:HD21	21:m:94:GLY:N	2.34	0.41
6:N:154:ILE:HD11	6:N:195:PRO:HG2	2.01	0.41
6:N:218:ALA:CB	6:N:240:MET:SD	3.08	0.41
7:O:267:THR:O	7:O:271:GLU:HG3	2.19	0.41
8:U:128:PHE:HZ	8:U:148:ILE:CD1	2.33	0.41
10:Y:91:ASN:HD22	10:Y:91:ASN:HA	1.71	0.41
12:d:108:THR:HG23	12:d:110:ALA:HB3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:e:33:CYS:O	13:e:34:HIS:C	2.62	0.41
17:i:20:ARG:HH11	17:i:20:ARG:HG3	1.84	0.41
22:n:56:ASP:O	22:n:59:ARG:N	2.54	0.41
22:n:114:MET:HG3	22:n:115:TYR:CD2	2.55	0.41
4:L:142:ILE:HG12	5:M:370:PRO:HB2	2.01	0.41
4:L:598:ILE:HD11	6:N:153:ILE:HD13	2.02	0.41
5:M:151:PHE:CZ	6:N:291:PHE:CB	2.97	0.41
5:M:177:MET:HB3	5:M:177:MET:HE3	1.70	0.41
5:M:270:ILE:HD11	5:M:395:LEU:HA	2.03	0.41
5:M:319:HIS:HA	5:M:322:THR:CG2	2.44	0.41
6:N:285:MET:HE1	6:N:288:LEU:HD22	2.03	0.41
7:O:146:ALA:CB	7:O:159:LEU:HD21	2.50	0.41
7:O:179:ILE:CD1	7:O:184:VAL:HG22	2.50	0.41
7:O:179:ILE:HD12	7:O:184:VAL:HG22	2.02	0.41
7:O:243:LYS:HB2	7:O:243:LYS:HE2	1.64	0.41
13:e:85:LYS:HG3	13:e:85:LYS:H	1.58	0.41
14:f:42:MET:HB3	24:p:71:VAL:HG23	2.02	0.41
21:m:42:ARG:O	21:m:43:LEU:C	2.62	0.41
23:o:15:VAL:HG13	23:o:110:GLN:HG2	2.01	0.41
1:D:49:GLY:O	6:N:173:THR:HG21	2.21	0.41
2:J:100:VAL:O	2:J:101:PHE:C	2.63	0.41
4:L:23:MET:HE1	26:L:705:CDL:H132	2.02	0.41
4:L:202:MET:HE3	4:L:265:PRO:CB	2.50	0.41
4:L:231:PRO:O	4:L:234:PRO:HD2	2.20	0.41
4:L:286:LEU:HG	4:L:290:ILE:HD11	2.01	0.41
25:L:707:3PE:H3C1	5:M:155:ILE:CD1	2.51	0.41
5:M:142:ARG:HG3	5:M:143:LEU:N	2.35	0.41
5:M:270:ILE:HD12	5:M:395:LEU:HD22	2.02	0.41
7:O:261:TRP:H	7:O:261:TRP:HE3	1.68	0.41
7:O:295:ARG:HH12	7:O:299:GLN:CB	2.33	0.41
8:U:87:LEU:C	8:U:89:LEU:N	2.78	0.41
8:U:105:MET:SD	8:U:139:MET:HE1	2.58	0.41
10:Y:20:CYS:O	10:Y:21:HIS:C	2.63	0.41
17:i:102:PRO:HB2	24:p:18:PRO:CG	2.51	0.41
21:m:124:LYS:O	21:m:126:ASN:N	2.54	0.41
23:o:4:HIS:HB3	23:o:16:GLU:OE1	2.21	0.41
23:o:26:PRO:C	23:o:28:ASP:N	2.75	0.41
23:o:53:LEU:HD23	23:o:56:ARG:NE	2.34	0.41
2:J:22:LYS:HE3	3:K:22:PHE:HA	2.02	0.41
2:J:29:GLY:O	2:J:33:ILE:HG13	2.21	0.41
2:J:168:GLU:OE2	2:J:171:ARG:HG3	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:85:LYS:O	5:M:85:LYS:HG2	2.21	0.41
5:M:247:SER:OG	5:M:304:GLN:NE2	2.53	0.41
7:O:117:PHE:CZ	7:O:173:MET:HE3	2.54	0.41
7:O:263:ALA:C	7:O:265:ASP:N	2.77	0.41
8:U:74:LEU:CD2	8:U:79:ILE:HD11	2.49	0.41
8:U:120:MET:HE1	22:n:24:LEU:HD12	2.03	0.41
18:j:40:ILE:HD12	18:j:40:ILE:HA	1.93	0.41
18:j:44:TYR:CD2	18:j:45:ARG:HG3	2.56	0.41
18:j:52:ARG:HG2	18:j:56:ILE:HD12	2.02	0.41
2:J:60:LEU:O	2:J:64:LEU:HB2	2.20	0.41
2:J:98:MET:HE2	2:J:98:MET:HB3	1.82	0.41
4:L:112:PRO:CD	22:n:97:TYR:CE2	3.03	0.41
4:L:182:PHE:HE2	4:L:186:MET:CE	2.32	0.41
4:L:258:PHE:O	4:L:261:VAL:HG22	2.20	0.41
4:L:296:ASN:CG	4:L:357:ARG:HE	2.28	0.41
4:L:466:PHE:HB2	18:j:68:TRP:CH2	2.50	0.41
5:M:4:ILE:CD1	5:M:41:LEU:HD21	2.51	0.41
5:M:178:ILE:O	5:M:179:LEU:C	2.60	0.41
5:M:250:LEU:HD12	5:M:250:LEU:C	2.39	0.41
5:M:301:ILE:HG22	5:M:301:ILE:O	2.19	0.41
6:N:152:THR:HG22	10:Y:138:PHE:HB3	2.02	0.41
6:N:233:LEU:CD2	6:N:241:LEU:HD12	2.26	0.41
7:O:164:TYR:CE1	7:O:201:PRO:HD3	2.56	0.41
9:X:162:LYS:HE3	9:X:163:HIS:CD2	2.55	0.41
11:c:69:TYR:O	11:c:73:ASN:ND2	2.54	0.41
13:e:49:GLY:O	13:e:52:ALA:N	2.53	0.41
14:f:5:GLN:O	14:f:9:GLU:HB2	2.20	0.41
15:g:71:PHE:CE2	15:g:73:GLY:HA2	2.55	0.41
17:i:74:HIS:O	17:i:78:PRO:HG2	2.20	0.41
17:i:106:PRO:HG3	17:i:120:MET:HG2	2.02	0.41
18:j:99:ILE:HA	23:o:108:LEU:CD2	2.51	0.41
1:D:50:ALA:C	1:D:51:VAL:HG13	2.45	0.41
2:J:87:LEU:HD23	2:J:87:LEU:C	2.46	0.41
4:L:253:VAL:HB	4:L:310:LEU:CD1	2.50	0.41
4:L:296:ASN:ND2	22:n:78:GLN:HB3	2.36	0.41
26:L:705:CDL:H361	16:h:72:LYS:HG3	2.03	0.41
5:M:210:TYR:HB2	5:M:268:GLY:HA3	2.03	0.41
5:M:329:LEU:HD23	5:M:437:MET:CE	2.49	0.41
6:N:83:THR:HG22	6:N:84:TRP:N	2.35	0.41
6:N:317:GLN:HB3	7:O:301:LYS:HB2	2.01	0.41
7:O:262:GLU:O	7:O:265:ASP:HB3	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:c:72:ARG:HD2	12:d:20:SER:CA	2.50	0.41
13:e:32:ARG:O	13:e:33:CYS:CB	2.69	0.41
13:e:93:THR:HA	13:e:94:PRO:HD3	1.92	0.41
18:j:47:PHE:O	18:j:48:PRO:C	2.62	0.41
18:j:102:ASP:O	18:j:103:ASP:HB2	2.21	0.41
20:l:122:THR:HG22	20:l:124:VAL:H	1.85	0.41
23:o:39:MET:CE	23:o:58:TYR:HA	2.51	0.41
24:p:91:GLN:O	24:p:91:GLN:HG2	2.21	0.41
2:J:92:LEU:HD23	2:J:92:LEU:C	2.46	0.41
4:L:368:PHE:HB3	4:L:445:GLU:OE1	2.20	0.41
4:L:519:TYR:O	4:L:520:SER:C	2.62	0.41
4:L:571:THR:O	4:L:574:THR:HG22	2.20	0.41
4:L:586:LEU:HD21	10:Y:47:PRO:HD3	2.03	0.41
25:L:707:3PE:H2A1	6:N:288:LEU:HD13	2.02	0.41
25:L:707:3PE:H341	25:L:707:3PE:H371	1.91	0.41
5:M:16:TRP:HZ2	25:M:502:3PE:C28	2.34	0.41
5:M:22:LYS:HE3	5:M:26:ASN:HD21	1.86	0.41
5:M:216:LEU:CG	5:M:220:HIS:CE1	2.88	0.41
5:M:264:LEU:HD23	21:m:98:LEU:HD21	2.01	0.41
5:M:350:MET:HE3	5:M:350:MET:HB2	1.80	0.41
6:N:81:LEU:CD2	13:e:60:PHE:HE1	2.33	0.41
6:N:103:SER:O	6:N:107:GLY:N	2.54	0.41
6:N:200:LEU:CD2	6:N:265:ILE:HG23	2.51	0.41
7:O:117:PHE:CE1	7:O:128:SER:CB	2.96	0.41
7:O:150:LEU:O	7:O:154:GLY:HA2	2.20	0.41
7:O:287:ASP:HB3	7:O:290:THR:HG23	2.02	0.41
13:e:65:GLU:OE2	13:e:71:LYS:N	2.54	0.41
14:f:36:ALA:O	14:f:37:PHE:C	2.61	0.41
15:g:148:PRO:O	24:p:167:ARG:NH2	2.53	0.41
17:i:102:PRO:CG	24:p:18:PRO:HD2	2.49	0.41
18:j:81:LEU:O	18:j:81:LEU:HD23	2.20	0.41
20:l:44:THR:HG23	20:l:46:GLU:HG2	2.03	0.41
20:l:63:GLU:O	20:l:64:PRO:C	2.63	0.41
2:J:33:ILE:HG12	2:J:64:LEU:HD23	2.02	0.41
2:J:107:ASN:O	2:J:108:TYR:C	2.63	0.41
4:L:3:ILE:HG22	4:L:49:LEU:CD2	2.51	0.41
4:L:61:TYR:HA	17:i:98:VAL:O	2.21	0.41
4:L:321:GLN:NE2	4:L:324:LEU:HD13	2.36	0.41
4:L:441:ILE:HD13	18:j:48:PRO:HD3	2.02	0.41
4:L:466:PHE:HE1	18:j:72:ARG:CZ	2.32	0.41
4:L:481:THR:CG2	23:o:95:TYR:CE2	3.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:570:HIS:O	4:L:573:MET:N	2.54	0.41
25:L:701:3PE:H122	17:i:89:HIS:CB	2.51	0.41
5:M:6:LEU:O	5:M:7:PRO:C	2.60	0.41
5:M:7:PRO:HG3	14:f:20:PHE:CA	2.51	0.41
5:M:72:LEU:O	5:M:76:MET:N	2.45	0.41
5:M:160:LEU:O	5:M:164:LEU:HD13	2.21	0.41
5:M:164:LEU:HB3	5:M:174:LEU:HD11	2.03	0.41
5:M:175:ASN:ND2	16:h:143:GLU:HG2	2.31	0.41
5:M:303:ILE:HG13	5:M:385:LEU:HD23	2.03	0.41
5:M:391:PHE:HE2	25:M:503:3PE:C23	2.34	0.41
6:N:89:GLN:HG2	13:e:60:PHE:CE2	2.56	0.41
6:N:124:LEU:CD2	6:N:176:ARG:HD3	2.51	0.41
6:N:131:LEU:O	6:N:135:LYS:HG3	2.21	0.41
6:N:194:LEU:HD13	6:N:201:THR:HG21	2.03	0.41
6:N:215:MET:HE3	6:N:215:MET:HB3	1.96	0.41
7:O:42:ALA:O	7:O:45:LEU:C	2.64	0.41
7:O:63:ASP:HB3	7:O:245:PHE:HE2	1.84	0.41
7:O:90:GLY:H	7:O:93:TYR:HB2	1.85	0.41
7:O:105:ASP:OD1	7:O:106:ILE:N	2.54	0.41
7:O:354:LEU:HD12	7:O:354:LEU:HA	1.95	0.41
8:U:83:VAL:HG13	8:U:122:MET:SD	2.61	0.41
8:U:128:PHE:CZ	8:U:148:ILE:CD1	3.04	0.41
10:Y:5:LYS:C	10:Y:7:PHE:N	2.77	0.41
10:Y:51:THR:HG23	10:Y:52:LEU:N	2.35	0.41
12:d:11:LEU:HD22	13:e:5:ASP:O	2.20	0.41
12:d:25:LYS:HE3	12:d:27:ASN:OD1	2.21	0.41
12:d:45:ASP:O	12:d:46:ASN:C	2.62	0.41
13:e:83:ARG:O	13:e:87:MET:HG3	2.20	0.41
17:i:29:SER:O	17:i:32:GLU:HB2	2.21	0.41
17:i:125:ASP:O	17:i:126:GLN:C	2.63	0.41
18:j:89:PRO:O	23:o:103:GLU:HG2	2.21	0.41
20:l:129:MET:HE3	20:l:129:MET:HB2	1.89	0.41
21:m:50:GLN:O	21:m:50:GLN:HG2	2.20	0.41
21:m:59:HIS:O	21:m:60:ILE:C	2.64	0.41
22:n:41:ALA:C	22:n:43:LEU:N	2.78	0.41
22:n:165:PRO:O	22:n:166:LEU:C	2.64	0.41
23:o:50:GLN:OE1	24:p:120:ASN:ND2	2.54	0.41
23:o:71:ARG:NH1	23:o:72:ASP:OD1	2.54	0.41
24:p:40:VAL:O	24:p:44:PRO:HG2	2.20	0.41
2:J:2:ASN:O	2:J:3:ASN:HB2	2.20	0.41
2:J:59:TYR:HH	3:K:34:GLU:C	2.28	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:52:LEU:O	4:L:53:MET:C	2.62	0.41
5:M:165:ILE:HG21	6:N:268:THR:HA	2.02	0.41
5:M:248:ILE:HG13	5:M:249:ILE:H	1.85	0.41
5:M:422:HIS:CE1	21:m:56:ARG:HH22	2.38	0.41
7:O:104:LEU:HD23	7:O:104:LEU:HA	1.90	0.41
7:O:263:ALA:C	7:O:265:ASP:H	2.29	0.41
7:O:268:LYS:HA	7:O:271:GLU:OE1	2.21	0.41
26:X:201:CDL:H521	26:X:201:CDL:H552	1.90	0.41
13:e:49:GLY:HA2	13:e:52:ALA:HB3	2.02	0.41
14:f:7:LEU:O	14:f:8:ARG:HB2	2.21	0.41
16:h:91:ILE:O	24:p:56:HIS:CD2	2.74	0.41
19:k:81:PHE:O	19:k:85:VAL:HG23	2.21	0.41
20:l:159:LYS:HE3	20:l:161:TYR:CE1	2.56	0.41
22:n:139:GLN:O	22:n:140:LEU:C	2.64	0.41
23:o:52:THR:O	23:o:53:LEU:C	2.62	0.41
3:K:51:SER:HA	13:e:32:ARG:NH1	2.34	0.40
4:L:68:TRP:CE3	4:L:76:LEU:CD2	3.04	0.40
4:L:283:LEU:HD12	20:l:140:MET:HE2	2.03	0.40
4:L:324:LEU:HB3	4:L:395:ILE:CD1	2.51	0.40
26:L:705:CDL:H162	26:L:705:CDL:H132	1.81	0.40
5:M:197:LEU:O	5:M:201:MET:HB2	2.21	0.40
6:N:189:TRP:CZ3	6:N:282:MET:HE3	2.57	0.40
6:N:224:SER:HB2	6:N:229:SER:HB2	2.01	0.40
6:N:323:ASN:OD1	6:N:323:ASN:C	2.61	0.40
9:X:169:PHE:HD1	9:X:169:PHE:O	2.04	0.40
14:f:56:TRP:CD1	16:h:134:GLU:OE1	2.73	0.40
15:g:112:MET:HE3	15:g:115:TRP:CE3	2.56	0.40
17:i:22:TRP:CE3	22:n:172:THR:CG2	3.04	0.40
17:i:32:GLU:OE2	22:n:117:ASP:N	2.53	0.40
17:i:69:LEU:HD23	17:i:69:LEU:N	2.36	0.40
22:n:157:ALA:O	22:n:158:ARG:HB2	2.21	0.40
23:o:95:TYR:O	23:o:99:MET:HG3	2.21	0.40
2:J:32:LEU:O	2:J:33:ILE:C	2.64	0.40
4:L:14:LEU:CD2	17:i:74:HIS:O	2.69	0.40
4:L:22:SER:HA	4:L:27:ILE:CG2	2.52	0.40
4:L:203:PHE:CE2	24:p:110:LEU:HD11	2.56	0.40
4:L:205:ASN:ND2	24:p:121:TYR:OH	2.52	0.40
4:L:210:LEU:O	4:L:211:ILE:C	2.62	0.40
4:L:400:ASN:HD22	4:L:409:LEU:HD11	1.85	0.40
5:M:162:ILE:CG2	6:N:271:MET:HE3	2.22	0.40
5:M:435:THR:HG23	5:M:436:LEU:N	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:111:ASP:OD1	8:U:112:SER:N	2.55	0.40
13:e:69:ARG:CD	13:e:72:THR:HG21	2.50	0.40
15:g:125:LYS:HD3	24:p:6:ASP:OD2	2.21	0.40
16:h:87:THR:O	16:h:91:ILE:HG13	2.21	0.40
16:h:148:GLU:O	16:h:152:LYS:HG3	2.21	0.40
19:k:57:TRP:HA	19:k:60:MET:HB3	2.02	0.40
20:l:122:THR:CG2	20:l:129:MET:HE1	2.45	0.40
21:m:6:TYR:HB3	21:m:18:LEU:HD21	2.01	0.40
24:p:43:TRP:HB3	24:p:44:PRO:HD3	2.03	0.40
2:J:63:MET:O	2:J:66:VAL:N	2.54	0.40
3:K:82:SER:HA	3:K:86:GLY:H	1.85	0.40
4:L:172:ILE:HG22	5:M:405:MET:HE1	2.04	0.40
4:L:553:LEU:HD21	21:m:93:ALA:O	2.22	0.40
5:M:53:SER:O	5:M:54:ASN:C	2.63	0.40
5:M:394:ILE:O	5:M:398:ILE:HG13	2.22	0.40
25:M:502:3PE:H2H2	25:M:502:3PE:H3I1	2.03	0.40
6:N:59:TYR:O	6:N:63:GLN:HG2	2.21	0.40
8:U:86:VAL:CB	8:U:122:MET:HE1	2.49	0.40
8:U:113:LEU:HD23	22:n:45:ARG:NH1	2.36	0.40
8:U:133:ILE:CG2	8:U:134:ASP:N	2.84	0.40
17:i:98:VAL:HG13	24:p:115:GLN:HG2	2.03	0.40
17:i:102:PRO:HG2	17:i:104:ILE:HG23	2.03	0.40
21:m:32:ALA:O	21:m:33:GLN:C	2.63	0.40
25:J:201:3PE:H332	25:J:201:3PE:O11	2.22	0.40
4:L:1:MET:HE1	4:L:59:MET:HE1	2.03	0.40
4:L:67:HIS:HD2	4:L:76:LEU:O	2.05	0.40
4:L:586:LEU:CD2	10:Y:47:PRO:HD3	2.50	0.40
5:M:259:TYR:HB2	5:M:260:PRO:HD3	2.03	0.40
7:O:78:ALA:CB	7:O:85:HIS:HB2	2.51	0.40
7:O:170:LEU:CD2	7:O:184:VAL:HG13	2.51	0.40
7:O:221:LYS:HD3	7:O:222:GLY:H	1.86	0.40
7:O:235:GLN:HE21	7:O:239:ASN:ND2	2.19	0.40
8:U:87:LEU:C	8:U:89:LEU:H	2.29	0.40
12:d:104:LYS:HB3	12:d:104:LYS:HE2	1.85	0.40
14:f:49:ARG:HG3	14:f:52:GLU:CG	2.51	0.40
14:f:53:GLU:C	14:f:54:VAL:HG13	2.46	0.40
17:i:101:LYS:HB2	23:o:50:GLN:HE21	1.87	0.40
18:j:71:TRP:HZ3	18:j:72:ARG:NH2	2.19	0.40
21:m:49:LEU:O	21:m:49:LEU:CD1	2.65	0.40
23:o:11:TRP:CD1	23:o:12:ASP:N	2.89	0.40
2:J:123:TRP:HB2	2:J:126:TYR:CE1	2.57	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:210:LEU:HD12	4:L:270:ASN:HD21	1.86	0.40
4:L:399:ILE:HG22	4:L:409:LEU:CD1	2.52	0.40
5:M:5:ILE:CG1	5:M:6:LEU:N	2.85	0.40
5:M:186:LEU:CB	5:M:253:LEU:HD13	2.52	0.40
5:M:285:LEU:CD2	5:M:410:MET:SD	3.09	0.40
6:N:220:MET:HG3	6:N:221:LEU:N	2.36	0.40
6:N:273:ASN:HD21	10:Y:143:VAL:HA	1.84	0.40
6:N:297:ILE:O	6:N:298:TYR:C	2.63	0.40
7:O:117:PHE:HE1	7:O:173:MET:HE1	1.80	0.40
7:O:247:PRO:O	7:O:248:LYS:C	2.65	0.40
7:O:276:LEU:C	7:O:276:LEU:HD12	2.46	0.40
12:d:11:LEU:HB2	13:e:9:LYS:HB2	2.04	0.40
13:e:65:GLU:OE2	13:e:71:LYS:HB2	2.21	0.40
19:k:56:ALA:O	19:k:60:MET:N	2.53	0.40
21:m:49:LEU:HD12	21:m:49:LEU:C	2.47	0.40
21:m:124:LYS:HG2	21:m:125:PHE:CD2	2.57	0.40
23:o:18:ASP:HB3	23:o:21:LYS:HE2	2.04	0.40
23:o:25:PHE:O	23:o:26:PRO:C	2.64	0.40
24:p:45:VAL:O	24:p:46:THR:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	D	36/463 (8%)	34 (94%)	2 (6%)	0	100	100
2	J	153/172 (89%)	144 (94%)	9 (6%)	0	100	100
3	K	95/98 (97%)	90 (95%)	5 (5%)	0	100	100
4	L	604/607 (100%)	573 (95%)	30 (5%)	1 (0%)	43	71
5	M	456/459 (99%)	438 (96%)	18 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	N	342/345 (99%)	330 (96%)	11 (3%)	1 (0%)	36	65
7	O	317/355 (89%)	303 (96%)	14 (4%)	0	100	100
8	U	82/156 (53%)	76 (93%)	6 (7%)	0	100	100
9	X	25/172 (14%)	24 (96%)	1 (4%)	0	100	100
10	Y	137/143 (96%)	133 (97%)	4 (3%)	0	100	100
11	c	45/76 (59%)	44 (98%)	1 (2%)	0	100	100
12	d	117/120 (98%)	115 (98%)	2 (2%)	0	100	100
13	e	102/106 (96%)	97 (95%)	5 (5%)	0	100	100
14	f	53/57 (93%)	50 (94%)	3 (6%)	0	100	100
15	g	100/151 (66%)	93 (93%)	7 (7%)	0	100	100
16	h	134/189 (71%)	127 (95%)	7 (5%)	0	100	100
17	i	90/128 (70%)	76 (84%)	13 (14%)	1 (1%)	11	39
18	j	63/105 (60%)	58 (92%)	5 (8%)	0	100	100
19	k	69/104 (66%)	67 (97%)	2 (3%)	0	100	100
20	l	156/186 (84%)	143 (92%)	13 (8%)	0	100	100
21	m	125/129 (97%)	117 (94%)	8 (6%)	0	100	100
22	n	176/179 (98%)	162 (92%)	13 (7%)	1 (1%)	21	52
23	o	118/137 (86%)	109 (92%)	9 (8%)	0	100	100
24	p	168/176 (96%)	153 (91%)	15 (9%)	0	100	100
All	All	3763/4813 (78%)	3556 (94%)	203 (5%)	4 (0%)	49	75

