



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 06:43 AM UTC

PDB ID : 8XO0 / pdb_00008xo0
EMDB ID : EMD-38521
Title : Respiratory complex Peripheral Arm of CI, close form B, focus-refined map of type I, PERK -/- mouse under Cold Acclimation
Authors : Shin, Y.-C.; Liao, M.
Deposited on : 2023-12-30
Resolution : 4.20 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:

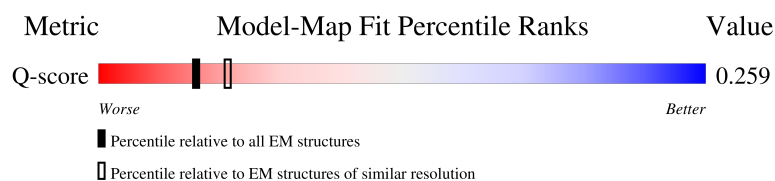
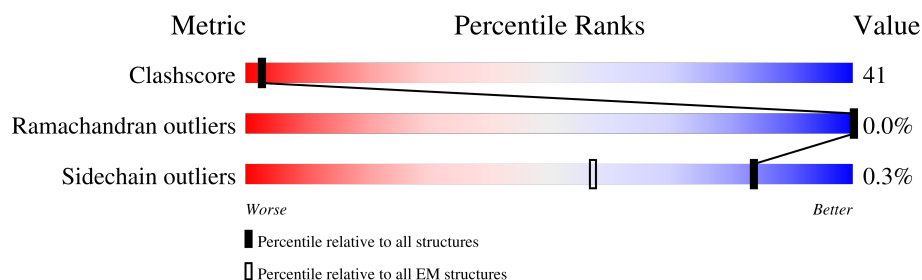
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 4.20 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.



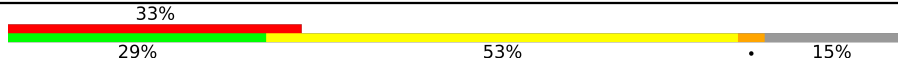
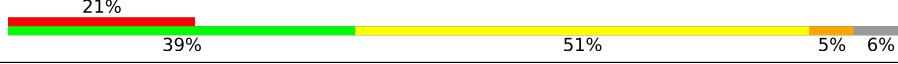
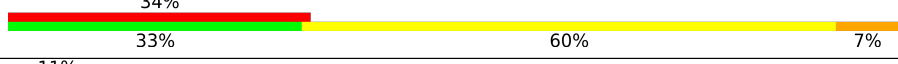
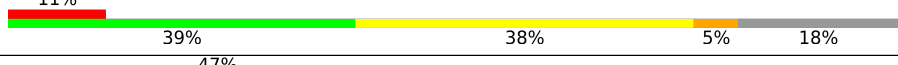
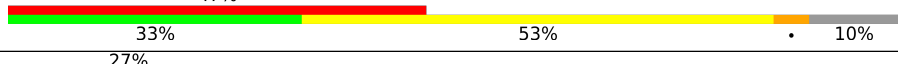
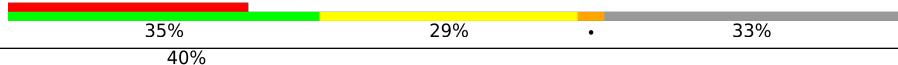
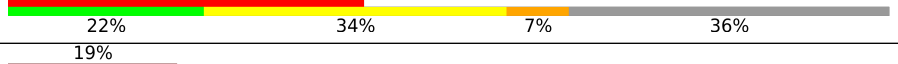
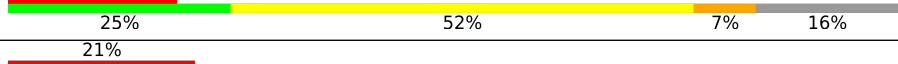
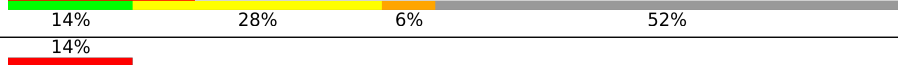
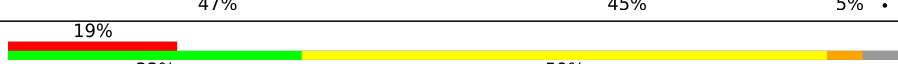
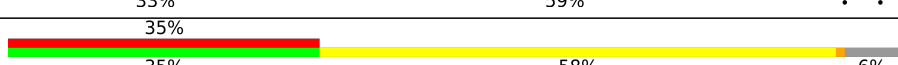
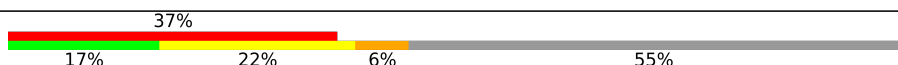
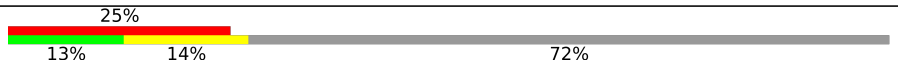
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5410 (3.70 - 4.70)

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	A	115	45% 23% 56% 21%
2	B	224	12% 31% 34% 30%
3	C	263	11% 40% 33% 25%
4	D	463	14% 34% 45% 5% 17%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	248	
6	F	464	
7	G	727	
8	H	318	
9	I	212	
10	P	377	
11	Q	175	
12	R	116	
13	S	99	
14	T	156	
15	V	116	
16	W	131	
17	X	172	
18	Z	144	
19	a	70	
20	b	84	
21	q	145	
22	r	113	
23	s	104	

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
24	SF4	B	301	-	-	X	-
24	SF4	F	502	-	-	X	-
24	SF4	G	802	-	-	X	-
24	SF4	I	303	-	-	X	-
26	FES	E	301	-	-	X	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	FES	G	803	-	-	X	-
30	CDL	q	201	-	-	X	-

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 33729 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-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	91	Total	C	N	O	S	0	0
			737	511	102	118	6		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	156	Total	C	N	O	S	0	0
			1247	796	223	214	14		

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	198	Total	C	N	O	S	0	0
			1641	1060	279	299	3		

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	385	Total	C	N	O	S	0	0
			3088	1970	533	562	23		

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	210	Total	C	N	O	S	0	0
			1635	1039	275	310	11		

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	424	Total	C	N	O	S	0	0
			3273	2062	586	603	22		

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	687	Total	C	N	O	S	0	0
			5287	3316	918	1012	41		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	317	Total	C	N	O	S	0	0
			2531	1701	383	425	22		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	173	Total	C	N	O	S	0	0
			1389	875	239	263	12		

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	P	339	Total	C	N	O	S	0	0
			2720	1759	476	478	7		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Q	118	Total	C	N	O	S	0	0
			957	608	165	180	4		

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	R	74	Total	C	N	O	S	0	0
			587	366	109	109	3		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	S	83	Total	C	N	O	S	0	0
			667	419	126	119	3		

- Molecule 14 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	75	Total	C	N	O	S	0	0
			604	388	89	122	5		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	V	112	Total	C	N	O	S	0	0
			915	596	152	164	3		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	W	114	Total	C	N	O	S	0	0
			970	619	180	165	6		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	X	142	Total	C	N	O	S	0	0
			1164	736	209	209	10		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Z	139	Total	C	N	O	S	0	0
			1152	741	204	199	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	a	67	Total	C	N	O	S	0	0
			548	356	97	91	4		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	b	79	Total	C	N	O	S	0	0
			620	408	98	110	4		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	q	122	Total	C	N	O	S	0	0
			1020	655	180	181	4		

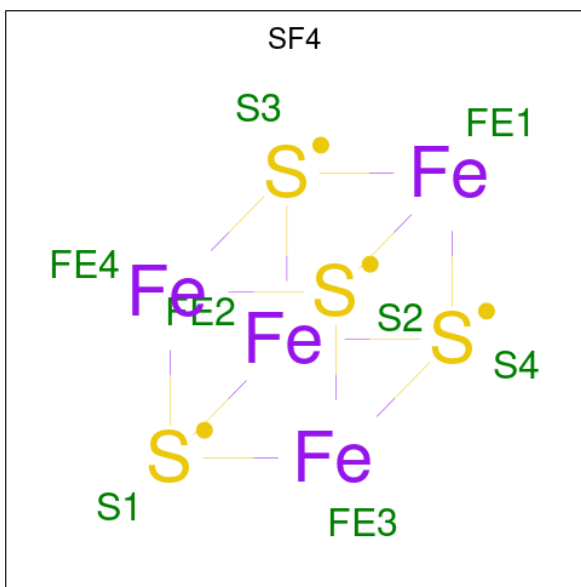
- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	r	51	Total	C	N	O	S	0	0
			418	266	78	73	1		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

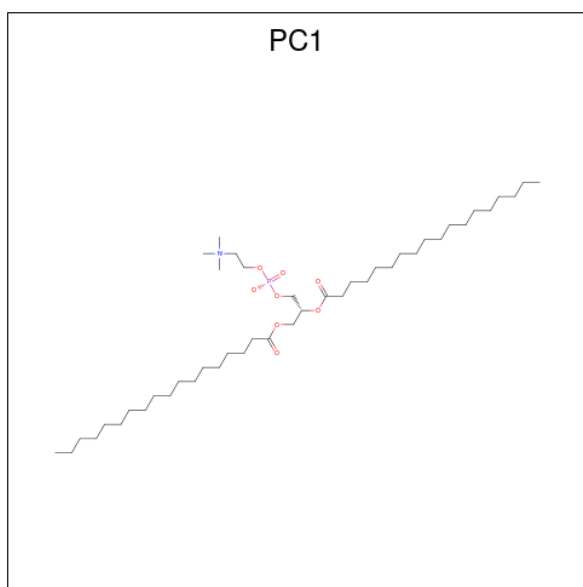
Mol	Chain	Residues	Atoms				AltConf	Trace
23	s	29	Total	C	N	O	0	0
			238	151	39	48		

- Molecule 24 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



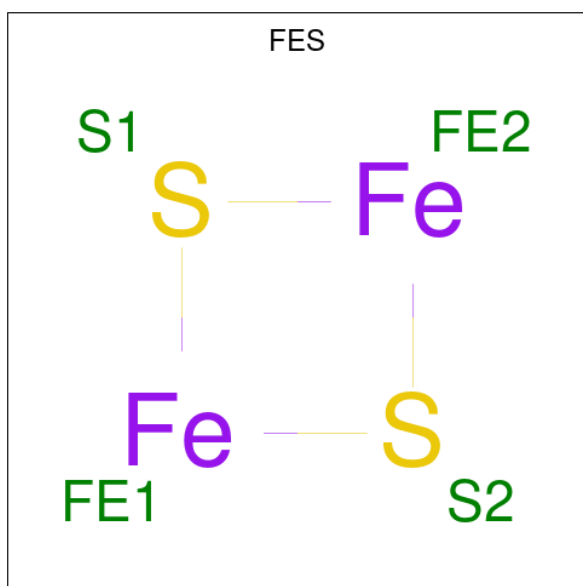
Mol	Chain	Residues	Atoms			AltConf
24	B	1	Total	Fe	S	0
			8	4	4	
24	F	1	Total	Fe	S	0
			8	4	4	
24	G	1	Total	Fe	S	0
			8	4	4	
24	G	1	Total	Fe	S	0
			8	4	4	
24	I	1	Total	Fe	S	0
			8	4	4	
24	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 25 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
25	B	1	Total	C	N	O	P	0
			35	25	1	8	1	
25	I	1	Total	C	N	O	P	0
			43	33	1	8	1	

- Molecule 26 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



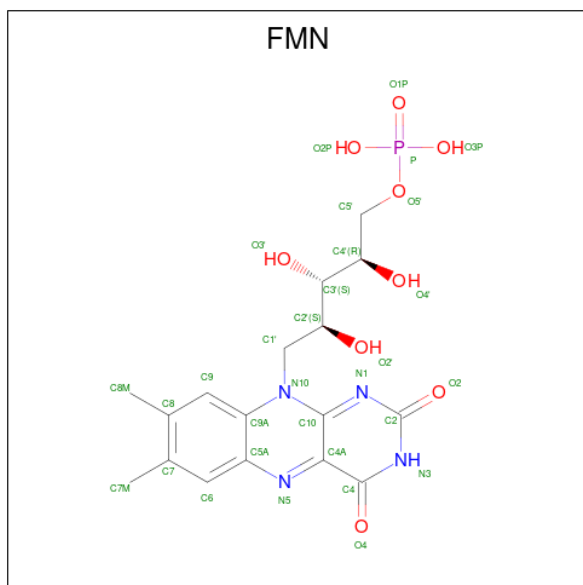
Mol	Chain	Residues	Atoms			AltConf
26	E	1	Total	Fe	S	0
			4	2	2	

Continued on next page...

Continued from previous page...

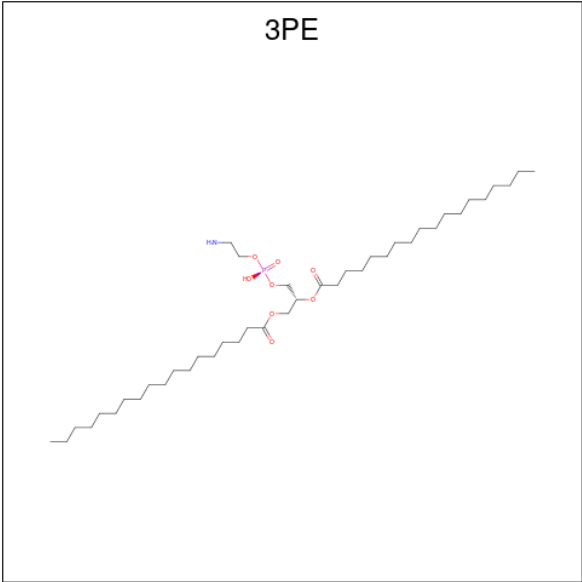
Mol	Chain	Residues	Atoms			AltConf
26	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 27 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



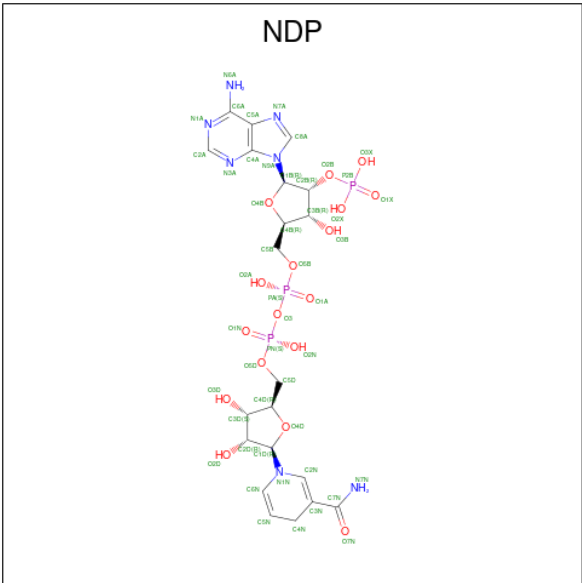
Mol	Chain	Residues	Atoms					AltConf
27	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 28 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
28	H	1	Total	C	N	O	P	0
			51	41	1	8	1	

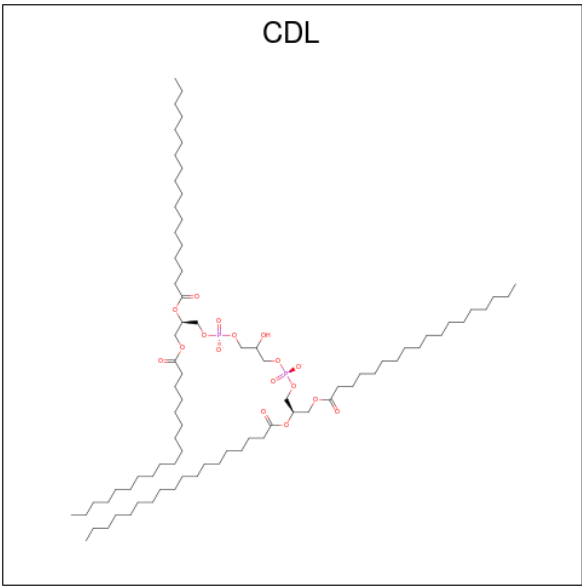
- Molecule 29 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
29	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 30 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand

of Interest" by depositor).