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	N	109	ALA
17	i	124	PRO
22	n	156	PRO
4	L	518	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 PDB entries followed by that with respect to all EM entries.

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	D	33/395 (8%)	33 (100%)	0	100	100
2	J	127/138 (92%)	125 (98%)	2 (2%)	55	72
3	K	87/88 (99%)	87 (100%)	0	100	100
4	L	549/550 (100%)	547 (100%)	2 (0%)	84	84
5	M	414/415 (100%)	413 (100%)	1 (0%)	87	88
6	N	307/308 (100%)	306 (100%)	1 (0%)	86	86
7	O	283/309 (92%)	283 (100%)	0	100	100
8	U	78/135 (58%)	78 (100%)	0	100	100
9	X	23/154 (15%)	23 (100%)	0	100	100
10	Y	104/107 (97%)	104 (100%)	0	100	100
11	c	41/67 (61%)	41 (100%)	0	100	100
12	d	106/107 (99%)	106 (100%)	0	100	100
13	e	91/94 (97%)	90 (99%)	1 (1%)	65	76
14	f	51/53 (96%)	51 (100%)	0	100	100
15	g	93/129 (72%)	93 (100%)	0	100	100
16	h	121/162 (75%)	121 (100%)	0	100	100
17	i	89/120 (74%)	88 (99%)	1 (1%)	65	76
18	j	61/87 (70%)	61 (100%)	0	100	100
19	k	54/78 (69%)	54 (100%)	0	100	100
20	l	142/161 (88%)	142 (100%)	0	100	100
21	m	112/114 (98%)	112 (100%)	0	100	100
22	n	163/164 (99%)	163 (100%)	0	100	100
23	o	110/121 (91%)	110 (100%)	0	100	100
24	p	154/158 (98%)	154 (100%)	0	100	100
All	All	3393/4214 (80%)	3385 (100%)	8 (0%)	85	88

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	J	60	LEU
2	J	65	VAL
4	L	3	ILE
4	L	69	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	M	218	LYS
6	N	105	LYS
13	e	91	LYS
17	i	72	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (95) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	36	GLN
1	D	38	GLN
2	J	3	ASN
2	J	107	ASN
3	K	7	ASN
4	L	2	ASN
4	L	25	ASN
4	L	102	GLN
4	L	135	ASN
4	L	136	ASN
4	L	139	GLN
4	L	170	GLN
4	L	192	ASN
4	L	194	ASN
4	L	199	GLN
4	L	209	ASN
4	L	264	HIS
4	L	269	ASN
4	L	296	ASN
4	L	321	GLN
4	L	354	GLN
4	L	400	ASN
4	L	452	ASN
4	L	572	ASN
4	L	579	ASN
5	M	26	ASN
5	M	44	GLN
5	M	51	ASN
5	M	81	GLN
5	M	92	GLN
5	M	170	HIS
5	M	175	ASN
5	M	213	HIS
5	M	279	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	M	293	HIS
5	M	304	GLN
5	M	415	GLN
6	N	112	HIS
6	N	120	GLN
6	N	150	ASN
6	N	204	ASN
6	N	273	ASN
6	N	289	ASN
6	N	317	GLN
6	N	342	GLN
7	O	54	HIS
7	O	85	HIS
7	O	132	GLN
7	O	175	ASN
7	O	225	HIS
7	O	239	ASN
7	O	286	GLN
7	O	292	HIS
7	O	299	GLN
7	O	306	ASN
7	O	323	GLN
8	U	101	ASN
9	X	151	ASN
10	Y	19	GLN
10	Y	21	HIS
10	Y	91	ASN
12	d	59	HIS
12	d	61	GLN
12	d	79	GLN
13	e	34	HIS
14	f	10	HIS
14	f	13	HIS
15	g	52	GLN
16	h	109	HIS
16	h	154	GLN
16	h	170	GLN
16	h	181	HIS
17	i	83	HIS
18	j	83	HIS
19	k	39	GLN
19	k	66	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	l	31	HIS
20	l	83	GLN
20	l	91	GLN
20	l	106	HIS
20	l	154	GLN
21	m	75	ASN
21	m	79	ASN
22	n	13	GLN
22	n	14	GLN
22	n	26	HIS
22	n	33	HIS
22	n	53	ASN
22	n	62	GLN
22	n	74	ASN
22	n	139	GLN
23	o	85	HIS
24	p	91	GLN
24	p	104	ASN
24	p	124	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

18 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
25	3PE	M	502	-	50,50,50	0.89	2 (4%)	53,55,55	1.16	4 (7%)
26	CDL	X	201	-	66,66,99	1.09	4 (6%)	72,78,111	1.27	6 (8%)
26	CDL	L	706	-	85,85,99	0.99	4 (4%)	91,97,111	1.14	7 (7%)
25	3PE	L	704	-	46,46,50	0.95	2 (4%)	49,51,55	1.09	3 (6%)
25	3PE	Y	201	-	39,39,50	1.02	2 (5%)	42,44,55	1.15	3 (7%)
26	CDL	h	201	-	69,69,99	1.09	4 (5%)	75,81,111	1.23	6 (8%)
25	3PE	M	503	-	50,50,50	0.93	2 (4%)	53,55,55	1.13	3 (5%)
27	ADP	O	402	-	28,29,29	1.42	4 (14%)	43,45,45	1.86	10 (23%)
25	3PE	L	703	-	50,50,50	0.90	2 (4%)	53,55,55	1.13	3 (5%)
25	3PE	L	701	-	41,41,50	0.99	2 (4%)	44,46,55	1.04	2 (4%)
25	3PE	L	707	-	44,44,50	0.96	2 (4%)	47,49,55	1.09	3 (6%)
26	CDL	L	705	-	76,76,99	1.02	5 (6%)	82,88,111	1.19	6 (7%)
25	3PE	O	401	-	30,30,50	1.17	2 (6%)	33,35,55	1.29	5 (15%)
28	EHZ	n	201	-	29,31,37	1.80	7 (24%)	37,41,47	1.93	12 (32%)
25	3PE	M	501	-	50,50,50	0.91	2 (4%)	53,55,55	1.12	5 (9%)
25	3PE	N	401	-	36,36,50	1.06	2 (5%)	39,41,55	1.20	5 (12%)
25	3PE	L	702	-	39,39,50	1.04	2 (5%)	42,44,55	1.12	5 (11%)
25	3PE	J	201	-	45,45,50	0.96	2 (4%)	48,50,55	1.07	3 (6%)

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
25	3PE	M	502	-	-	13/54/54/54	-
26	CDL	X	201	-	-	24/77/77/110	-
26	CDL	L	706	-	-	26/96/96/110	-
25	3PE	L	704	-	-	13/50/50/54	-
25	3PE	Y	201	-	-	5/43/43/54	-
26	CDL	h	201	-	-	24/80/80/110	-
25	3PE	M	503	-	-	18/54/54/54	-
27	ADP	O	402	-	-	3/16/32/32	0/3/3/3
25	3PE	L	703	-	-	14/54/54/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	3PE	L	701	-	-	11/45/45/54	-
25	3PE	L	707	-	-	11/48/48/54	-
26	CDL	L	705	-	-	23/87/87/110	-
25	3PE	O	401	-	-	9/34/34/54	-
28	EHZ	n	201	-	-	21/39/39/45	-
25	3PE	M	501	-	-	15/54/54/54	-
25	3PE	N	401	-	-	8/40/40/54	-
25	3PE	L	702	-	-	7/43/43/54	-
25	3PE	J	201	-	-	12/49/49/54	-

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	n	201	EHZ	C15-N2	5.00	1.45	1.33
28	n	201	EHZ	C12-N1	4.98	1.45	1.33
27	O	402	ADP	C5-C4	4.70	1.47	1.39
25	M	503	3PE	O31-C31	4.32	1.45	1.33
25	J	201	3PE	O31-C31	4.27	1.45	1.33
26	L	706	CDL	OB8-CB7	4.27	1.45	1.33
26	L	705	CDL	OB8-CB7	4.25	1.45	1.33
25	L	702	3PE	O31-C31	4.25	1.45	1.33
25	Y	201	3PE	O31-C31	4.23	1.45	1.33
25	M	501	3PE	O31-C31	4.19	1.45	1.33
25	L	704	3PE	O31-C31	4.19	1.45	1.33
26	L	706	CDL	OA8-CA7	4.19	1.45	1.33
26	X	201	CDL	OB6-CB5	4.17	1.46	1.34
25	L	707	3PE	O31-C31	4.17	1.45	1.33
25	O	401	3PE	O31-C31	4.15	1.45	1.33
25	M	502	3PE	O31-C31	4.15	1.45	1.33
25	L	701	3PE	O31-C31	4.14	1.45	1.33
26	h	201	CDL	OA8-CA7	4.12	1.45	1.33
26	h	201	CDL	OB8-CB7	4.12	1.45	1.33
26	L	705	CDL	OA8-CA7	4.12	1.45	1.33
26	L	706	CDL	OB6-CB5	4.12	1.45	1.34
25	L	701	3PE	O21-C21	4.10	1.45	1.34
26	X	201	CDL	OB8-CB7	4.09	1.45	1.33
26	L	706	CDL	OA6-CA5	4.08	1.45	1.34
25	N	401	3PE	O21-C21	4.08	1.45	1.34
25	N	401	3PE	O31-C31	4.08	1.45	1.33
26	h	201	CDL	OB6-CB5	4.08	1.45	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	M	503	3PE	O21-C21	4.06	1.45	1.34
26	X	201	CDL	OA8-CA7	4.06	1.45	1.33
25	L	702	3PE	O21-C21	4.05	1.45	1.34
25	L	703	3PE	O21-C21	4.03	1.45	1.34
25	L	704	3PE	O21-C21	4.02	1.45	1.34
26	h	201	CDL	OA6-CA5	4.02	1.45	1.34
25	L	703	3PE	O31-C31	4.01	1.45	1.33
25	J	201	3PE	O21-C21	3.99	1.45	1.34
25	O	401	3PE	O21-C21	3.99	1.45	1.34
26	L	705	CDL	OB6-CB5	3.98	1.45	1.34
25	M	501	3PE	O21-C21	3.95	1.45	1.34
25	L	707	3PE	O21-C21	3.94	1.45	1.34
25	Y	201	3PE	O21-C21	3.93	1.45	1.34
26	X	201	CDL	OA6-CA5	3.90	1.45	1.34
25	M	502	3PE	O21-C21	3.86	1.45	1.34
26	L	705	CDL	OA6-CA5	3.73	1.44	1.34
27	O	402	ADP	C5-C6	2.74	1.48	1.41
28	n	201	EHZ	P1-O7	2.66	1.64	1.54
28	n	201	EHZ	O4-C15	-2.53	1.18	1.23
28	n	201	EHZ	O3-C12	-2.43	1.18	1.23
28	n	201	EHZ	C9-S1	2.40	1.81	1.76
28	n	201	EHZ	P1-OP3	-2.34	1.46	1.54
27	O	402	ADP	C5-N7	-2.29	1.34	1.39
27	O	402	ADP	C8-N7	2.19	1.35	1.31
26	L	705	CDL	OA6-CA4	-2.02	1.41	1.46