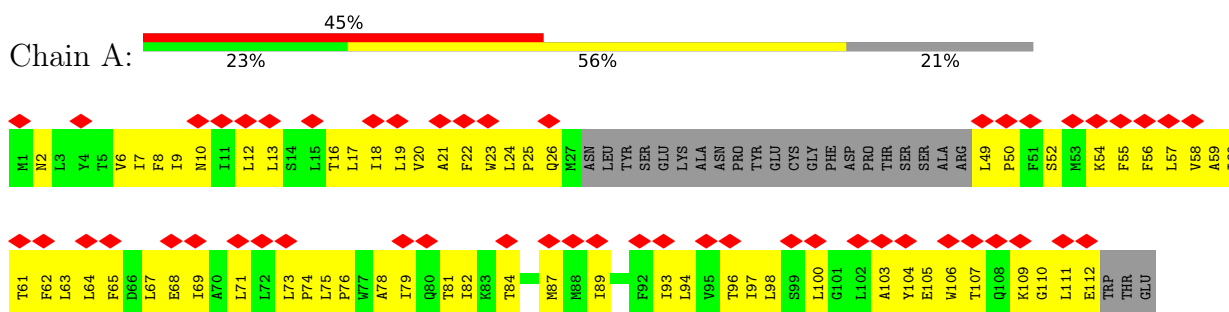


Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
30	q	1	57	38	17	2	0

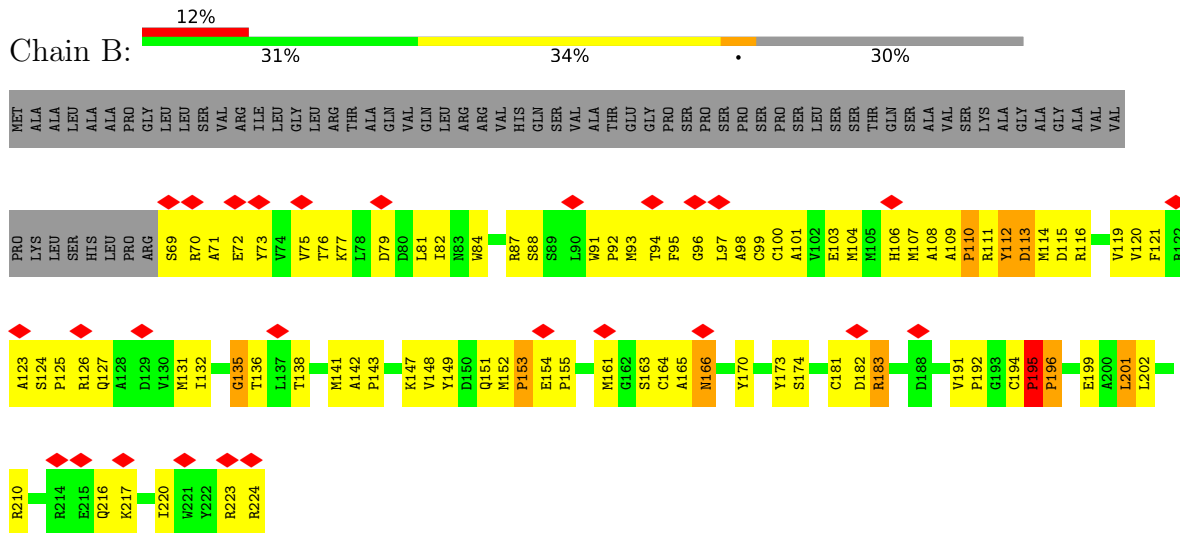
3 Residue-property plots

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

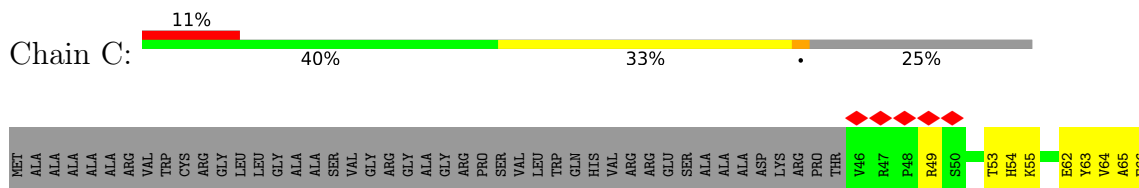
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3

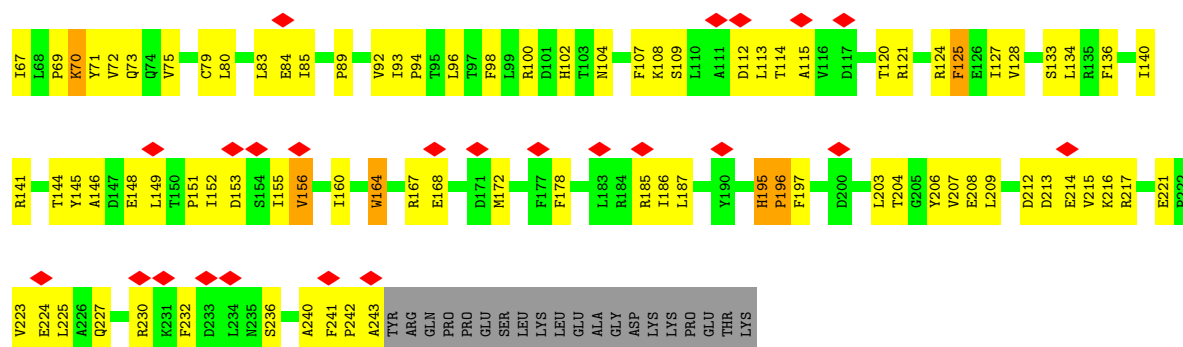


- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

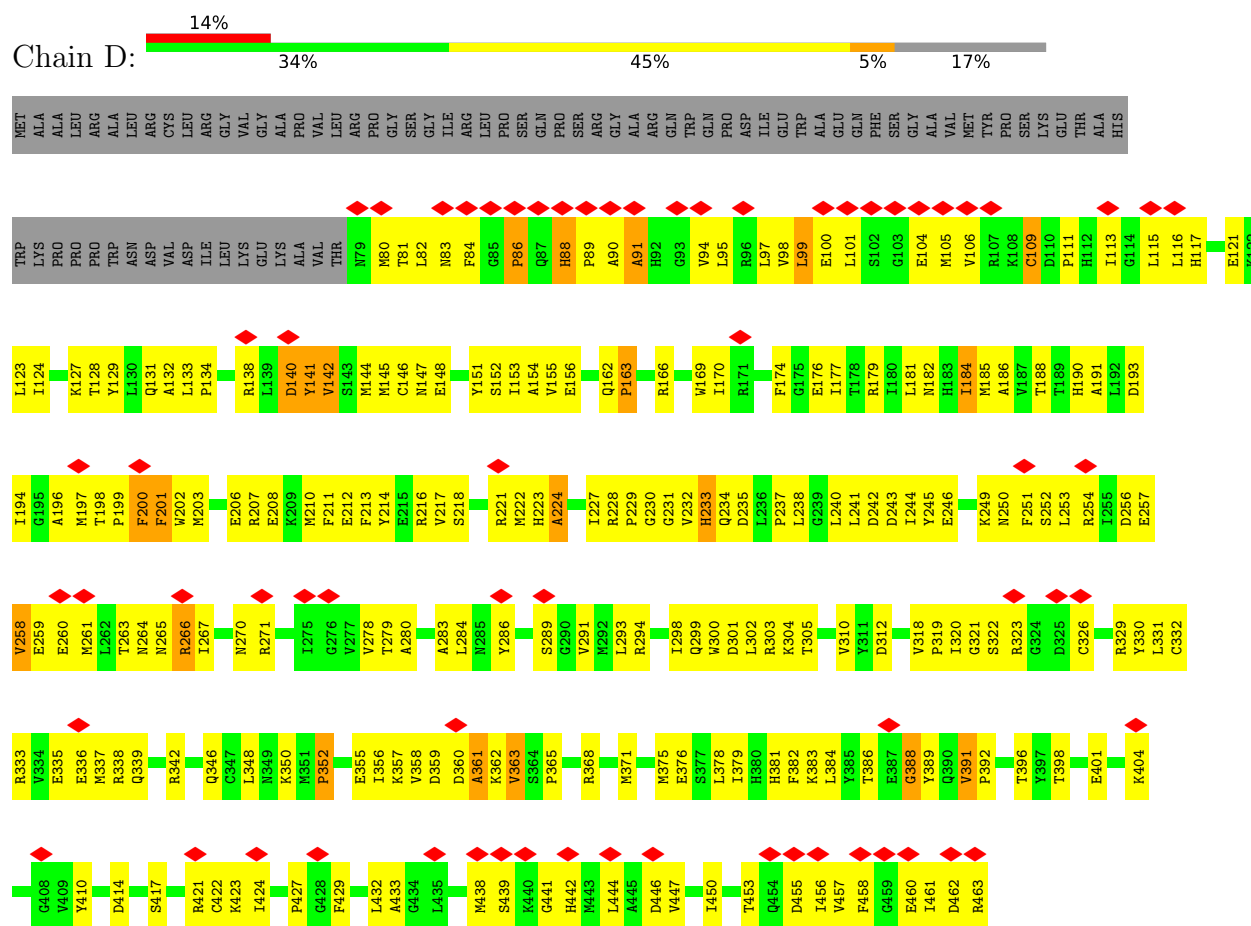


- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

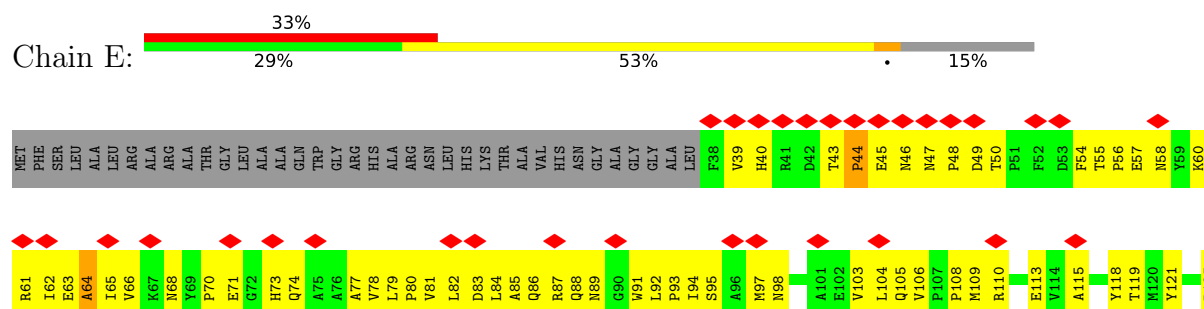


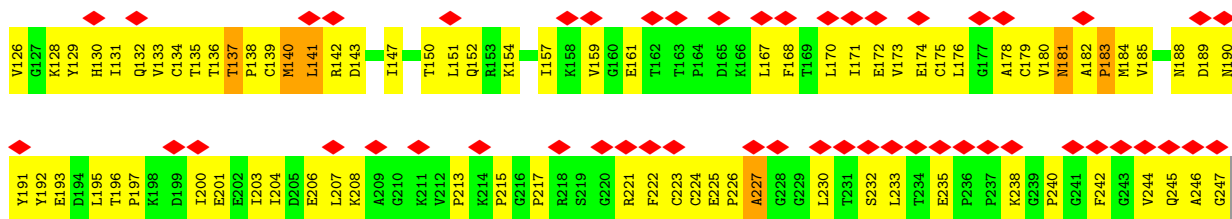


• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

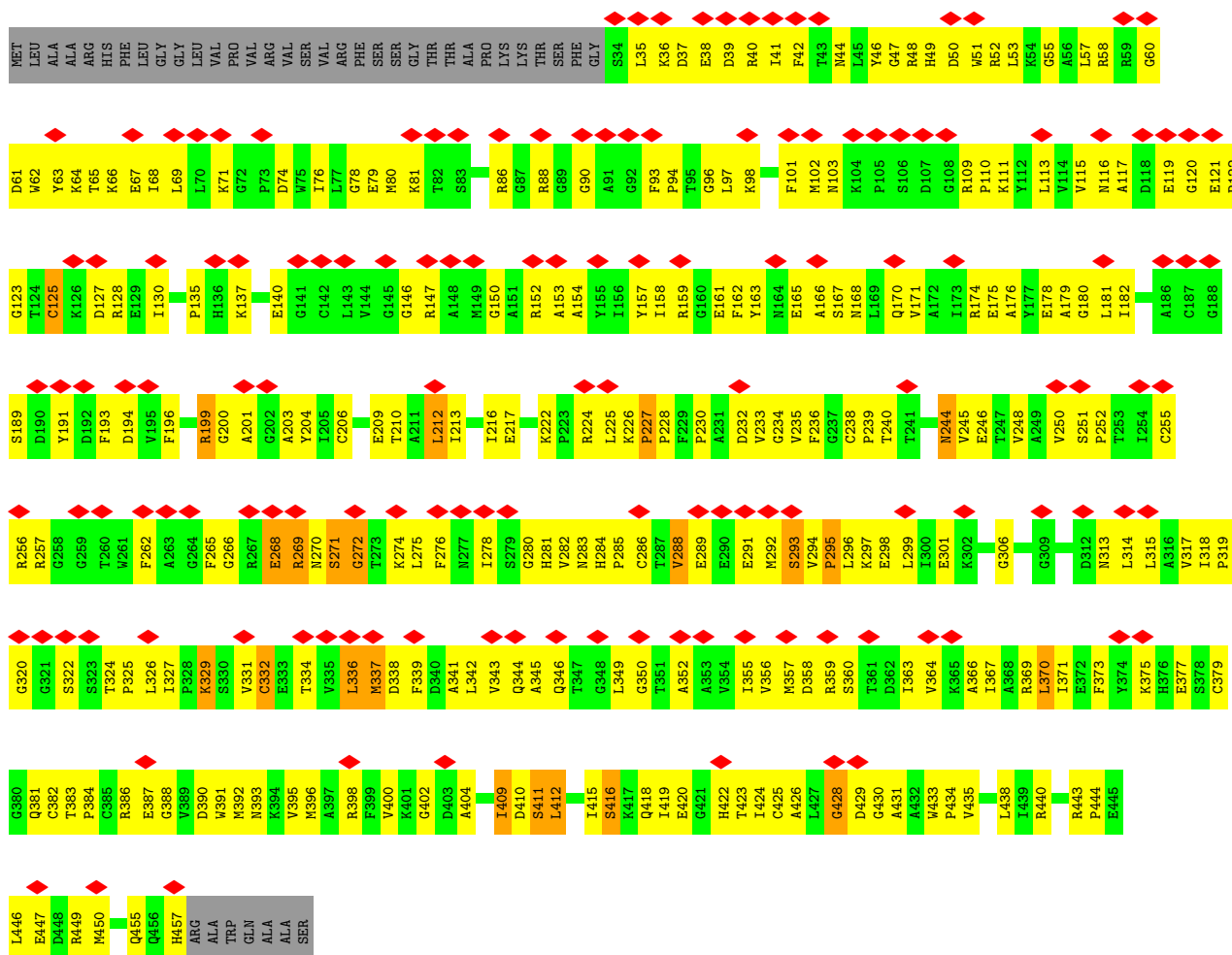


• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

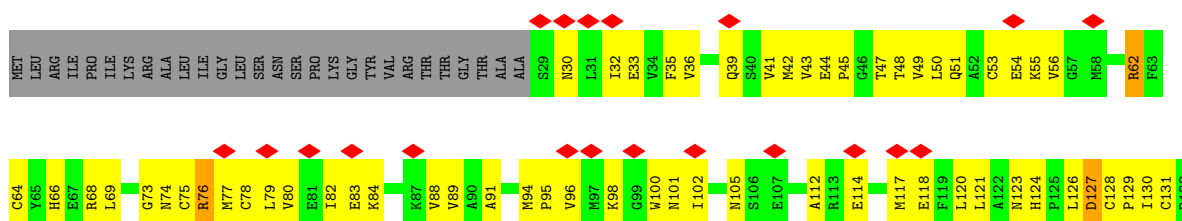


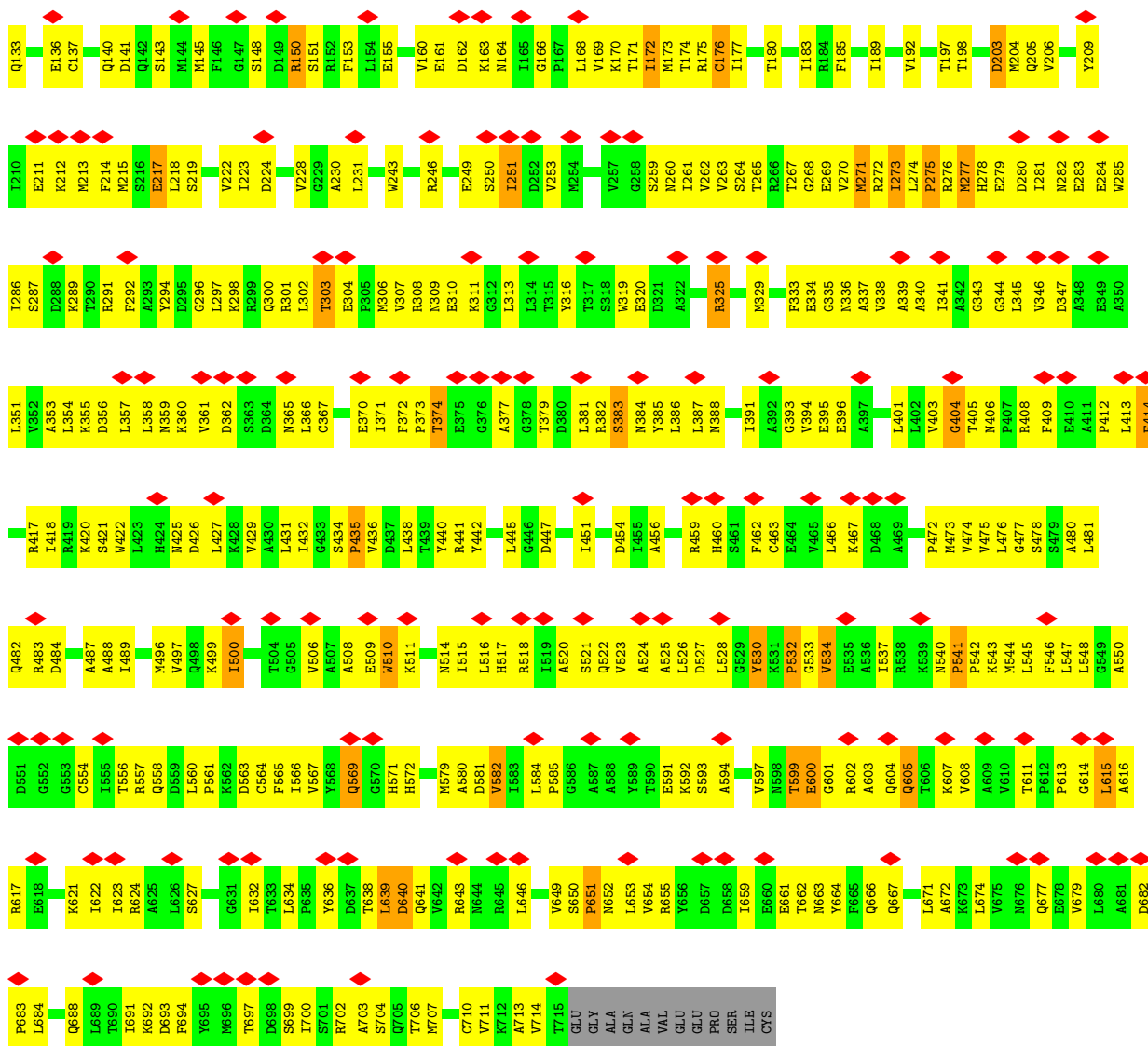


• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

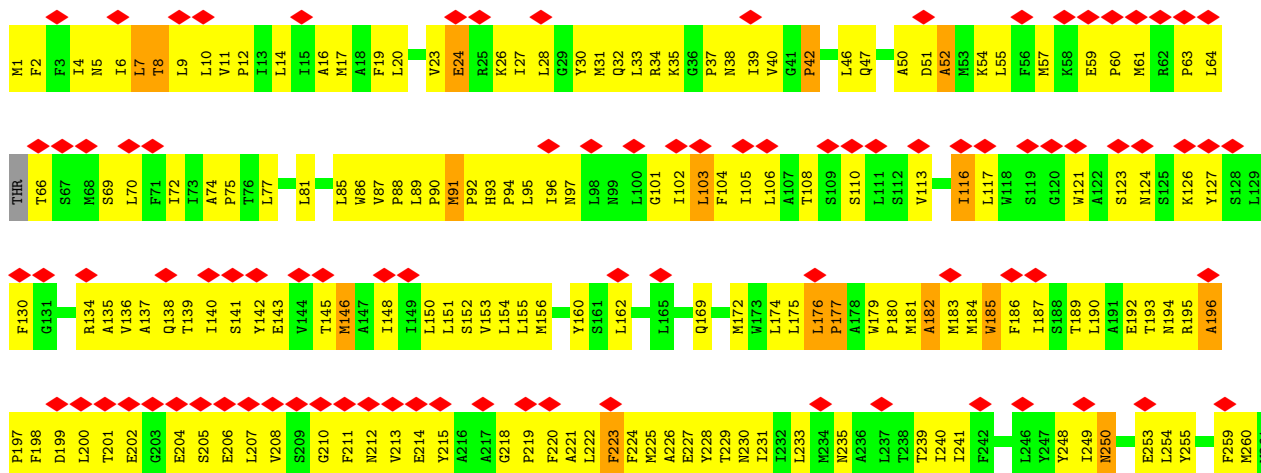