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	n	201	EHZ	C8-C9-S1	6.23	121.43	113.56
27	O	402	ADP	C5-C4-N3	-6.05	118.39	126.72
26	X	201	CDL	OA6-CA5-C11	5.00	122.30	111.48
27	O	402	ADP	N3-C4-N9	4.73	135.21	127.17
25	M	503	3PE	O21-C21-C22	4.49	121.20	111.48
26	h	201	CDL	OB6-CB5-C51	4.45	121.11	111.48
25	N	401	3PE	O21-C21-C22	4.36	120.92	111.48
25	M	502	3PE	O21-C21-C22	4.36	120.91	111.48
25	L	703	3PE	O21-C21-C22	4.35	120.89	111.48
25	O	401	3PE	O21-C21-C22	4.31	120.80	111.48
26	X	201	CDL	OB6-CB5-C51	4.22	120.61	111.48
26	L	706	CDL	OA6-CA5-C11	4.20	120.56	111.48
26	L	706	CDL	OB6-CB5-C51	4.19	120.55	111.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	J	201	3PE	O21-C21-C22	4.00	120.14	111.48
26	h	201	CDL	OA6-CA5-C11	3.95	120.03	111.48
25	M	501	3PE	O21-C21-C22	3.85	119.82	111.48
26	X	201	CDL	CA4-OA6-CA5	-3.81	108.67	117.80
27	O	402	ADP	C2-N3-C4	3.76	121.01	111.83
25	L	704	3PE	O21-C21-C22	3.74	119.58	111.48
25	Y	201	3PE	O21-C21-C22	3.74	119.58	111.48
25	L	707	3PE	O21-C21-C22	3.63	119.34	111.48
25	L	701	3PE	O21-C21-C22	3.62	119.30	111.48
27	O	402	ADP	C4-C5-N7	-3.59	106.48	110.58
25	L	702	3PE	O21-C21-C22	3.58	119.22	111.48
26	L	705	CDL	OA6-CA5-C11	3.58	119.22	111.48
26	L	705	CDL	CA4-OA6-CA5	-3.51	109.40	117.80
25	M	502	3PE	C2-O21-C21	-3.42	109.60	117.80
26	L	705	CDL	OB6-CB5-C51	3.38	118.79	111.48
28	n	201	EHZ	O2-C9-C8	-3.22	118.67	123.74
27	O	402	ADP	N3-C2-N1	-3.22	123.71	128.58
25	M	501	3PE	O31-C31-C32	3.20	121.58	111.83
26	L	705	CDL	OB8-CB7-C71	3.19	121.55	111.83
25	M	503	3PE	O31-C31-C32	3.13	121.38	111.83
25	L	702	3PE	O31-C31-C32	3.13	121.37	111.83
28	n	201	EHZ	C14-C13-C12	-3.05	107.31	112.39
25	O	401	3PE	O31-C31-C32	3.02	121.04	111.83
28	n	201	EHZ	OP3-P1-O9	-2.95	99.35	110.83
25	N	401	3PE	O31-C31-C32	2.95	120.82	111.83
25	M	501	3PE	C2-O21-C21	-2.94	110.76	117.80
28	n	201	EHZ	C7-C8-C9	-2.93	107.33	113.86
26	L	706	CDL	OB8-CB7-C71	2.92	120.73	111.83
26	h	201	CDL	OB8-CB7-C71	2.91	120.72	111.83
26	L	706	CDL	OA8-CA7-C31	2.91	120.69	111.83
28	n	201	EHZ	C13-C12-N1	2.89	121.62	116.34
25	Y	201	3PE	O31-C31-C32	2.84	120.49	111.83
25	L	703	3PE	O31-C31-C32	2.83	120.47	111.83
25	J	201	3PE	C2-O21-C21	-2.83	111.03	117.80
25	L	701	3PE	O31-C31-C32	2.79	120.34	111.83
25	L	704	3PE	O31-C31-C32	2.76	120.26	111.83
25	Y	201	3PE	C2-O21-C21	-2.70	111.32	117.80
26	L	705	CDL	OA8-CA7-C31	2.70	120.07	111.83
26	X	201	CDL	OA8-CA7-C31	2.70	120.06	111.83
26	h	201	CDL	CA4-OA6-CA5	-2.68	111.38	117.80
25	L	707	3PE	C2-O21-C21	-2.66	111.43	117.80
25	L	704	3PE	C2-O21-C21	-2.62	111.53	117.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	h	201	CDL	OA8-CA7-C31	2.59	119.73	111.83
26	h	201	CDL	CB4-OB6-CB5	-2.58	111.62	117.80
25	M	502	3PE	O31-C31-C32	2.53	119.54	111.83
27	O	402	ADP	C5-N7-C8	2.51	107.40	103.45
27	O	402	ADP	C3'-C2'-C1'	2.48	106.15	101.46
26	X	201	CDL	OA6-CA5-OA7	-2.42	118.05	123.70
26	L	706	CDL	CB4-OB6-CB5	-2.42	112.01	117.80
28	n	201	EHZ	C5-C6-C7	-2.42	108.02	114.68
25	J	201	3PE	O31-C31-C32	2.39	119.13	111.83
28	n	201	EHZ	C10-S1-C9	2.39	108.91	101.84
27	O	402	ADP	C4-N9-C8	2.39	108.25	105.74
27	O	402	ADP	O4'-C1'-N9	2.35	112.59	108.09
25	L	703	3PE	O21-C21-O22	-2.34	118.24	123.70
25	L	707	3PE	O31-C31-C32	2.33	118.95	111.83
25	M	502	3PE	O21-C21-O22	-2.33	118.26	123.70
25	N	401	3PE	C2-O21-C21	-2.31	112.26	117.80
26	X	201	CDL	OB8-CB7-C71	2.31	118.87	111.83
25	O	401	3PE	C2-O21-C21	-2.22	112.47	117.80
25	M	503	3PE	O21-C21-O22	-2.20	118.56	123.70
28	n	201	EHZ	O6-P1-O9	2.19	112.36	106.44
28	n	201	EHZ	O2-C9-S1	-2.18	119.91	122.68
25	L	702	3PE	O21-C21-O22	-2.16	118.66	123.70
25	N	401	3PE	O31-C31-O32	-2.13	118.30	123.63
28	n	201	EHZ	C11-N1-C12	-2.13	118.86	122.82
25	L	702	3PE	C2-O21-C21	-2.12	112.72	117.80
25	M	501	3PE	O21-C21-O22	-2.12	118.76	123.70
28	n	201	EHZ	O3-C12-N1	-2.04	119.02	123.03
26	L	706	CDL	OB6-CB5-OB7	-2.04	118.93	123.70
25	L	702	3PE	O31-C31-O32	-2.02	118.56	123.63
27	O	402	ADP	C6-C5-N7	2.02	135.99	132.09
26	L	706	CDL	CA4-OA6-CA5	-2.02	112.95	117.80
26	L	705	CDL	OB8-CB7-OB9	-2.02	118.58	123.63
25	O	401	3PE	O31-C31-O32	-2.01	118.59	123.63
25	M	501	3PE	O31-C31-O32	-2.01	118.60	123.63
25	N	401	3PE	O21-C21-O22	-2.01	119.01	123.70
25	O	401	3PE	O21-C21-O22	-2.00	119.02	123.70

There are no chirality outliers.

All (257) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	J	201	3PE	C11-O13-P-O11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	L	701	3PE	C1-O11-P-O12
25	L	701	3PE	C1-O11-P-O13
25	L	701	3PE	C1-O11-P-O14
25	L	702	3PE	C11-O13-P-O11
25	L	702	3PE	C11-O13-P-O14
25	L	703	3PE	C1-O11-P-O13
25	L	703	3PE	C1-O11-P-O14
25	L	703	3PE	O22-C21-O21-C2
25	L	703	3PE	C22-C21-O21-C2
25	L	704	3PE	C1-O11-P-O12
25	L	704	3PE	C1-O11-P-O13
25	L	707	3PE	C11-O13-P-O11
25	L	707	3PE	C11-O13-P-O12
25	M	501	3PE	C1-O11-P-O12
25	M	501	3PE	C1-O11-P-O13
25	M	501	3PE	C1-O11-P-O14
25	M	501	3PE	C11-O13-P-O11
25	M	501	3PE	C11-O13-P-O12
25	M	501	3PE	C11-O13-P-O14
25	M	502	3PE	C11-O13-P-O12
25	M	502	3PE	C11-O13-P-O14
25	M	503	3PE	C1-O11-P-O12
25	M	503	3PE	C1-O11-P-O13
25	M	503	3PE	C1-O11-P-O14
25	M	503	3PE	C11-O13-P-O11
25	M	503	3PE	C11-O13-P-O12
25	M	503	3PE	C11-O13-P-O14
25	M	503	3PE	C22-C21-O21-C2
25	N	401	3PE	C11-O13-P-O11
25	N	401	3PE	C11-O13-P-O12
25	N	401	3PE	C11-O13-P-O14
25	O	401	3PE	C11-O13-P-O12
25	O	401	3PE	C11-O13-P-O14
25	O	401	3PE	C22-C21-O21-C2
26	L	705	CDL	CA2-OA2-PA1-OA3
26	L	705	CDL	CA2-OA2-PA1-OA4
26	L	705	CDL	CA2-OA2-PA1-OA5
26	L	705	CDL	CA3-OA5-PA1-OA2
26	L	705	CDL	CA3-OA5-PA1-OA3
26	L	705	CDL	C11-CA5-OA6-CA4
26	L	705	CDL	C51-CB5-OB6-CB4
26	L	706	CDL	CA2-OA2-PA1-OA4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	L	706	CDL	CA3-OA5-PA1-OA4
26	L	706	CDL	C11-CA5-OA6-CA4
26	L	706	CDL	CB2-OB2-PB2-OB4
26	L	706	CDL	CB2-OB2-PB2-OB5
26	L	706	CDL	OB7-CB5-OB6-CB4
26	L	706	CDL	C51-CB5-OB6-CB4
26	X	201	CDL	CA3-OA5-PA1-OA2
26	X	201	CDL	CB2-OB2-PB2-OB3
26	X	201	CDL	CB3-OB5-PB2-OB2
26	X	201	CDL	CB3-OB5-PB2-OB3
26	X	201	CDL	CB3-OB5-PB2-OB4
26	X	201	CDL	C51-CB5-OB6-CB4
26	X	201	CDL	OB9-CB7-OB8-CB6
26	X	201	CDL	C71-CB7-OB8-CB6
26	h	201	CDL	CA2-OA2-PA1-OA3
26	h	201	CDL	CA2-OA2-PA1-OA4
26	h	201	CDL	CA2-OA2-PA1-OA5
26	h	201	CDL	CA3-OA5-PA1-OA2
26	h	201	CDL	CA3-OA5-PA1-OA4
26	h	201	CDL	CB2-OB2-PB2-OB3
26	h	201	CDL	CB3-OB5-PB2-OB3
26	h	201	CDL	C51-CB5-OB6-CB4
27	O	402	ADP	C5'-O5'-PA-O2A
27	O	402	ADP	C5'-O5'-PA-O3A
28	n	201	EHZ	O1-C7-C8-C9
28	n	201	EHZ	C6-C7-C8-C9
28	n	201	EHZ	S1-C10-C11-N1
28	n	201	EHZ	C16-C17-C20-O6
28	n	201	EHZ	C20-O6-P1-O7
28	n	201	EHZ	C20-O6-P1-O9
28	n	201	EHZ	C20-O6-P1-OP3
25	O	401	3PE	O32-C31-O31-C3
25	O	401	3PE	C32-C31-O31-C3
26	L	705	CDL	OA9-CA7-OA8-CA6
25	M	503	3PE	O22-C21-O21-C2
25	O	401	3PE	O22-C21-O21-C2
26	L	705	CDL	OA7-CA5-OA6-CA4
26	L	705	CDL	OB7-CB5-OB6-CB4
26	L	706	CDL	OA7-CA5-OA6-CA4
26	X	201	CDL	OB7-CB5-OB6-CB4
26	h	201	CDL	OB7-CB5-OB6-CB4
25	M	502	3PE	C32-C31-O31-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	J	201	3PE	C22-C21-O21-C2
26	L	705	CDL	C31-CA7-OA8-CA6
26	X	201	CDL	C31-CA7-OA8-CA6
25	Y	201	3PE	O32-C31-O31-C3
25	Y	201	3PE	C32-C31-O31-C3
25	M	502	3PE	O32-C31-O31-C3
26	X	201	CDL	OA9-CA7-OA8-CA6
25	J	201	3PE	O22-C21-O21-C2
26	h	201	CDL	CA4-CA3-OA5-PA1
26	h	201	CDL	C71-CB7-OB8-CB6
25	Y	201	3PE	C23-C24-C25-C26
26	L	705	CDL	C13-C14-C15-C16
25	L	703	3PE	C32-C31-O31-C3
25	M	501	3PE	C22-C21-O21-C2
26	h	201	CDL	OB9-CB7-OB8-CB6
25	M	501	3PE	O22-C21-O21-C2
26	X	201	CDL	CB6-CB4-OB6-CB5
25	L	703	3PE	O32-C31-O31-C3
25	L	703	3PE	C24-C25-C26-C27
26	h	201	CDL	C18-C19-C20-C21
26	X	201	CDL	C61-C62-C63-C64
25	L	702	3PE	C22-C21-O21-C2
25	M	501	3PE	C23-C24-C25-C26
26	X	201	CDL	C11-CA5-OA6-CA4
26	L	706	CDL	CB5-C51-C52-C53
25	M	503	3PE	C39-C3A-C3B-C3C
26	X	201	CDL	OA7-CA5-OA6-CA4
25	L	704	3PE	C31-C32-C33-C34
25	L	707	3PE	C32-C31-O31-C3
25	L	704	3PE	C27-C28-C29-C2A
25	L	702	3PE	O22-C21-O21-C2
25	M	501	3PE	C3C-C3D-C3E-C3F
26	L	706	CDL	C31-CA7-OA8-CA6
26	L	705	CDL	C56-C57-C58-C59
26	L	705	CDL	CB6-CB4-OB6-CB5
25	Y	201	3PE	C2A-C2B-C2C-C2D
26	L	706	CDL	C72-C73-C74-C75
25	N	401	3PE	C37-C38-C39-C3A
25	L	704	3PE	C38-C39-C3A-C3B
25	J	201	3PE	C32-C31-O31-C3
25	M	503	3PE	C2C-C2D-C2E-C2F
28	n	201	EHZ	N2-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	L	707	3PE	O32-C31-O31-C3
26	L	706	CDL	OA9-CA7-OA8-CA6
25	M	503	3PE	C2D-C2E-C2F-C2G
25	N	401	3PE	C32-C33-C34-C35
25	J	201	3PE	O21-C2-C3-O31
27	O	402	ADP	PB-O3A-PA-O5'
28	n	201	EHZ	C3-C4-C5-C6
25	N	401	3PE	C32-C31-O31-C3
26	h	201	CDL	C14-C15-C16-C17
25	L	704	3PE	C22-C21-O21-C2
26	h	201	CDL	CB3-CB4-OB6-CB5
25	J	201	3PE	O32-C31-O31-C3
25	L	703	3PE	C28-C29-C2A-C2B
25	J	201	3PE	C22-C23-C24-C25
25	J	201	3PE	C12-C11-O13-P
25	M	502	3PE	C12-C11-O13-P
25	L	701	3PE	O21-C2-C3-O31
25	J	201	3PE	C25-C26-C27-C28
26	L	705	CDL	C16-C17-C18-C19
25	L	704	3PE	C22-C23-C24-C25
25	N	401	3PE	O32-C31-O31-C3
28	n	201	EHZ	O4-C15-C16-O5
25	L	704	3PE	O22-C21-O21-C2
28	n	201	EHZ	C18-C17-C20-O6
28	n	201	EHZ	C19-C17-C20-O6
25	L	701	3PE	C24-C25-C26-C27
25	L	701	3PE	C2-C1-O11-P
26	L	705	CDL	CA4-CA3-OA5-PA1
26	h	201	CDL	CB4-CB3-OB5-PB2
28	n	201	EHZ	C11-C10-S1-C9
26	X	201	CDL	C59-C60-C61-C62
25	L	703	3PE	C34-C35-C36-C37
26	L	705	CDL	C77-C78-C79-C80
25	L	701	3PE	C1-C2-C3-O31
25	J	201	3PE	C11-O13-P-O14
25	L	702	3PE	C1-O11-P-O14
25	L	702	3PE	C11-O13-P-O12
25	L	703	3PE	C1-O11-P-O12
25	L	704	3PE	C1-O11-P-O14
25	L	707	3PE	C11-O13-P-O14
25	M	502	3PE	C11-O13-P-O11
25	M	502	3PE	O13-C11-C12-N