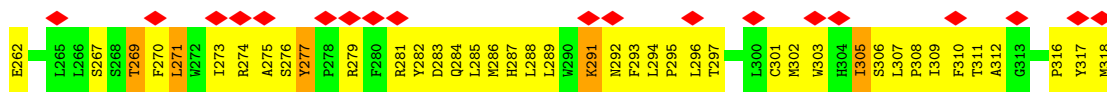
• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



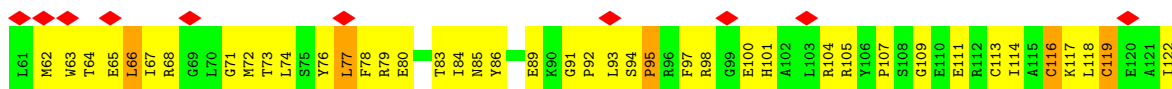
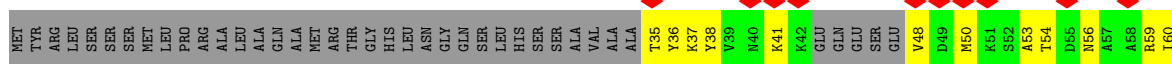


• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

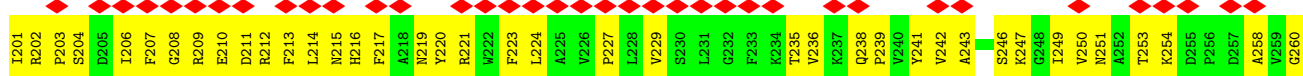
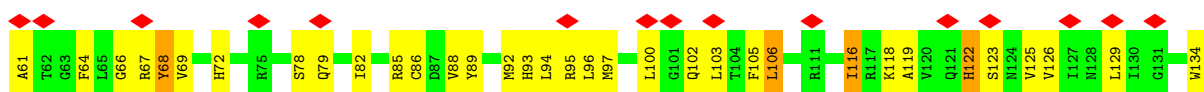
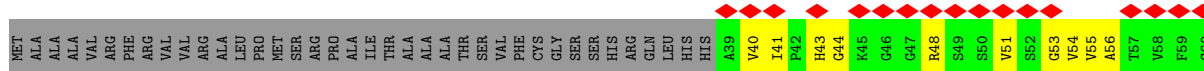




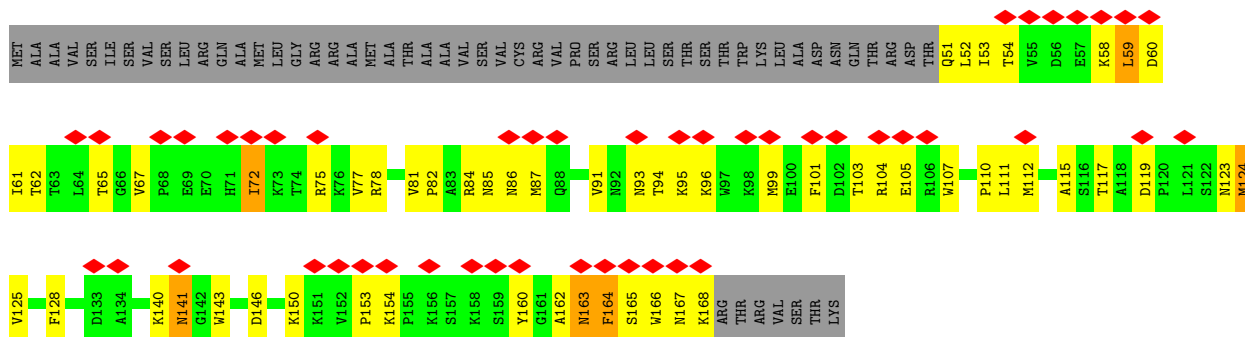
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



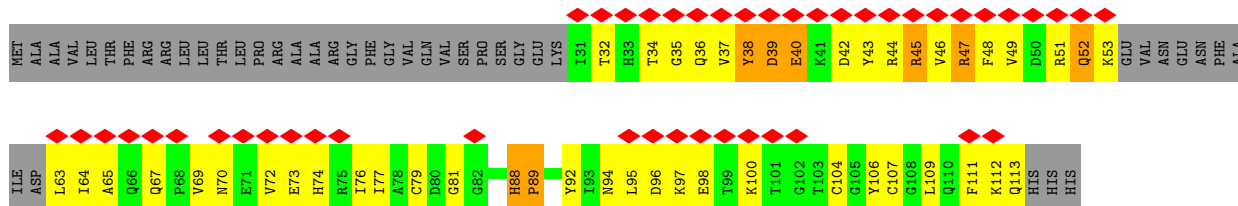
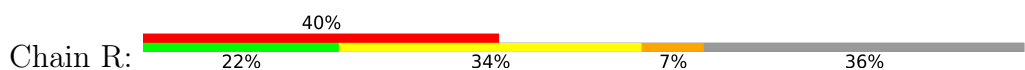
- Molecule 10: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial



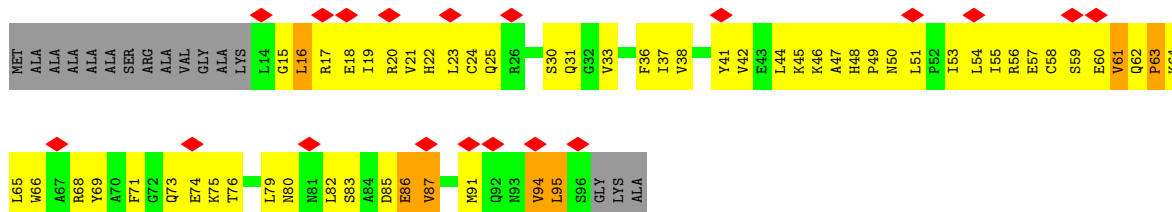
- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



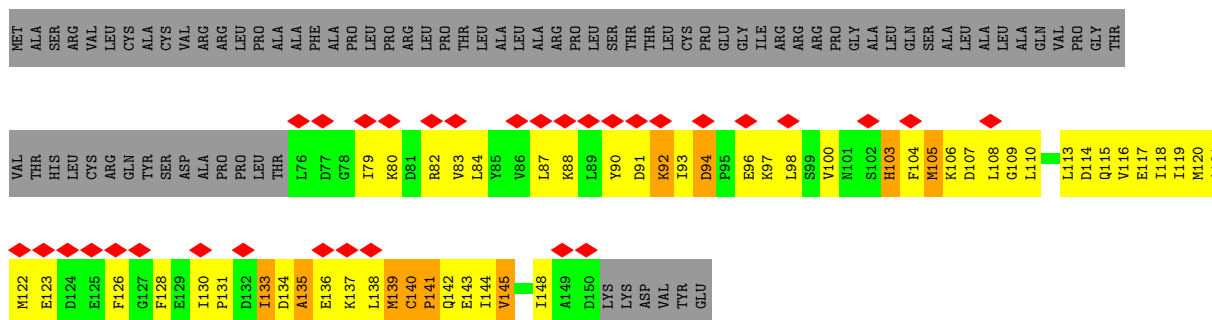
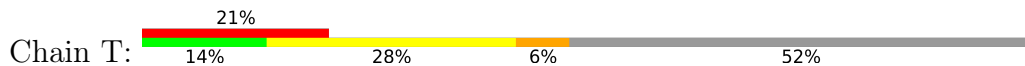
- Molecule 12: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



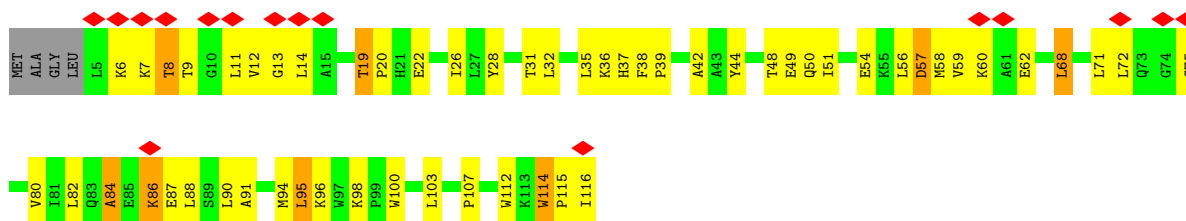
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



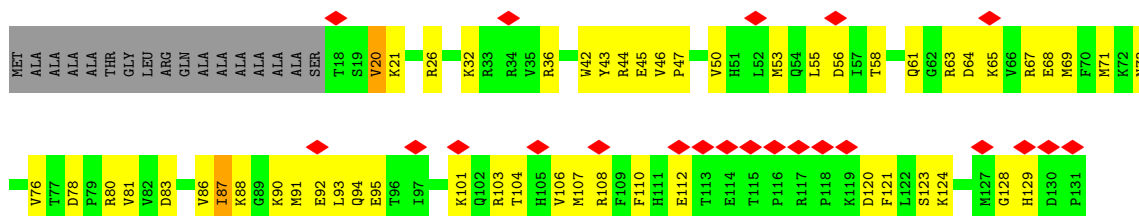
- Molecule 14: Acyl carrier protein, mitochondrial



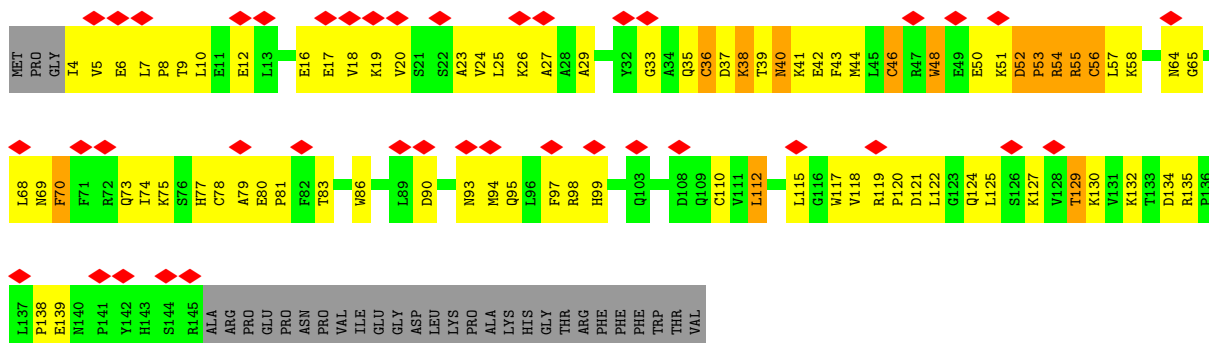
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



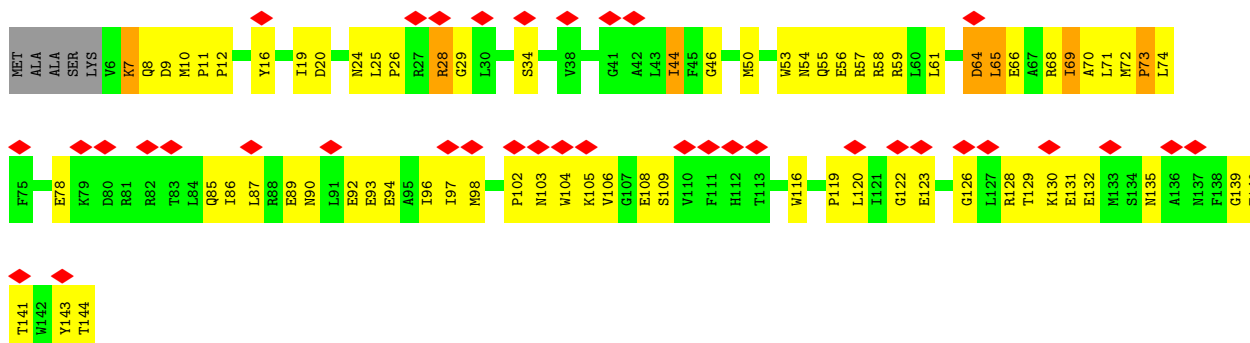
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



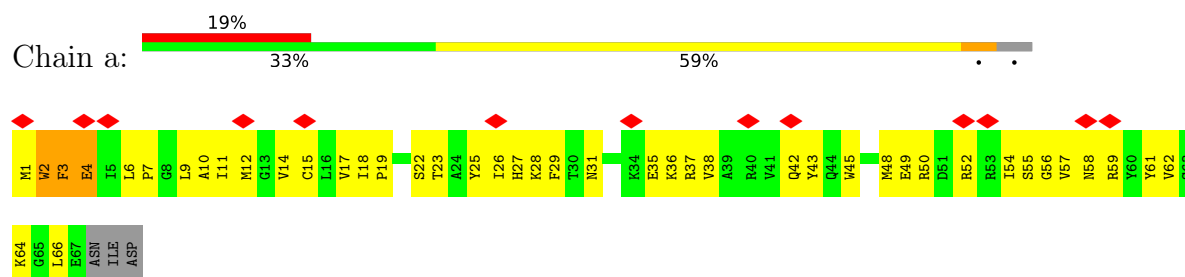
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