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	O	401	3PE	C11-O13-P-O11
26	L	705	CDL	CA3-OA5-PA1-OA4
26	L	706	CDL	CA2-OA2-PA1-OA3
26	L	706	CDL	CA2-OA2-PA1-OA5
26	L	706	CDL	CB2-OB2-PB2-OB3
26	X	201	CDL	CA2-OA2-PA1-OA4
26	X	201	CDL	CA3-OA5-PA1-OA3
26	h	201	CDL	CA3-OA5-PA1-OA3
26	h	201	CDL	CB2-OB2-PB2-OB5
26	h	201	CDL	CB3-OB5-PB2-OB2
26	h	201	CDL	CB3-OB5-PB2-OB4
26	L	706	CDL	C56-C57-C58-C59
26	L	705	CDL	C1-CA2-OA2-PA1
28	n	201	EHZ	C5-C6-C7-O1
26	L	706	CDL	C71-CB7-OB8-CB6
25	L	703	3PE	C3C-C3D-C3E-C3F
25	M	503	3PE	C32-C31-O31-C3
25	L	707	3PE	C22-C21-O21-C2
25	M	503	3PE	O32-C31-O31-C3
25	L	707	3PE	C36-C37-C38-C39
25	O	401	3PE	C32-C33-C34-C35
25	J	201	3PE	C1-C2-C3-O31
25	M	503	3PE	C26-C27-C28-C29
26	L	706	CDL	OB9-CB7-OB8-CB6
26	L	705	CDL	C33-C34-C35-C36
25	L	704	3PE	C29-C2A-C2B-C2C
26	L	706	CDL	C1-CA2-OA2-PA1
28	n	201	EHZ	C2-C3-C4-C5
25	M	503	3PE	C21-C22-C23-C24
25	M	501	3PE	O11-C1-C2-O21
26	L	705	CDL	OB9-CB7-OB8-CB6
25	L	707	3PE	O21-C2-C3-O31
25	L	704	3PE	C32-C33-C34-C35
25	M	501	3PE	C2B-C2C-C2D-C2E
25	O	401	3PE	C2-C1-O11-P
25	M	502	3PE	C34-C35-C36-C37
26	L	706	CDL	C74-C75-C76-C77
25	J	201	3PE	C28-C29-C2A-C2B
28	n	201	EHZ	N2-C15-C16-O5
25	M	503	3PE	C38-C39-C3A-C3B
25	L	701	3PE	C3-C2-O21-C21
25	L	707	3PE	O22-C21-O21-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	L	706	CDL	CB4-CB3-OB5-PB2
28	n	201	EHZ	O2-C9-S1-C10
26	L	705	CDL	C71-CB7-OB8-CB6
25	L	702	3PE	C38-C39-C3A-C3B
25	Y	201	3PE	C27-C28-C29-C2A
26	h	201	CDL	C31-CA7-OA8-CA6
26	X	201	CDL	CB4-CB3-OB5-PB2
25	M	502	3PE	C25-C26-C27-C28
25	L	707	3PE	C1-C2-C3-O31
25	M	501	3PE	C26-C27-C28-C29
26	h	201	CDL	OA9-CA7-OA8-CA6
25	M	501	3PE	O11-C1-C2-C3
25	L	703	3PE	C3D-C3E-C3F-C3G
25	L	701	3PE	C36-C37-C38-C39
25	M	503	3PE	C33-C34-C35-C36
25	N	401	3PE	C33-C34-C35-C36
26	L	706	CDL	C34-C35-C36-C37
28	n	201	EHZ	C15-C16-C17-C18
26	L	706	CDL	C19-C20-C21-C22
26	L	706	CDL	C55-C56-C57-C58
25	L	701	3PE	C32-C31-O31-C3
26	X	201	CDL	OA6-CA4-CA6-OA8
25	M	502	3PE	O21-C21-C22-C23
25	L	704	3PE	C2-C1-O11-P
28	n	201	EHZ	O5-C16-C17-C18
26	L	706	CDL	C52-C51-CB5-OB6
26	X	201	CDL	C12-C11-CA5-OA6
25	M	502	3PE	C22-C21-O21-C2
25	L	701	3PE	O32-C31-O31-C3
25	L	707	3PE	C39-C3A-C3B-C3C
28	n	201	EHZ	O4-C15-C16-C17
25	M	502	3PE	C39-C3A-C3B-C3C
25	L	703	3PE	C39-C3A-C3B-C3C
25	M	501	3PE	C39-C3A-C3B-C3C
26	X	201	CDL	C52-C51-CB5-OB6
28	n	201	EHZ	C15-C16-C17-C20
26	L	705	CDL	C20-C21-C22-C23
26	X	201	CDL	C12-C11-CA5-OA7
25	M	502	3PE	O22-C21-C22-C23
26	L	706	CDL	C52-C51-CB5-OB7
25	M	503	3PE	C3C-C3D-C3E-C3F
25	L	703	3PE	C2B-C2C-C2D-C2E

Continued on next page...

Continued from previous page...

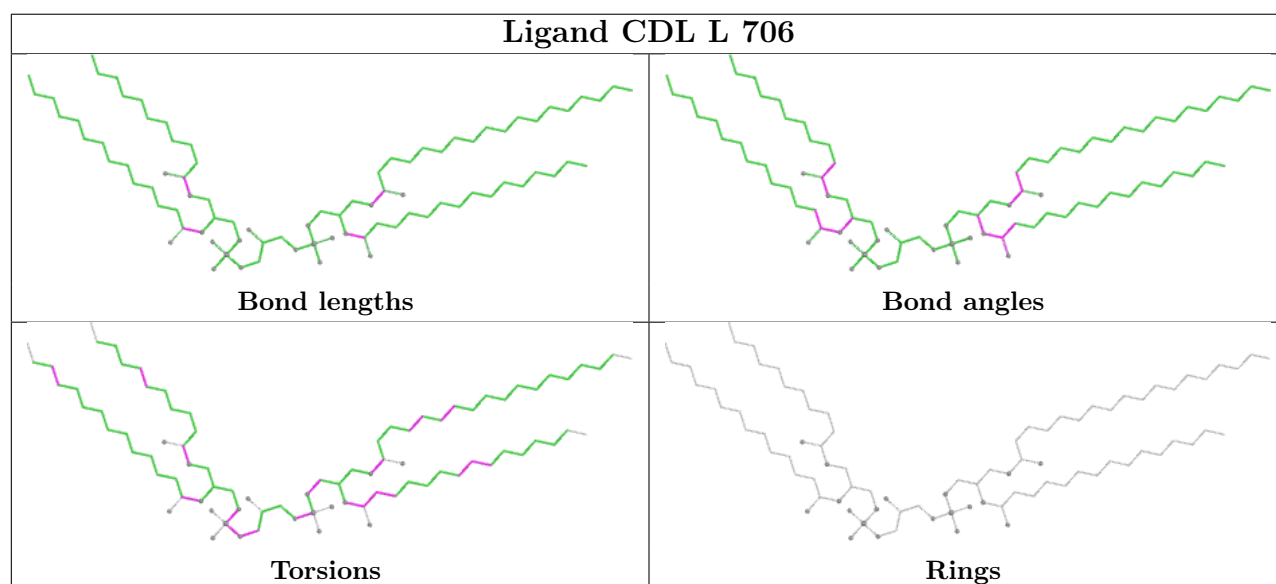
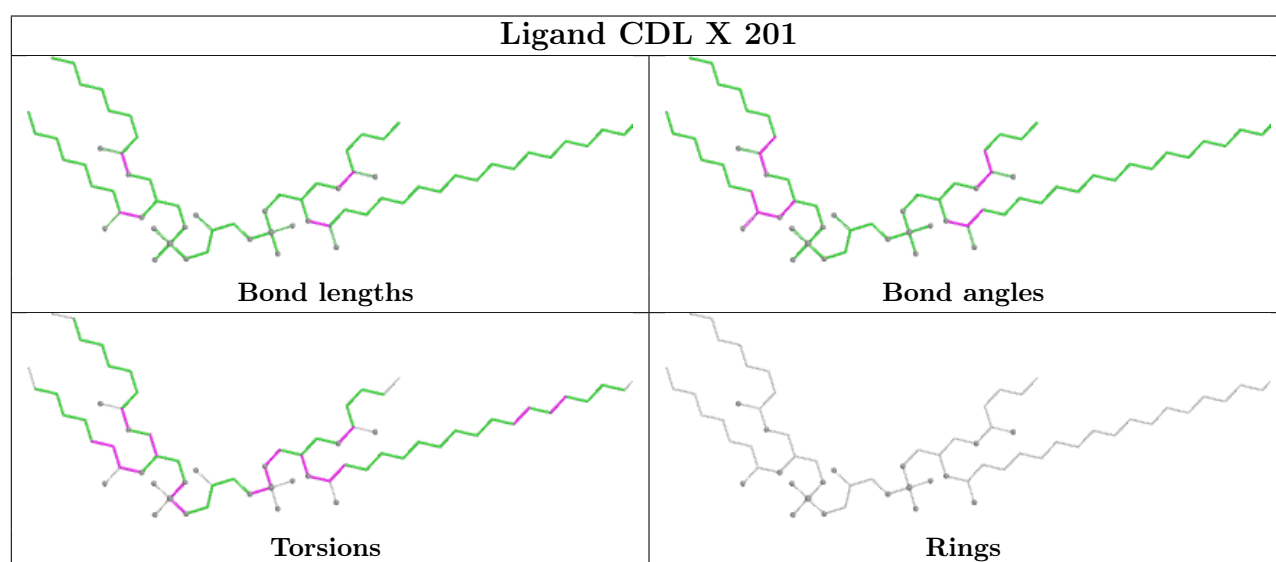
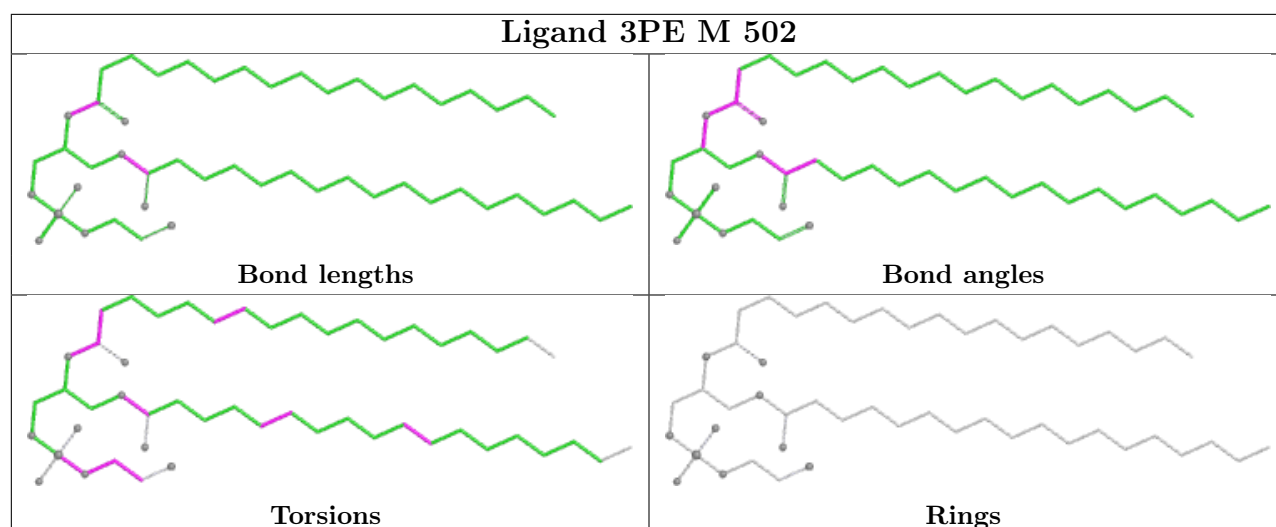
Mol	Chain	Res	Type	Atoms
26	h	201	CDL	C72-C71-CB7-OB8
25	L	704	3PE	C2B-C2C-C2D-C2E
26	h	201	CDL	C11-C12-C13-C14
26	X	201	CDL	CA5-C11-C12-C13

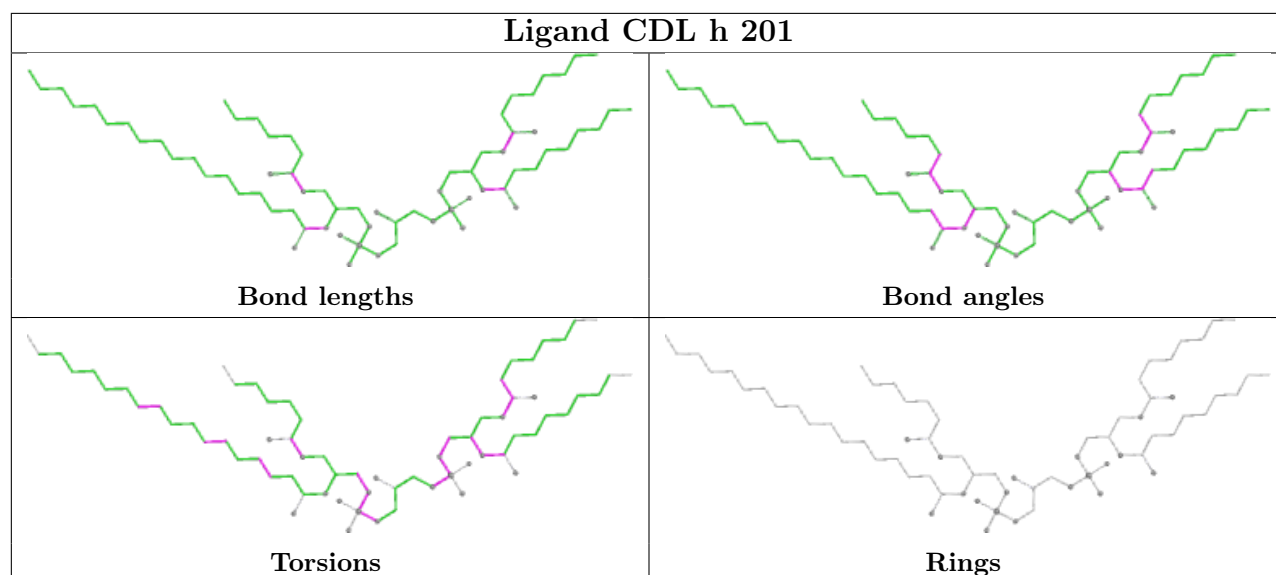
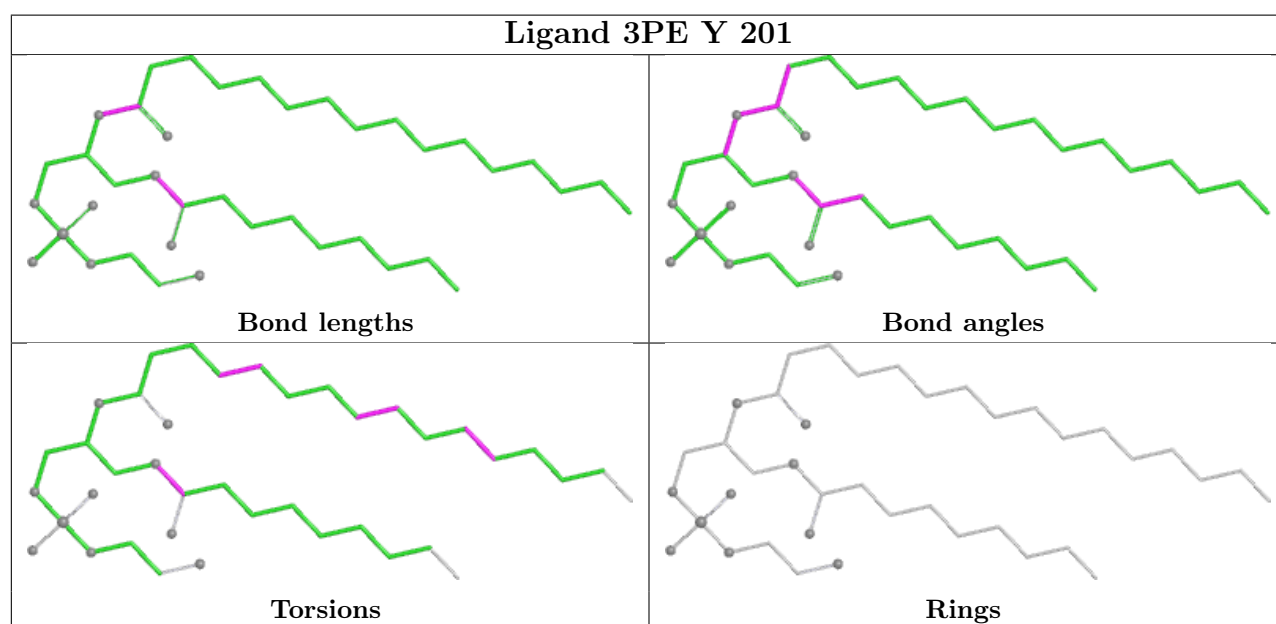
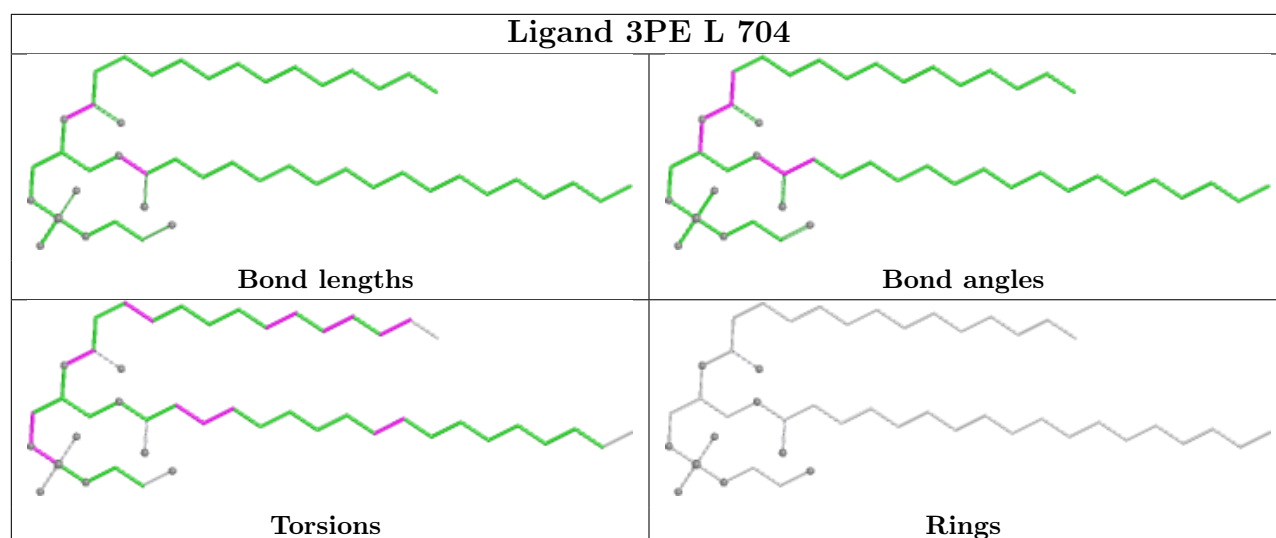
There are no ring outliers.

17 monomers are involved in 184 short contacts:

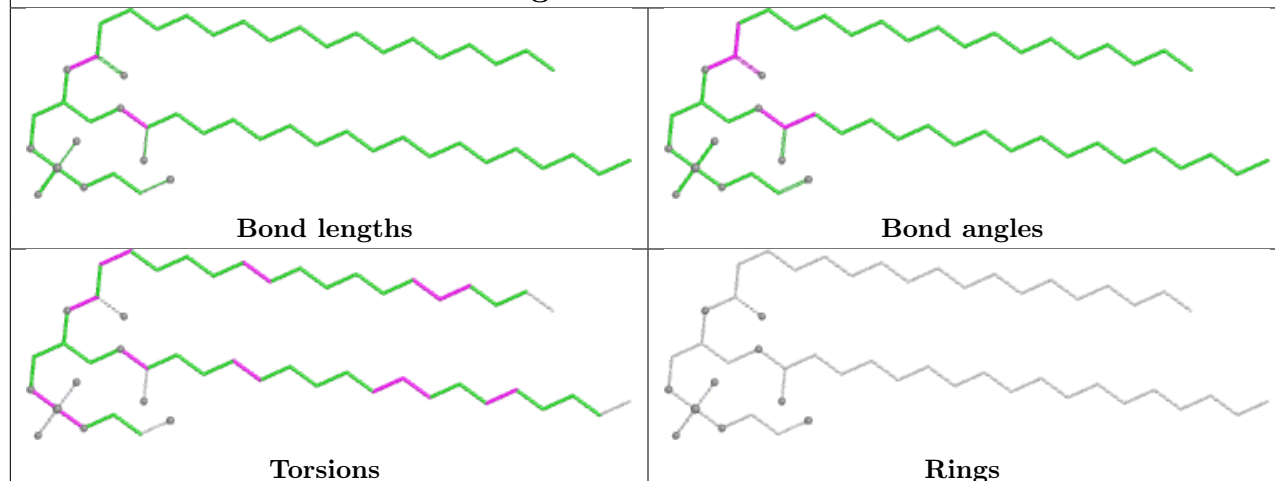
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	M	502	3PE	14	0
26	X	201	CDL	9	0
26	L	706	CDL	19	0
25	L	704	3PE	8	0
25	Y	201	3PE	20	0
26	h	201	CDL	15	0
25	M	503	3PE	6	0
27	O	402	ADP	6	0
25	L	703	3PE	10	0
25	L	701	3PE	23	0
25	L	707	3PE	10	0
26	L	705	CDL	19	0
25	O	401	3PE	5	0
25	M	501	3PE	6	0
25	N	401	3PE	14	0
25	L	702	3PE	6	0
25	J	201	3PE	5	0

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

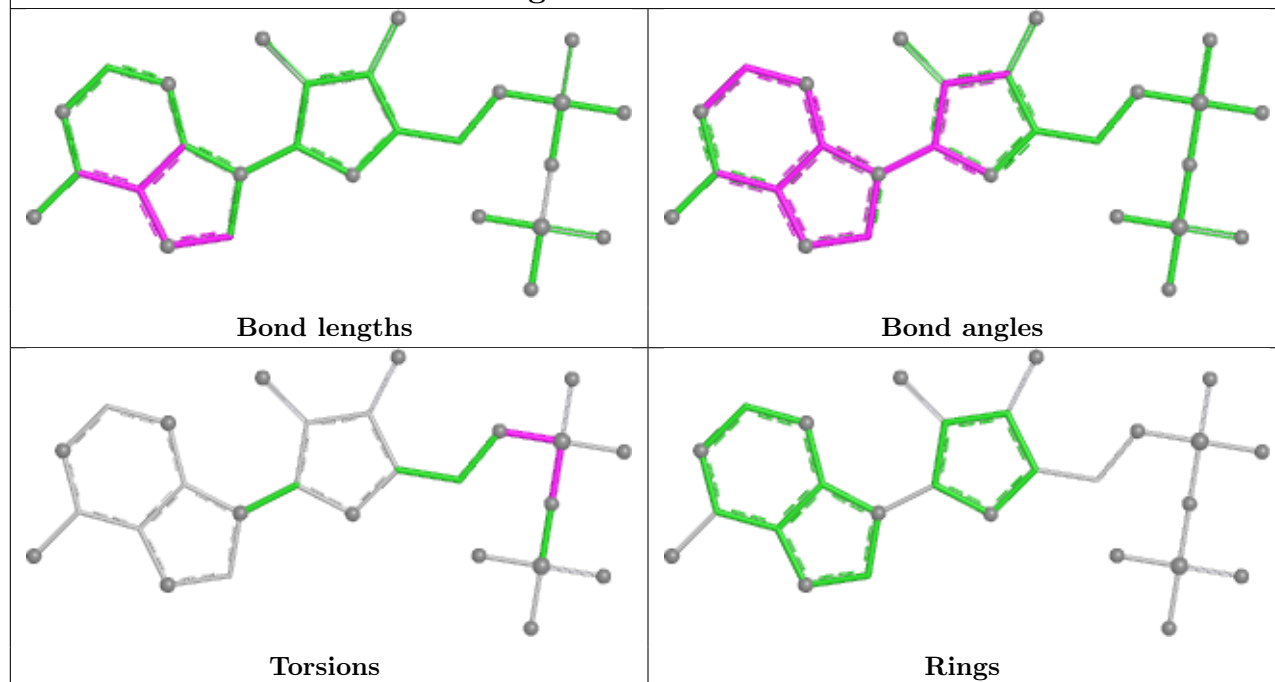




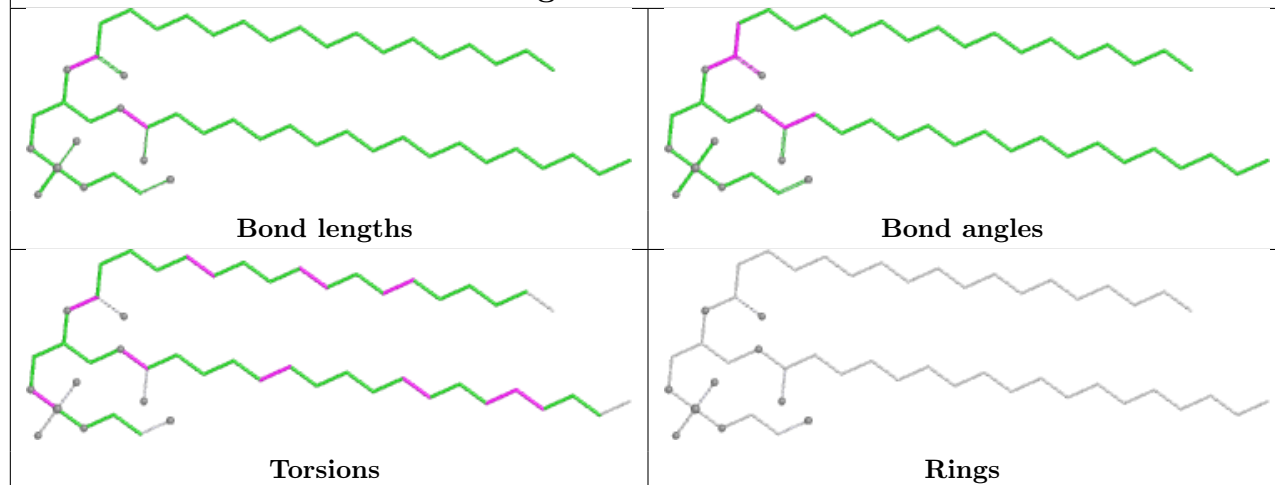
Ligand 3PE M 503

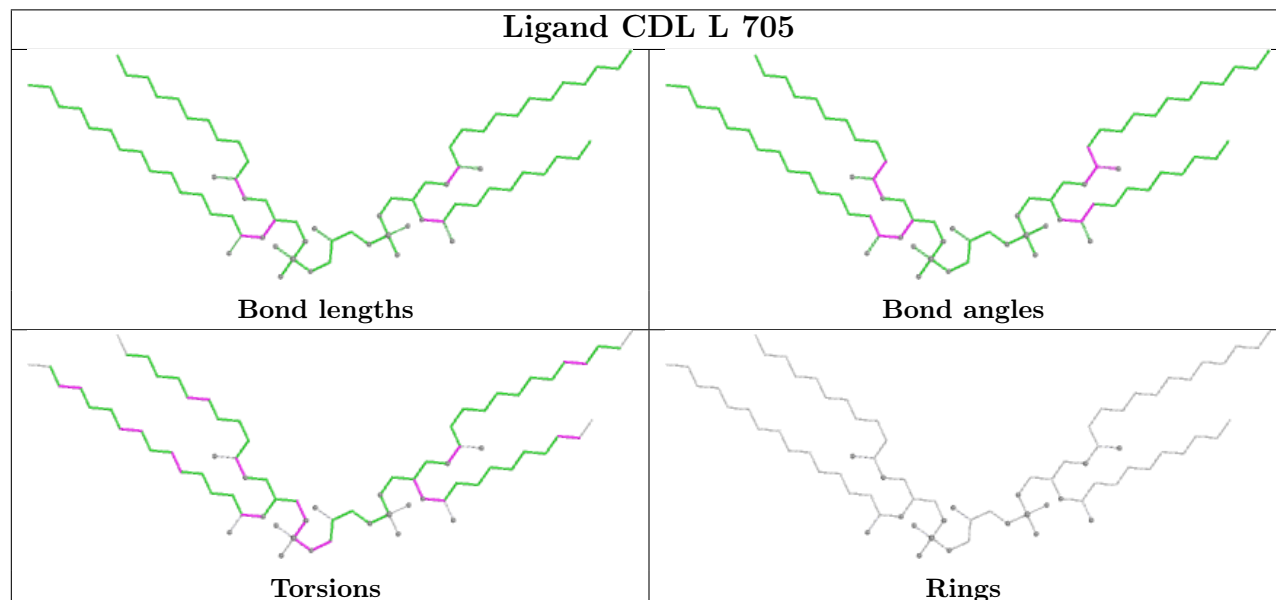
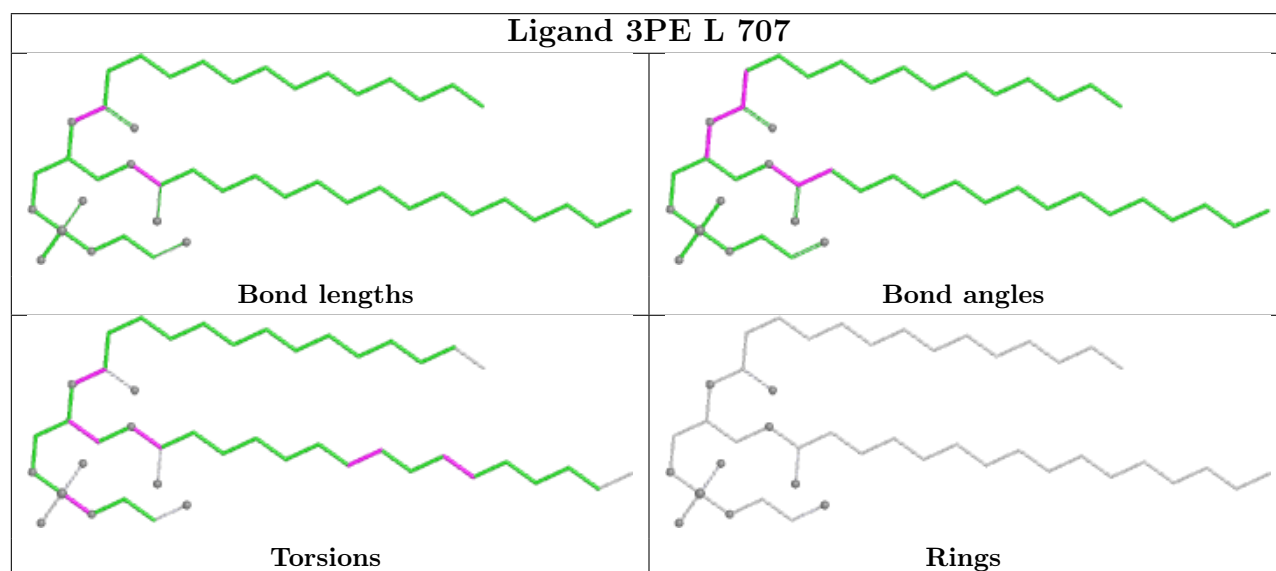
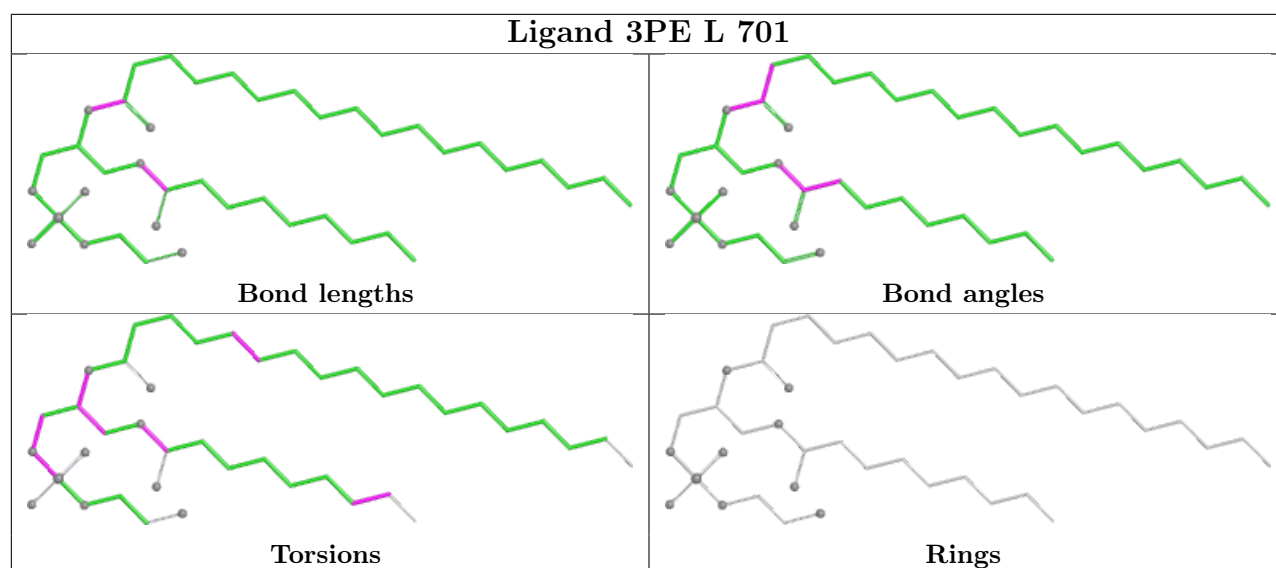