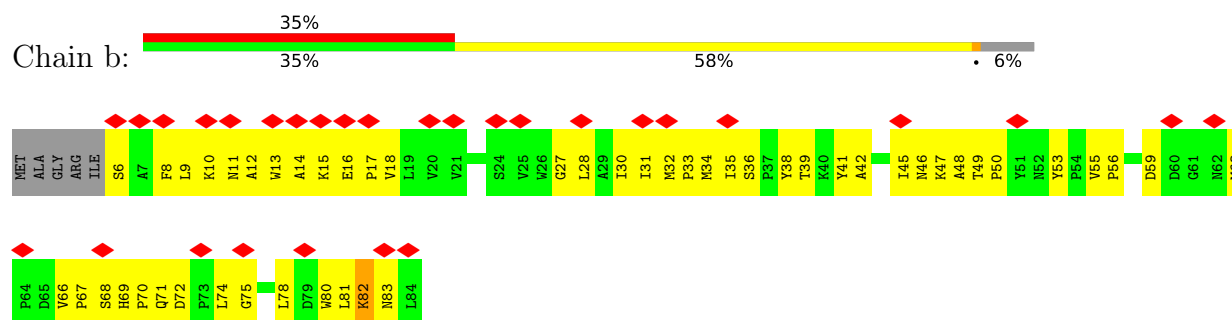
- Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



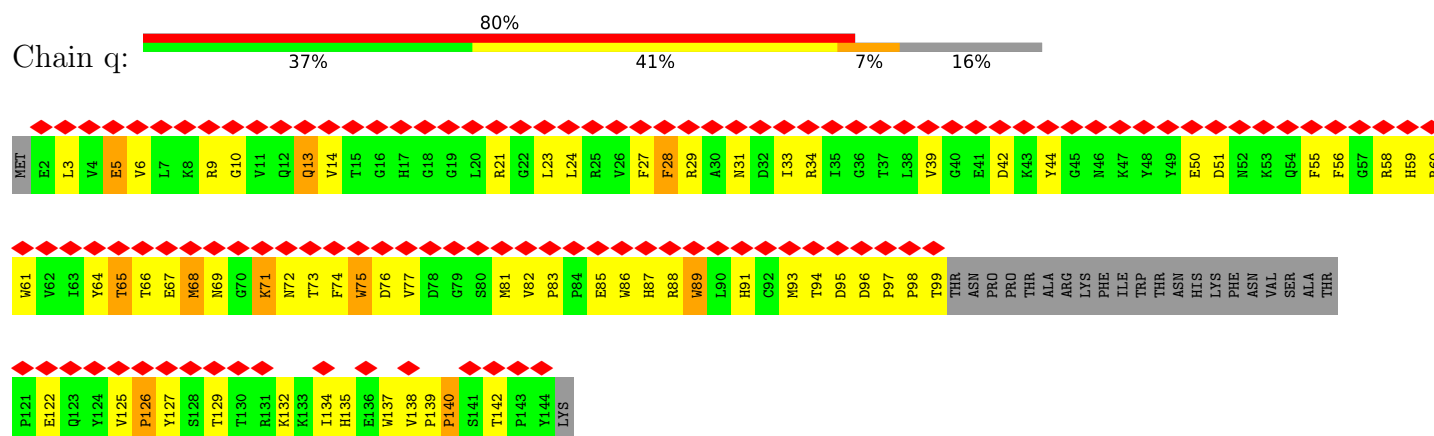
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



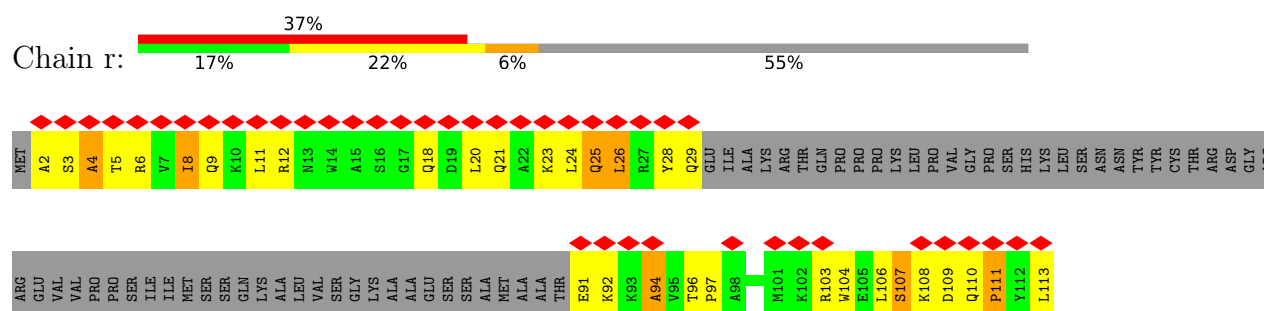
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



- Molecule 23: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



MET	ALA	VAL	SER	LEU	LEU	ARG	GLY	GLY	ARG	ILE	ARG	ALA	LEU	LYS	ALA	VAL	LEU	LEU	GLU	ALA	ARG	VAL	PHE	PRO	GLY	GLY	LEU	VAL	SER	VAL	VAL	ARG	LEU	SER	THR	GLU	SER	GLY	LYS	SER	ALA	LYS	GLU	LYS	GLU	LEU	HIS	PRO	LYS	THR	GLN	SER	SER	VAL	LEU	LYS	GLU	PRO	GLU
PRO	THR	ASP	THR	THR	THR	TYR	LYS	ASN	LEU	GLN	HIS	HIS	D39	Y40	N41	T42	Y43	T44	F45	L46	D47	L48	N49	L50	D51	L52	S53	K54	F55	R56	L57	P58	Q59	P60	S61	S62	G63	R64	E65	S66	P67	ARG	HIS																

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	7071	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.2	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.664	Depositor
Minimum map value	-0.623	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.064	Depositor
Recommended contour level	0.4	Depositor
Map size ($\text{\AA}$)	424.96, 424.96, 424.96	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.83, 0.83, 0.83	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, NDP, CDL, FES, SF4, FMN, PC1

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.67	0/755	0.96	3/1029 (0.3%)
2	B	0.96	4/1278 (0.3%)	1.30	11/1730 (0.6%)
3	C	0.88	1/1687 (0.1%)	1.28	13/2297 (0.6%)
4	D	0.95	5/3162 (0.2%)	1.40	34/4276 (0.8%)
5	E	0.82	3/1675 (0.2%)	1.16	19/2282 (0.8%)
6	F	0.82	4/3347 (0.1%)	1.32	41/4522 (0.9%)
7	G	0.88	8/5374 (0.1%)	1.49	85/7281 (1.2%)
8	H	0.83	2/2607 (0.1%)	1.22	31/3561 (0.9%)
9	I	0.91	1/1418 (0.1%)	1.49	18/1915 (0.9%)
10	P	0.79	4/2793 (0.1%)	1.17	23/3787 (0.6%)
11	Q	0.88	1/980 (0.1%)	1.28	12/1324 (0.9%)
12	R	1.05	3/596 (0.5%)	1.36	12/799 (1.5%)
13	S	0.94	2/678 (0.3%)	1.47	11/915 (1.2%)
14	T	1.04	1/613 (0.2%)	1.56	12/826 (1.5%)
15	V	0.87	0/937	1.47	14/1270 (1.1%)
16	W	0.73	0/993	0.95	2/1335 (0.1%)
17	X	0.96	2/1191 (0.2%)	1.50	27/1605 (1.7%)
18	Z	0.82	1/1183 (0.1%)	1.22	12/1597 (0.8%)
19	a	0.88	0/561	1.38	8/755 (1.1%)
20	b	0.70	0/643	0.94	1/884 (0.1%)
21	q	1.05	2/1054 (0.2%)	1.53	20/1431 (1.4%)
22	r	1.16	3/426 (0.7%)	1.71	13/573 (2.3%)
23	s	0.46	0/244	1.09	2/331 (0.6%)
All	All	0.88	47/34195 (0.1%)	1.34	424/46325 (0.9%)