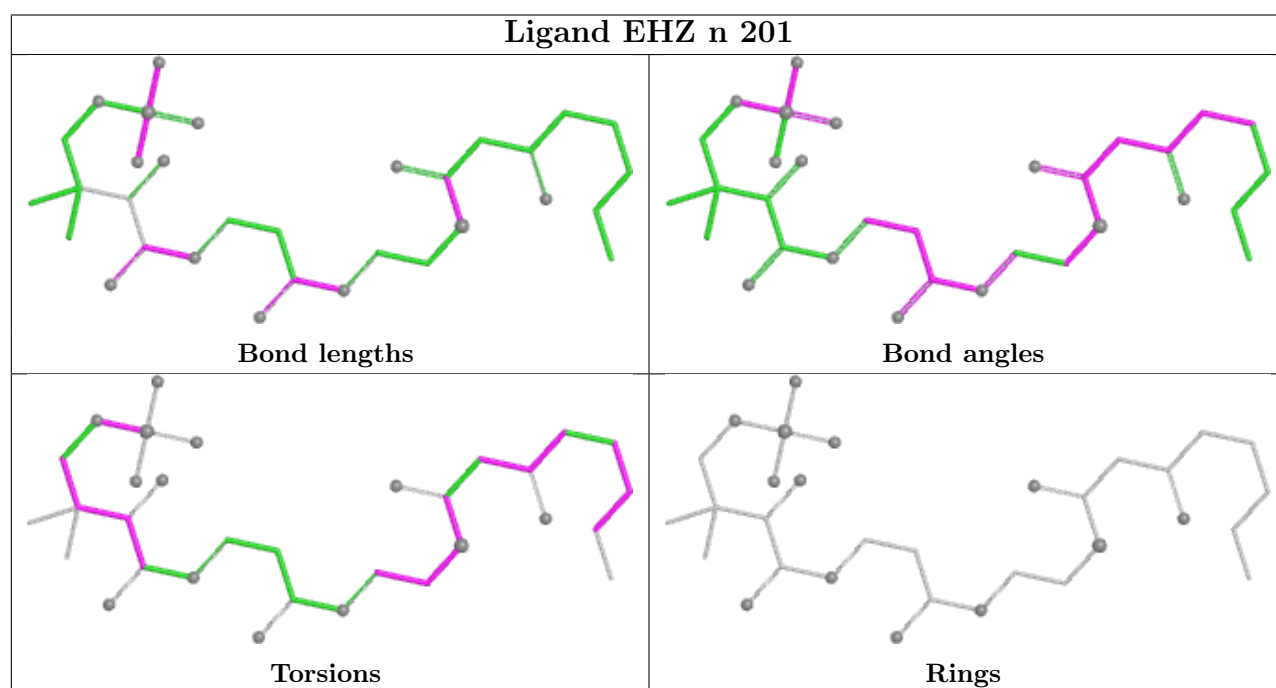
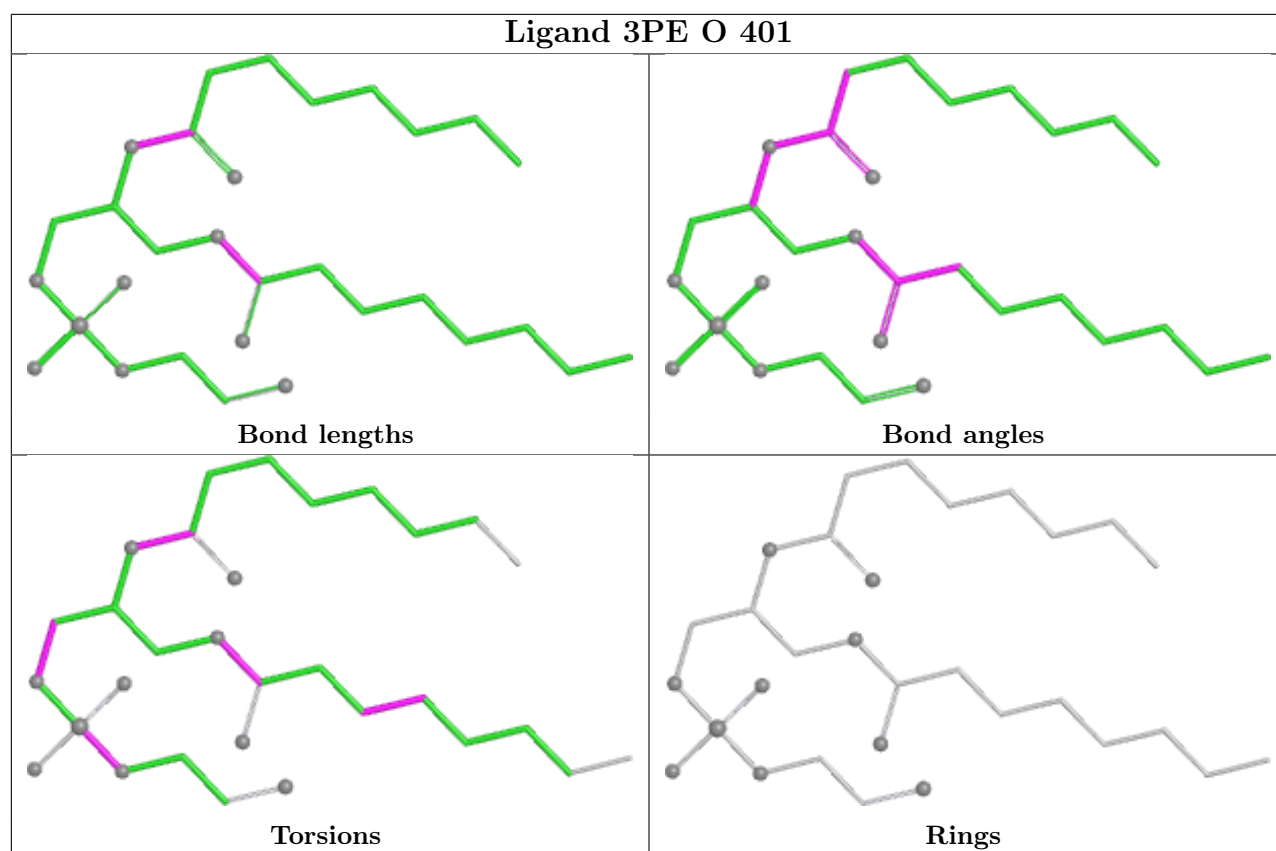
Ligand ADP O 402

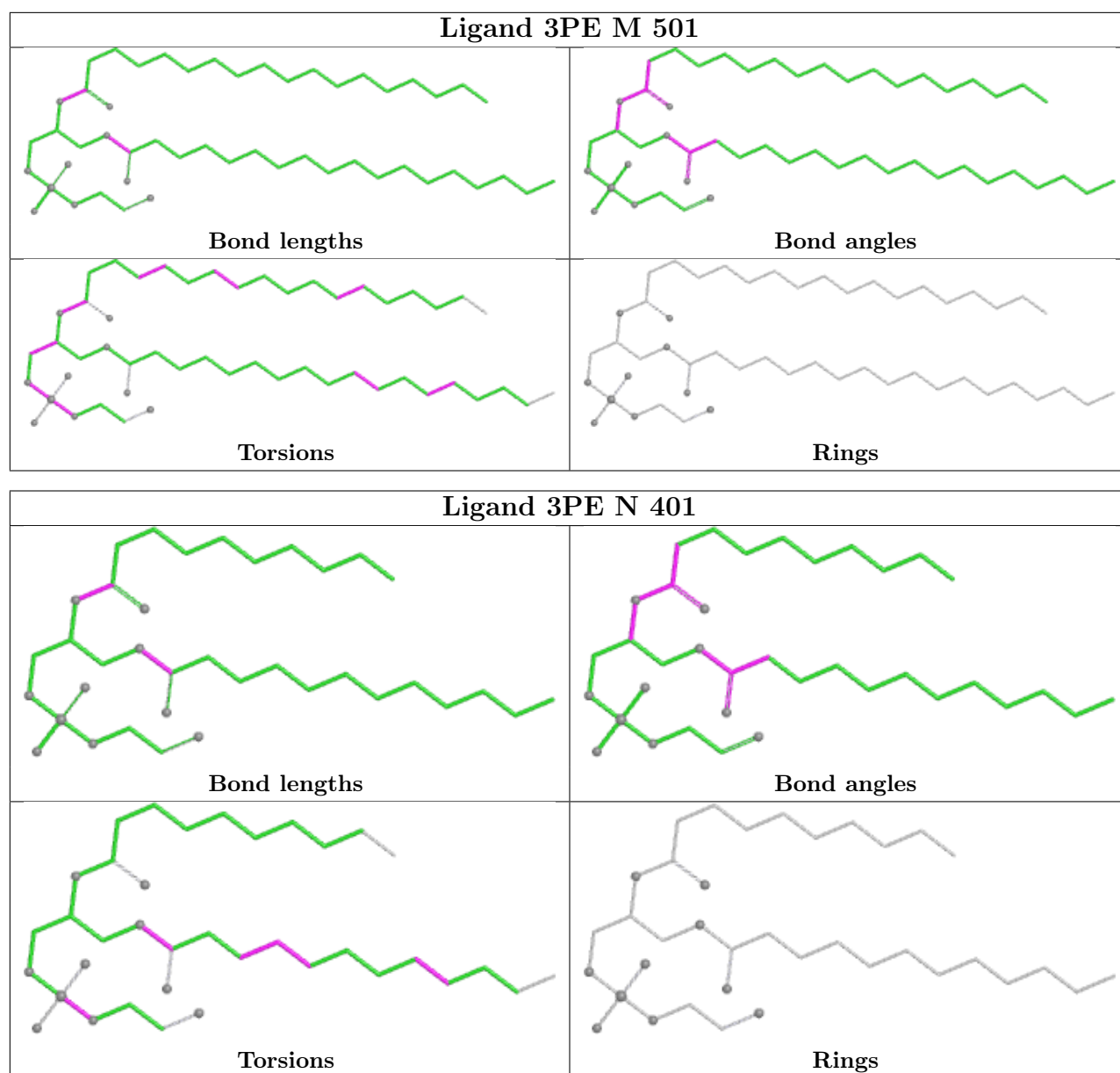


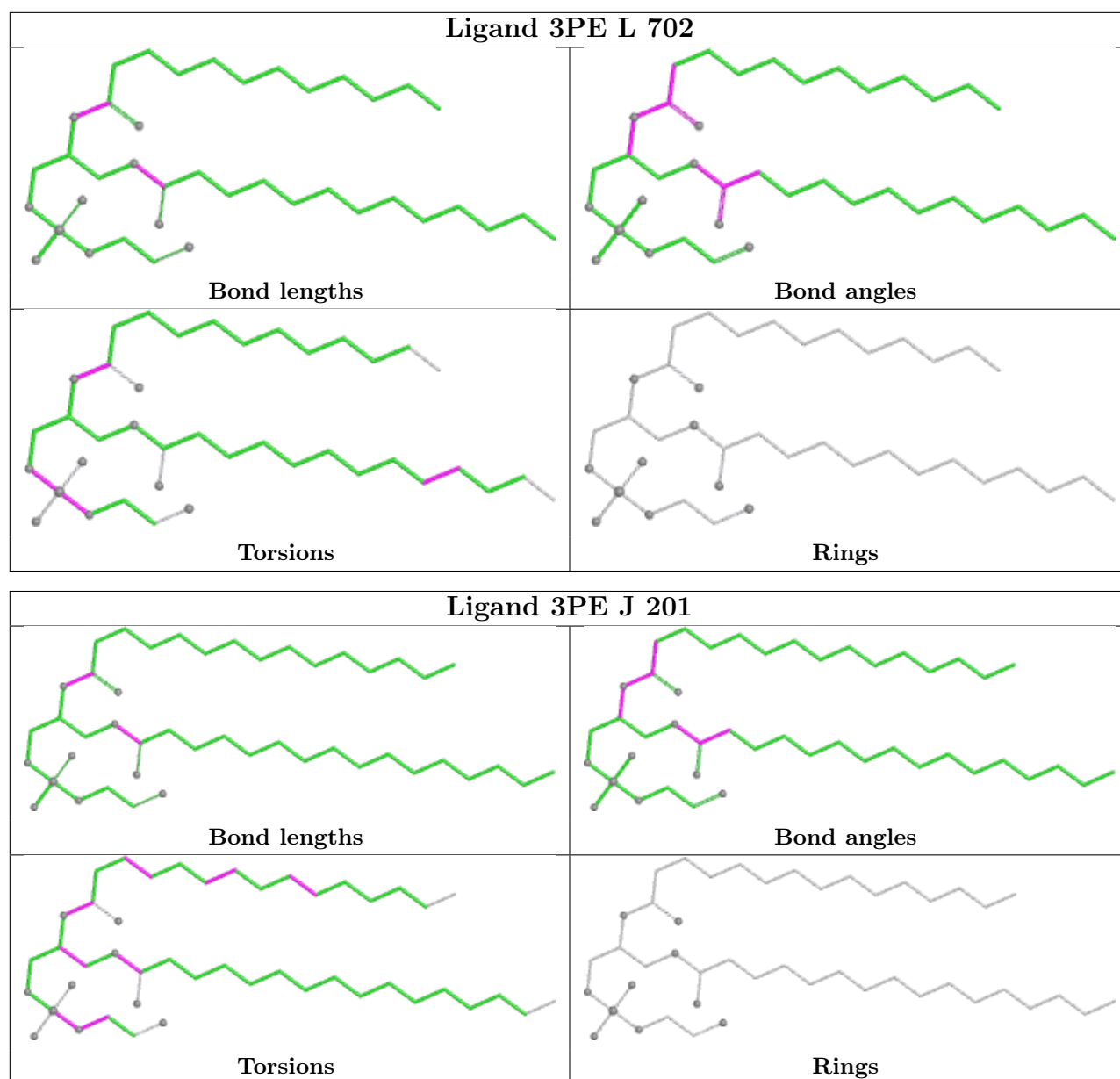
Ligand 3PE L 703











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.

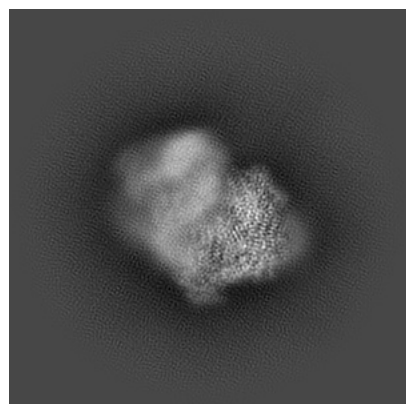
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35333. These allow visual inspection of the internal detail of the map and identification of artifacts.

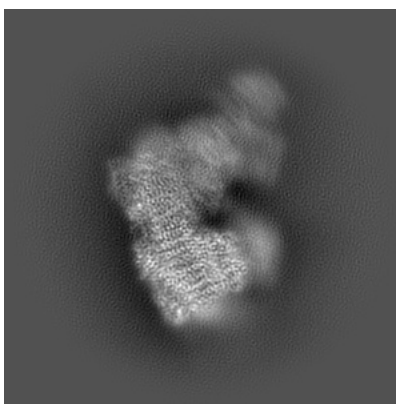
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

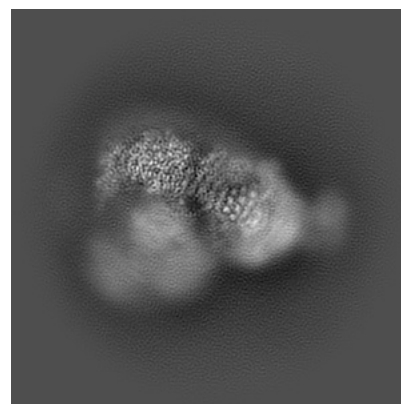
6.1.1 Primary map



X

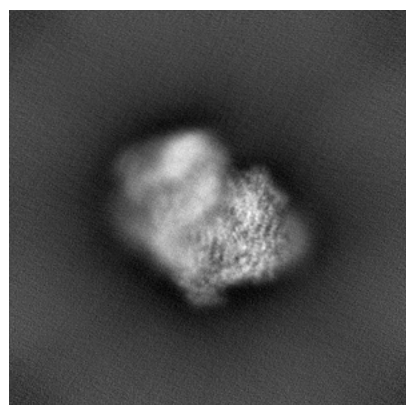


Y

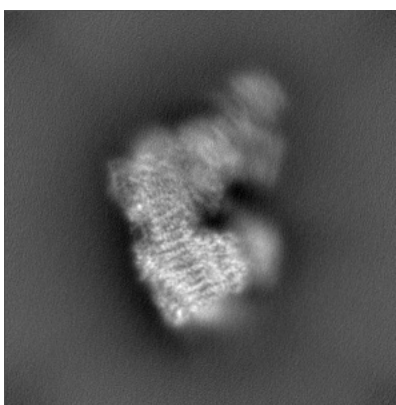


Z

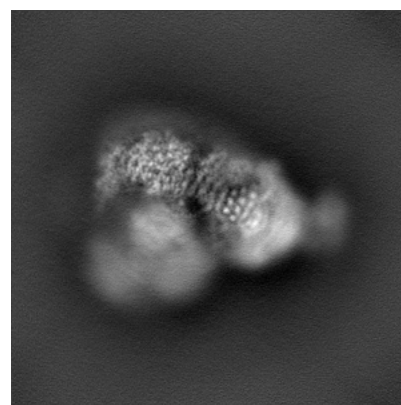
6.1.2 Raw map



X



Y

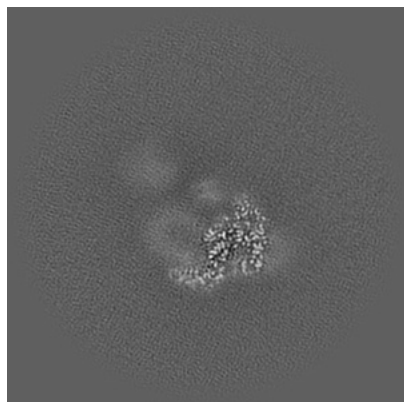


Z

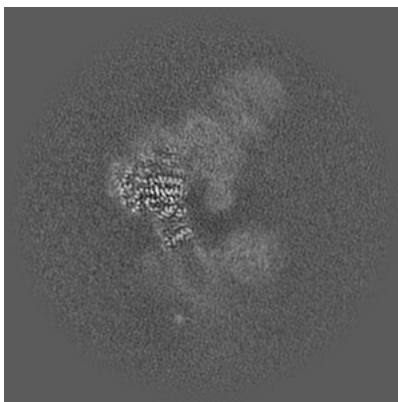
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

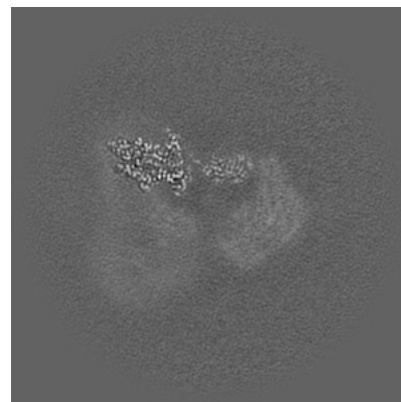
6.2.1 Primary map



X Index: 192

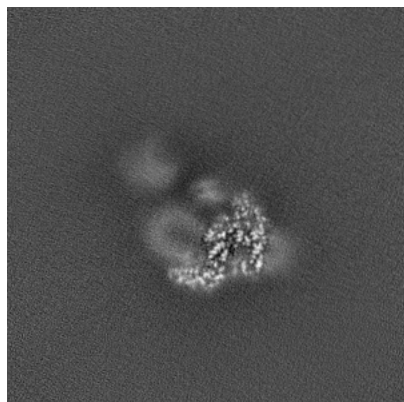


Y Index: 192



Z Index: 192

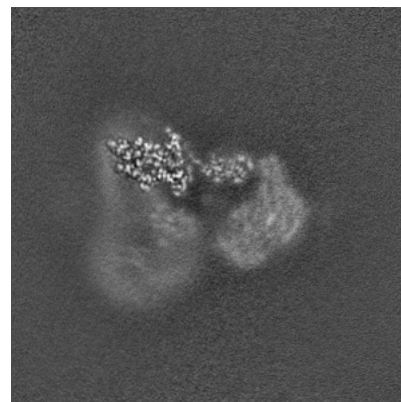
6.2.2 Raw map



X Index: 192



Y Index: 192

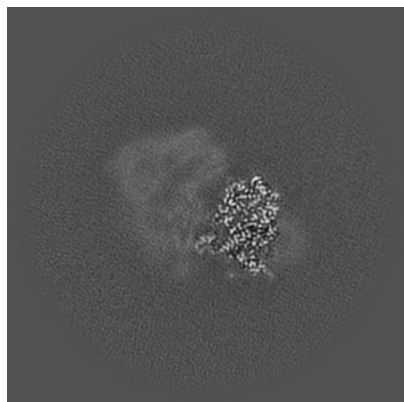


Z Index: 192

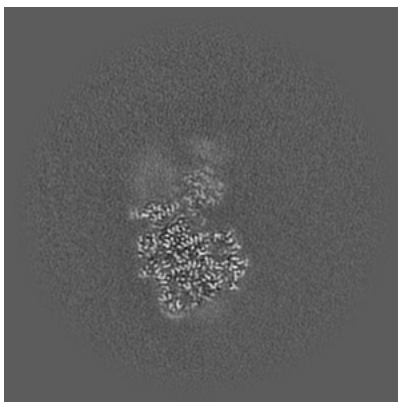
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

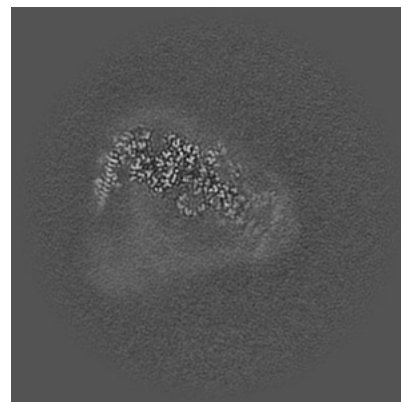
6.3.1 Primary map



X Index: 159

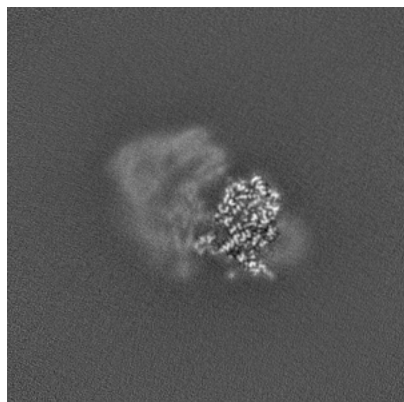


Y Index: 236

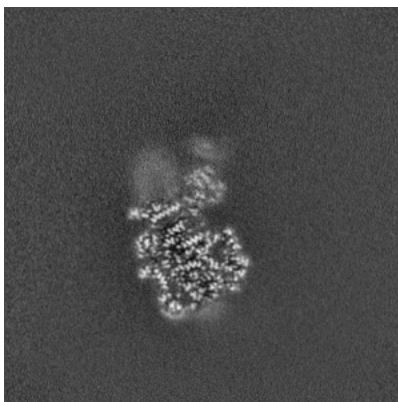


Z Index: 166

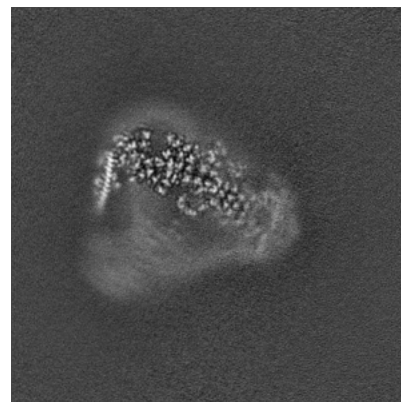
6.3.2 Raw map



X Index: 159



Y Index: 237

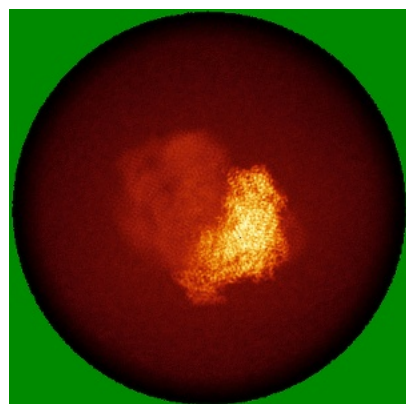


Z Index: 167

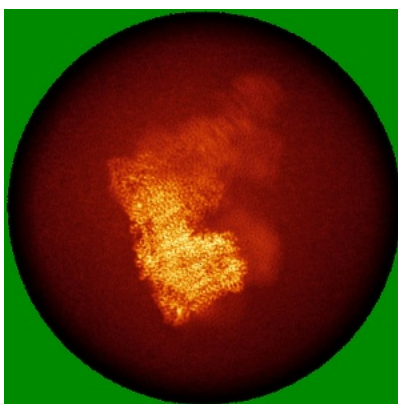
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

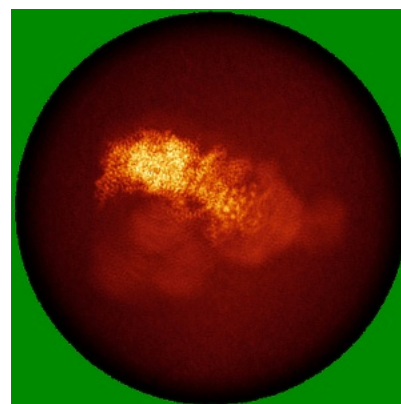
6.4.1 Primary map



X

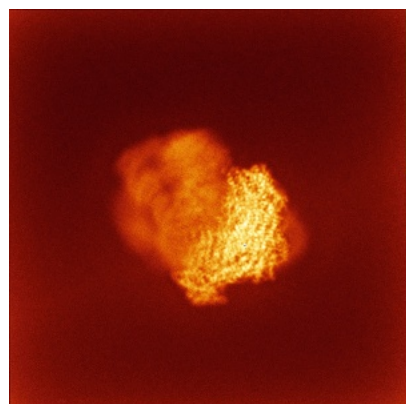


Y

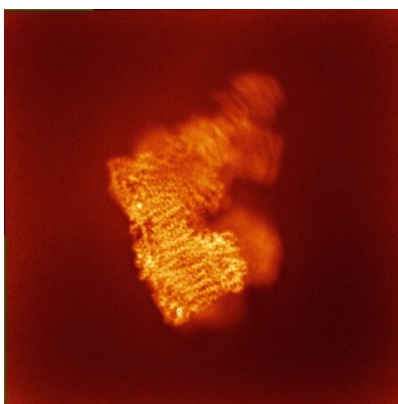


Z

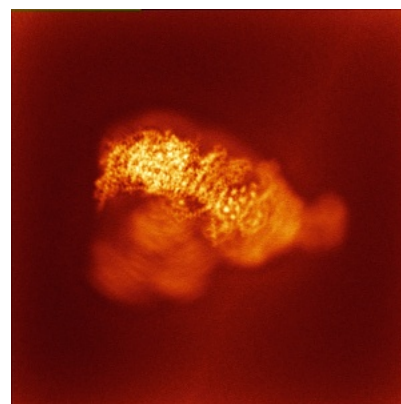
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

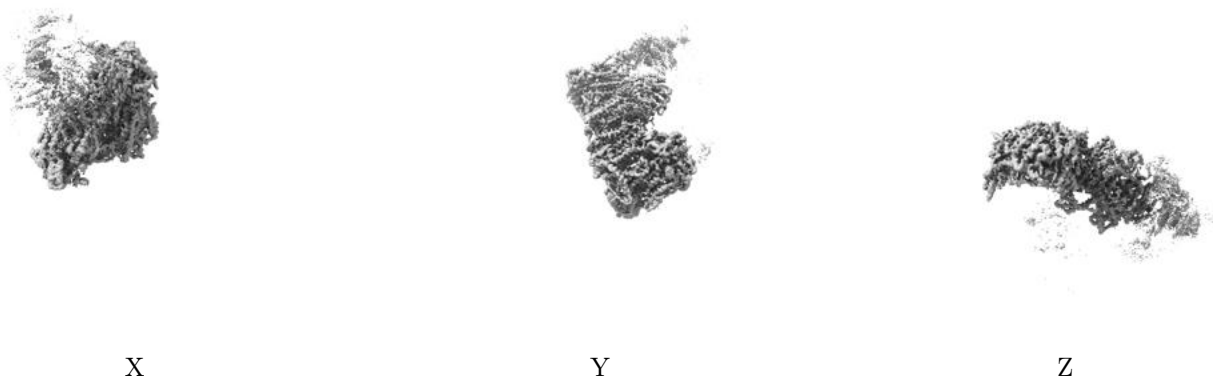
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.55. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

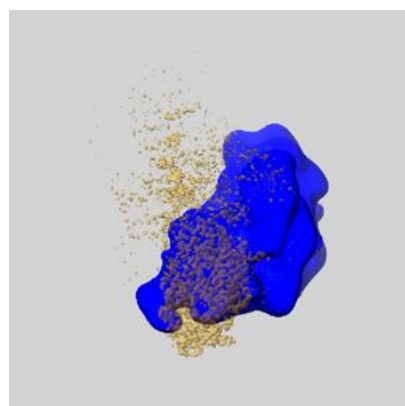
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

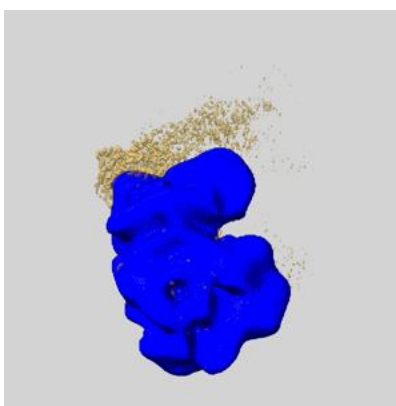
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

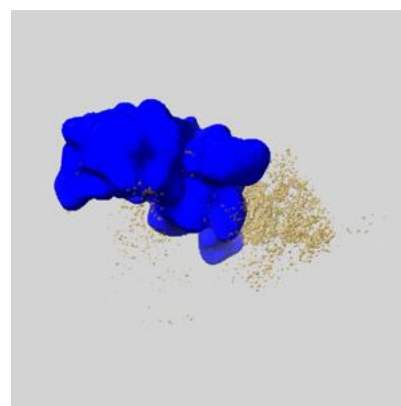
6.6.1 emd_35333_msk_1.map [i](#)



X



Y

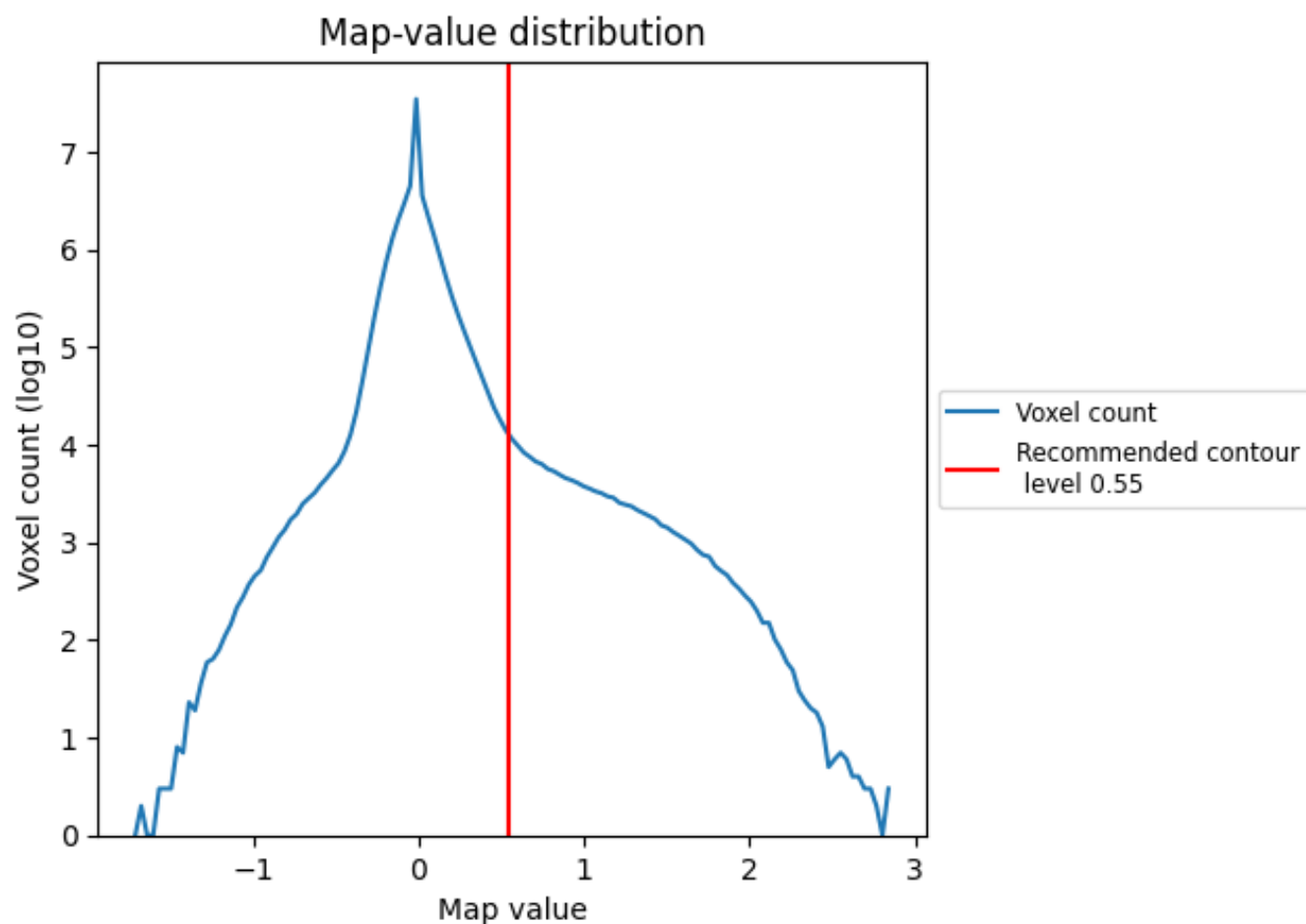


Z

7 Map analysis [i](#)

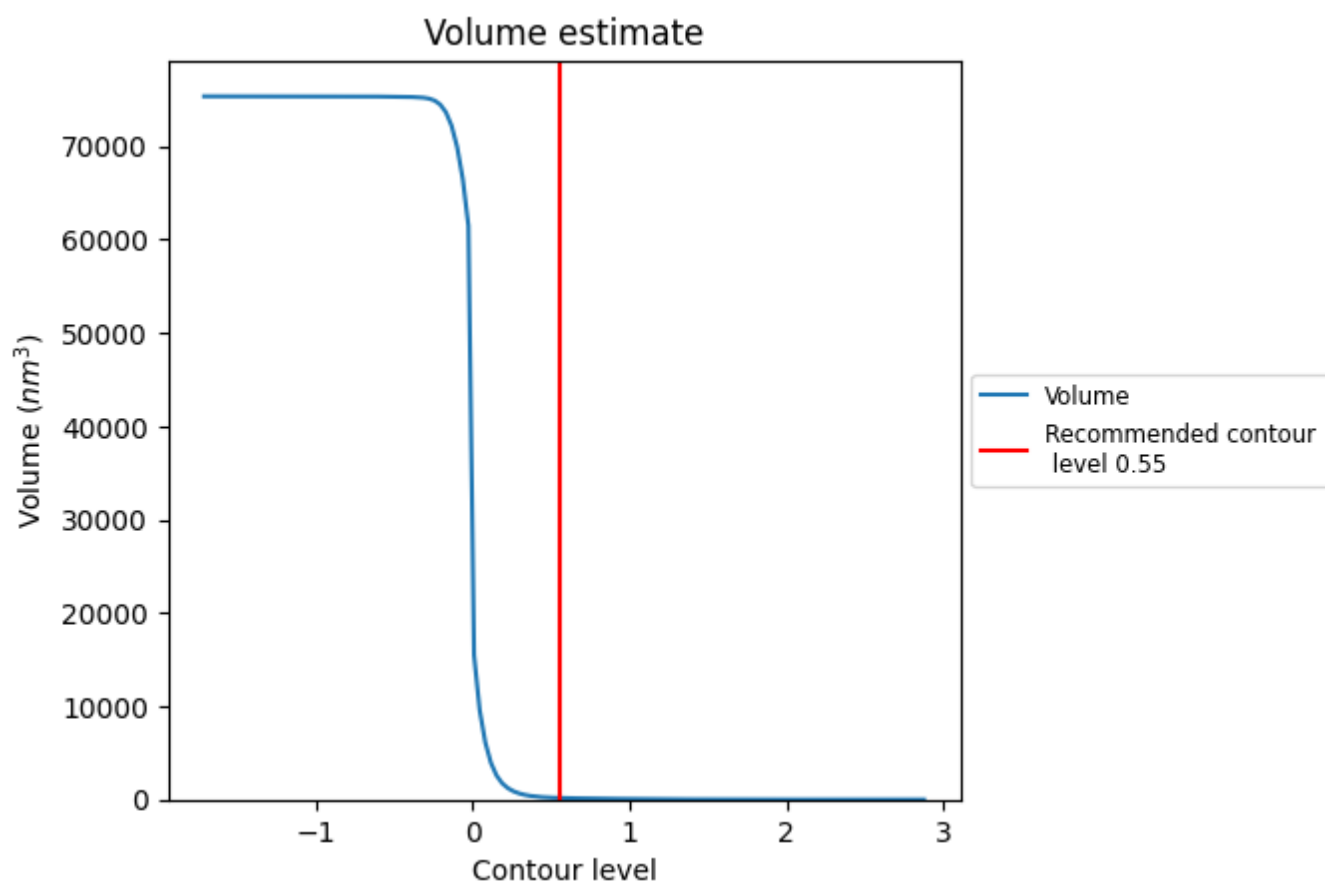
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

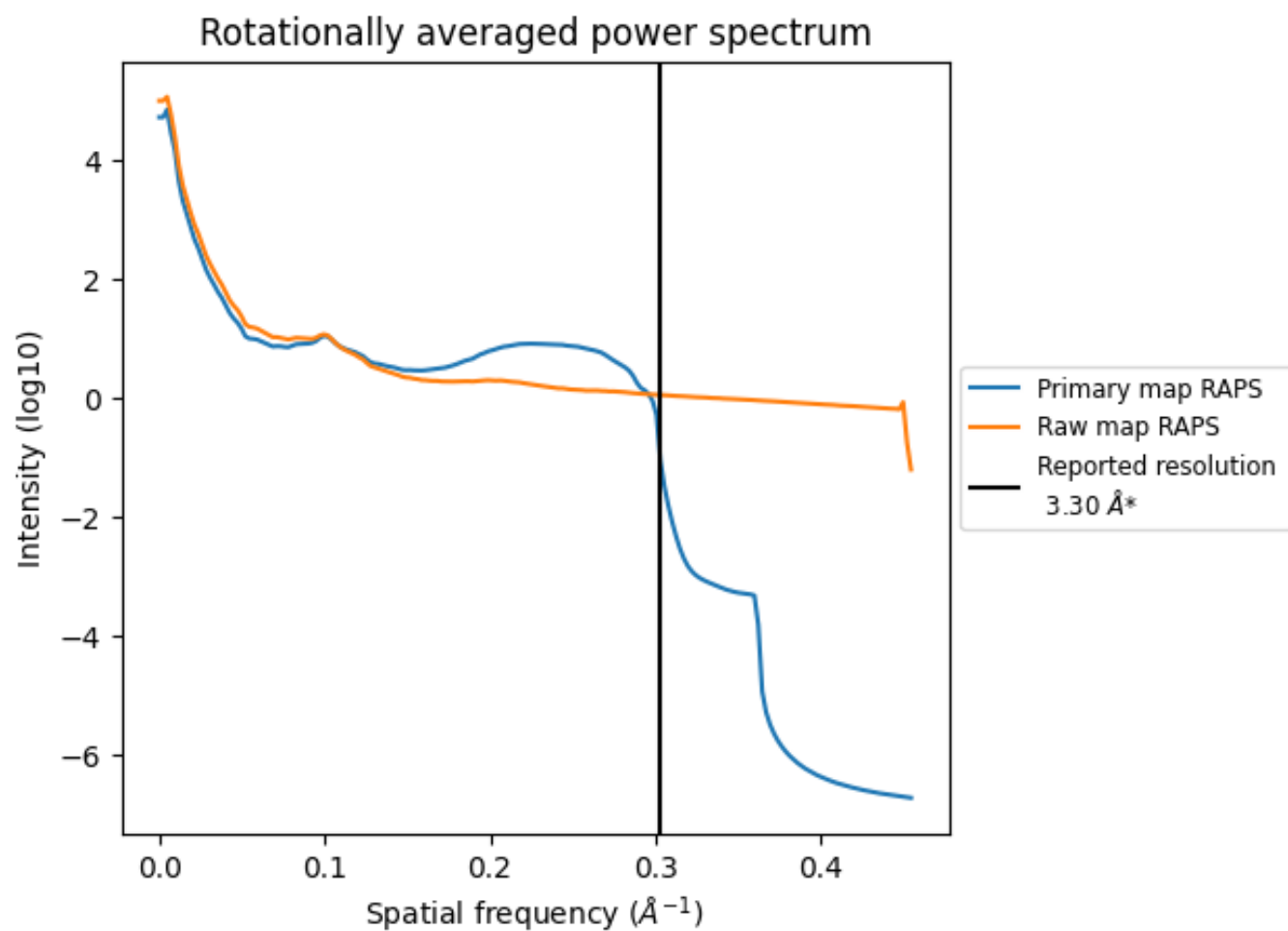
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 176 nm³; this corresponds to an approximate mass of 159 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

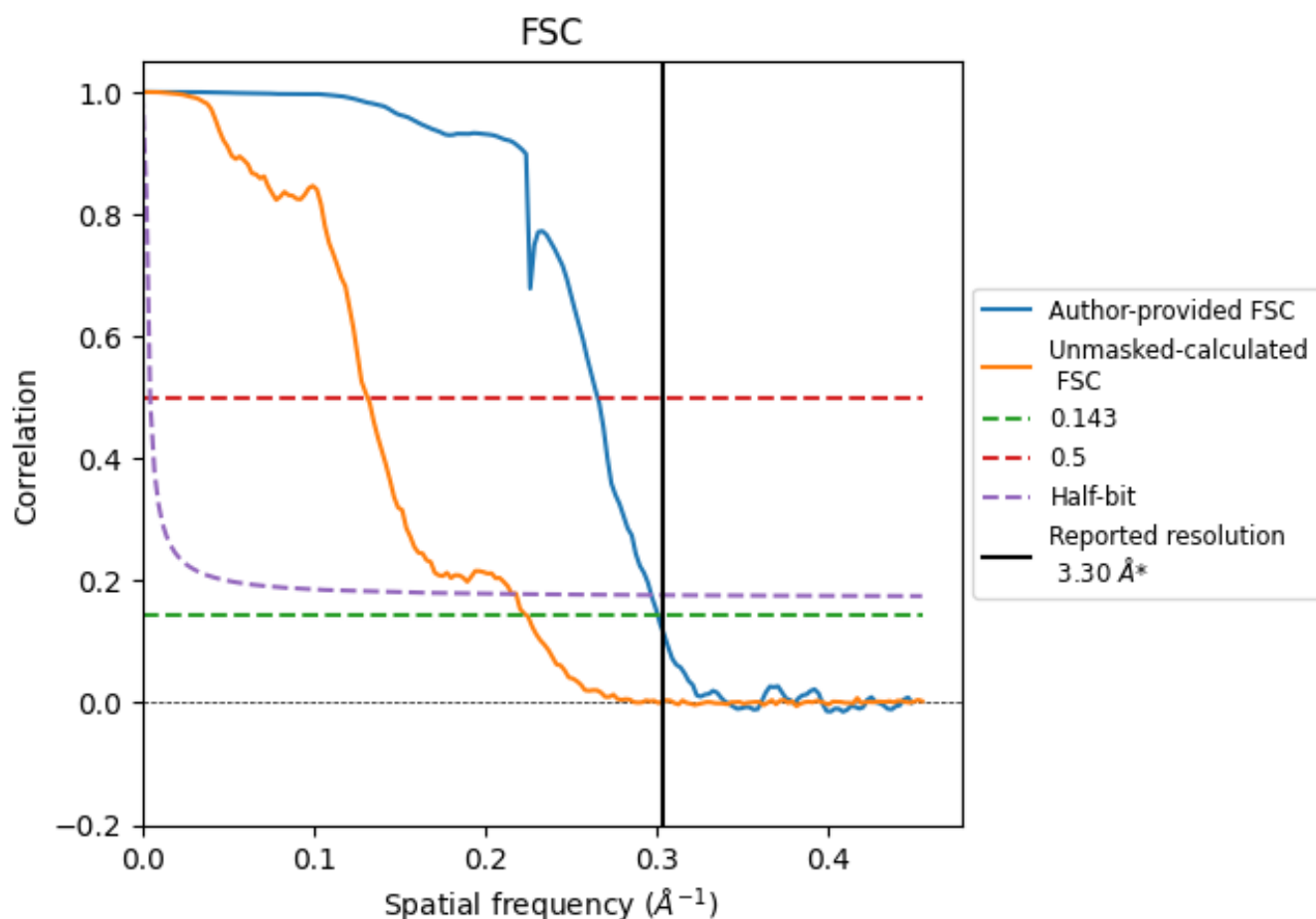


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

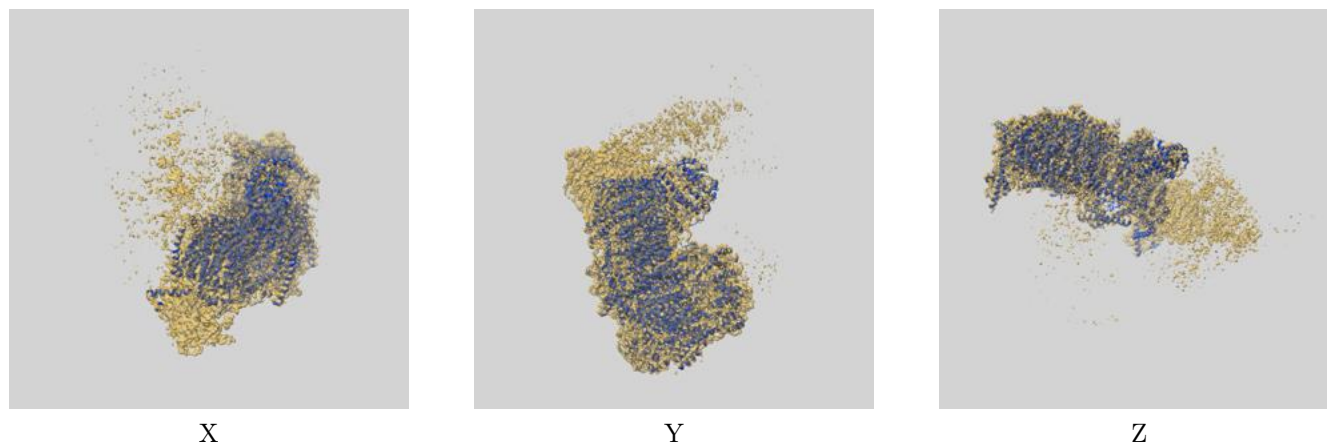
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.33	3.77	3.37
Unmasked-calculated*	4.47	7.62	4.64

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.47 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

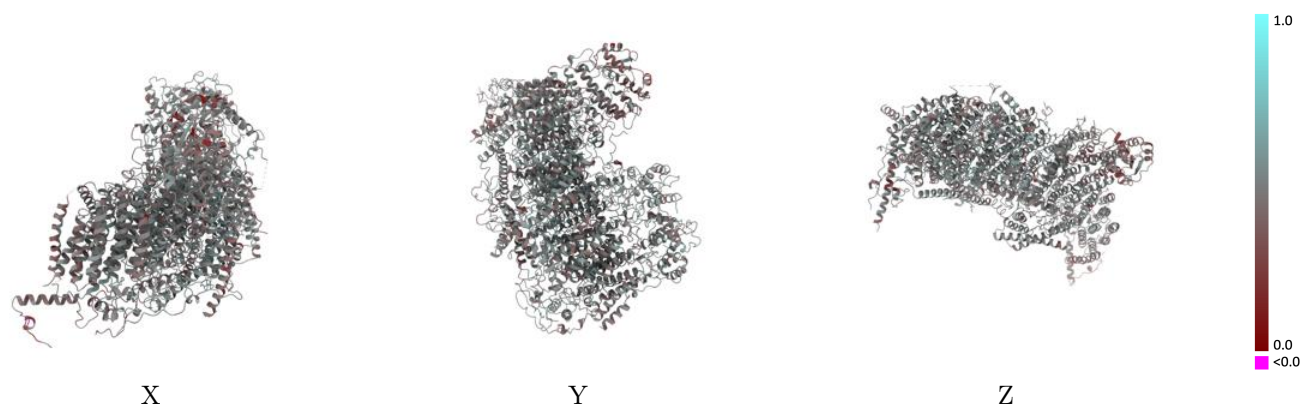
This section contains information regarding the fit between EMDB map EMD-35333 and PDB model 8IB6. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



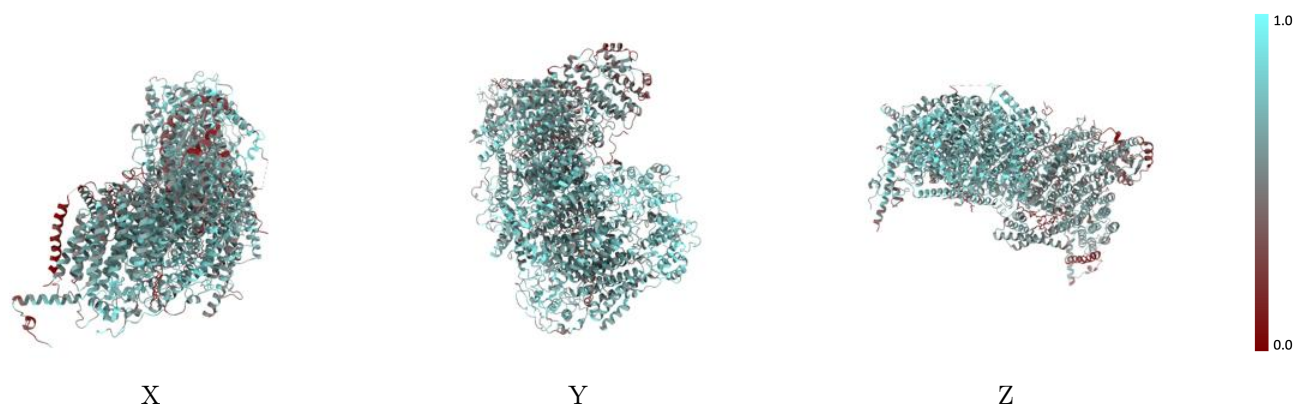
The images above show the 3D surface view of the map at the recommended contour level 0.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



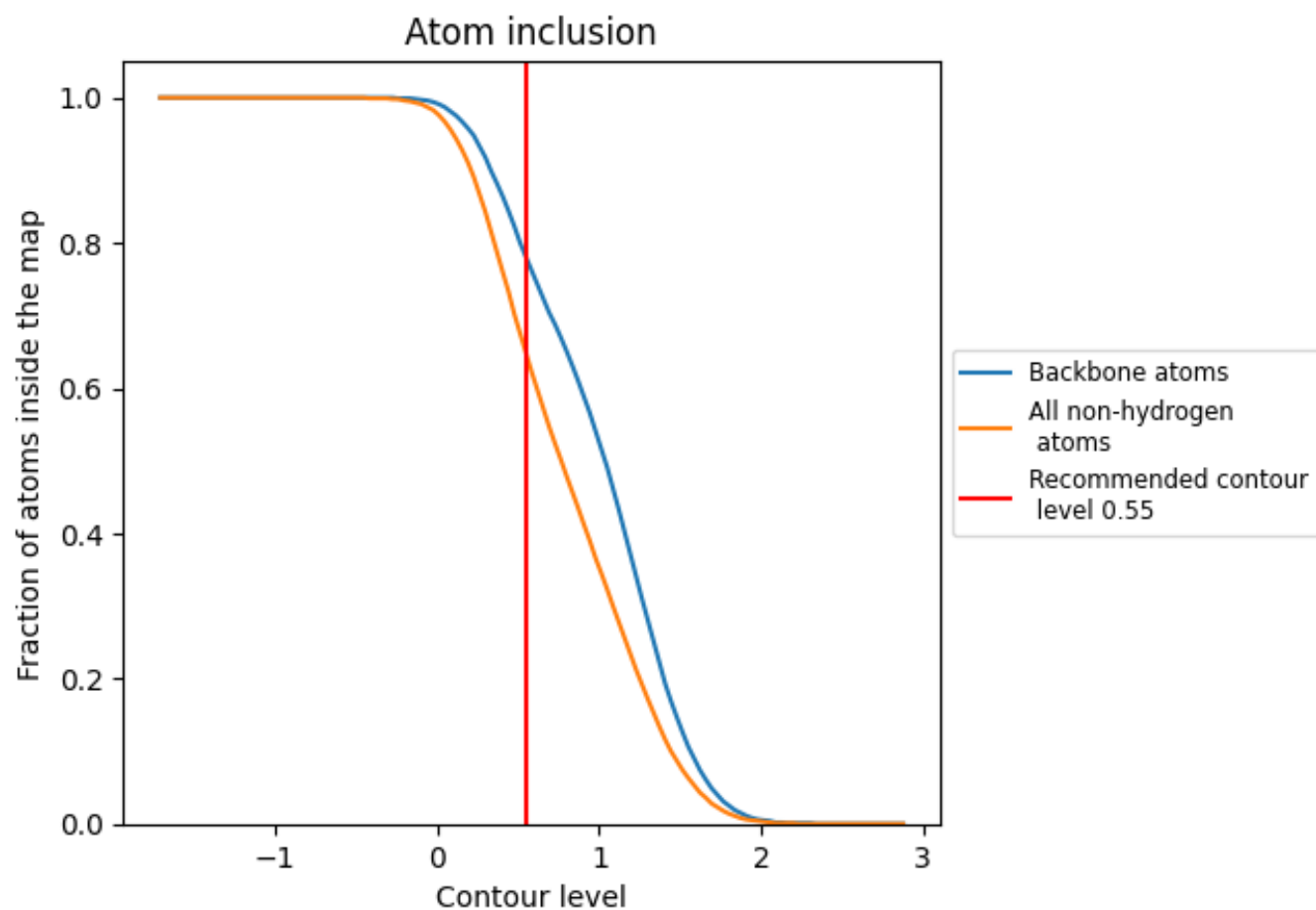
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.55).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 64% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6450	 0.4730
D	 0.4180	 0.4860
J	 0.4610	 0.4320
K	 0.6360	 0.4730
L	 0.6470	 0.4810
M	 0.6940	 0.5030
N	 0.6560	 0.4770
O	 0.4960	 0.4230
U	 0.7410	 0.4930
X	 0.6430	 0.4920
Y	 0.5440	 0.4630
c	 0.5290	 0.4090
d	 0.6900	 0.5000
e	 0.6040	 0.4330
f	 0.5950	 0.4710
g	 0.6700	 0.4770
h	 0.6970	 0.4650
i	 0.6840	 0.4840
j	 0.6610	 0.4540
k	 0.7220	 0.4740
l	 0.7290	 0.4990
m	 0.7000	 0.4760
n	 0.7510	 0.4900
o	 0.6750	 0.4700
p	 0.6820	 0.4550