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	X	53	PRO	N-CD	-19.18	1.20	1.47
5	E	227	ALA	C-O	15.80	1.42	1.24
12	R	89	PRO	N-CD	-15.19	1.26	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	q	139	PRO	N-CD	-13.61	1.28	1.47
10	P	371	PRO	N-CD	12.85	1.65	1.47
7	G	532	PRO	N-CD	-12.62	1.30	1.47
14	T	141	PRO	N-CD	11.85	1.64	1.47
6	F	295	PRO	N-CD	-11.25	1.32	1.47
8	H	42	PRO	N-CD	10.86	1.62	1.47
22	r	91	GLU	N-CA	9.97	1.65	1.46
6	F	227	PRO	N-CD	9.86	1.61	1.47
10	P	290	PRO	N-CD	9.60	1.61	1.47
5	E	44	PRO	N-CD	-9.54	1.34	1.47
7	G	275	PRO	N-CD	-9.48	1.34	1.47
6	F	319	PRO	N-CD	9.02	1.60	1.47
10	P	204	SER	C-O	-8.64	1.13	1.23
9	I	107	PRO	N-CD	8.52	1.59	1.47
4	D	163	PRO	N-CD	-8.35	1.36	1.47
18	Z	73	PRO	N-CD	8.03	1.58	1.47
13	S	63	PRO	N-CD	-7.97	1.36	1.47
12	R	39	ASP	CA-C	7.96	1.64	1.53
11	Q	53	ILE	C-O	7.87	1.33	1.24
12	R	40	GLU	N-CA	7.87	1.56	1.46
4	D	352	PRO	N-CD	-7.81	1.36	1.47
2	B	88	SER	C-N	-7.67	1.20	1.33
22	r	111	PRO	N-CD	-7.39	1.37	1.47
2	B	96	GLY	CA-C	-7.28	1.47	1.52
7	G	541	PRO	N-CD	-6.88	1.38	1.47
7	G	203	ASP	CA-C	6.67	1.62	1.52
7	G	600	GLU	CA-C	6.49	1.61	1.52
3	C	66	GLU	C-N	6.41	1.42	1.33
7	G	127	ASP	CA-C	6.32	1.62	1.52
2	B	153	PRO	N-CD	-6.29	1.39	1.47
4	D	266	ARG	C-O	-6.23	1.16	1.24
6	F	384	PRO	N-CD	-6.22	1.39	1.47
2	B	110	PRO	C-O	-6.18	1.16	1.24
7	G	76	ARG	CA-C	6.08	1.61	1.53
5	E	93	PRO	N-CD	-5.93	1.39	1.47
22	r	25	GLN	CA-C	5.89	1.60	1.52
8	H	291	LYS	C-O	-5.75	1.16	1.24
10	P	204	SER	CA-C	-5.59	1.46	1.53
7	G	683	PRO	N-CD	-5.50	1.40	1.47
13	S	95	LEU	CA-C	5.41	1.59	1.52
4	D	392	PRO	C-O	-5.39	1.20	1.24
21	q	126	PRO	N-CD	5.34	1.55	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	266	ARG	CA-C	-5.23	1.45	1.52
17	X	54	ARG	CA-C	5.14	1.59	1.52

All (424) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	142	VAL	N-CA-CB	19.30	132.46	110.65
4	D	142	VAL	N-CA-C	-19.05	92.51	110.42
7	G	174	THR	N-CA-C	-17.44	89.10	114.39
6	F	332	CYS	N-CA-C	15.56	130.01	111.02
17	X	53	PRO	N-CA-CB	-14.59	89.89	103.46
22	r	91	GLU	N-CA-CB	14.54	135.22	110.50
21	q	139	PRO	N-CA-CB	-13.59	95.58	103.19
7	G	251	ILE	N-CA-C	13.22	126.69	108.17
17	X	53	PRO	CA-N-CD	12.86	130.00	112.00
9	I	164	VAL	N-CA-C	-12.71	100.25	112.83
7	G	77	MET	N-CA-C	-12.49	97.43	113.17
7	G	500	ILE	N-CA-C	-12.45	98.83	110.53
19	a	3	PHE	CB-CA-C	-12.37	89.64	110.68
10	P	106	LEU	N-CA-C	12.17	128.67	109.07
7	G	204	MET	N-CA-C	-11.68	91.37	109.25
6	F	449	ARG	N-CA-C	-11.60	98.72	111.36
6	F	288	VAL	N-CA-C	11.57	121.53	110.42
6	F	334	THR	N-CA-CB	11.45	127.22	109.82
7	G	599	THR	N-CA-C	11.38	126.26	112.38
11	Q	60	ASP	N-CA-C	-11.36	90.27	109.24
15	V	57	ASP	N-CA-C	-11.00	99.30	111.07
9	I	160	GLU	N-CA-C	10.76	124.14	111.02
9	I	77	LEU	N-CA-C	-10.43	99.72	111.71
2	B	195	PRO	N-CA-C	-10.40	98.01	110.70
14	T	139	MET	N-CA-C	-10.38	97.49	113.89
5	E	68	ASN	N-CA-C	-10.38	99.97	111.07
7	G	280	ASP	N-CA-C	10.35	122.56	111.28
4	D	140	ASP	CB-CA-C	-10.26	97.98	111.42
4	D	337	MET	N-CA-C	-10.25	100.10	111.07
7	G	414	PHE	N-CA-C	-10.18	101.36	113.88
23	s	55	PHE	N-CA-C	10.18	125.69	112.26
10	P	366	ILE	N-CA-C	10.15	120.97	110.62
14	T	135	ALA	N-CA-C	-10.08	100.29	111.28
9	I	161	ALA	N-CA-C	10.03	122.21	111.28
19	a	4	GLU	N-CA-C	10.01	124.75	112.54
14	T	133	ILE	N-CA-C	9.98	119.91	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	166	ALA	N-CA-C	-9.86	100.80	113.12
5	E	64	ALA	N-CA-C	-9.80	99.35	111.11
7	G	325	ARG	N-CA-C	-9.79	100.30	110.97
21	q	138	VAL	CA-C-N	-9.79	112.51	119.66
21	q	138	VAL	C-N-CA	-9.79	112.51	119.66
16	W	87	ILE	N-CA-C	-9.77	101.05	110.42
19	a	2	TRP	N-CA-C	-9.68	101.47	113.28
7	G	654	VAL	N-CA-C	9.67	123.18	111.09
6	F	418	GLN	N-CA-C	-9.55	100.82	111.14
8	H	91	MET	N-CA-C	-9.51	96.50	110.20
8	H	52	ALA	N-CA-C	-9.50	100.91	111.07
17	X	70	PHE	N-CA-C	-9.49	99.72	111.11
12	R	38	TYR	N-CA-C	-9.45	96.35	110.24
4	D	427	PRO	N-CA-C	-9.41	95.72	110.50
21	q	139	PRO	CA-N-CD	9.39	125.15	112.00
10	P	367	GLU	N-CA-C	9.38	122.70	111.82
7	G	694	PHE	N-CA-C	9.35	121.48	111.28
17	X	112	LEU	N-CA-C	-9.35	101.04	111.14
18	Z	69	ILE	N-CA-C	-9.27	100.62	110.36
5	E	85	ALA	N-CA-C	-9.20	101.34	111.36
10	P	369	THR	N-CA-CB	9.18	123.39	110.17
6	F	103	ASN	N-CA-C	-9.17	101.01	113.30
7	G	692	LYS	N-CA-C	-9.16	100.68	112.23
7	G	640	ASP	N-CA-C	-9.16	101.38	111.36
10	P	371	PRO	N-CA-CB	9.10	111.80	103.34
17	X	55	ARG	N-CA-C	9.05	130.07	110.80
19	a	57	VAL	N-CA-C	-8.97	105.19	113.71
6	F	411	SER	N-CA-C	-8.93	101.52	111.07
7	G	133	GLN	N-CA-CB	8.83	121.58	110.45
7	G	212	LYS	N-CA-C	-8.79	94.58	108.90
16	W	20	VAL	N-CA-C	8.69	120.79	108.36
9	I	154	TYR	N-CA-CB	-8.68	99.21	111.62
19	a	3	PHE	CA-CB-CG	8.65	122.45	113.80
13	S	18	GLU	N-CA-C	8.57	123.36	109.40
13	S	86	GLU	N-CA-C	-8.56	102.03	111.36
2	B	100	CYS	N-CA-C	-8.52	102.65	113.72
10	P	373	LYS	N-CA-C	8.46	121.86	110.35
3	C	70	LYS	N-CA-C	8.43	121.53	111.33
17	X	48	TRP	N-CA-C	8.41	120.53	111.36
3	C	108	LYS	N-CA-C	8.36	120.01	111.07
7	G	532	PRO	CA-N-CD	8.34	123.68	112.00
11	Q	54	THR	N-CA-C	8.34	123.31	109.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	X	99	HIS	N-CA-C	-8.33	102.28	111.36
8	H	196	ALA	N-CA-C	8.24	128.03	109.81
7	G	558	GLN	N-CA-C	-8.24	102.25	111.07
7	G	484	ASP	N-CA-C	8.20	121.14	111.71
3	C	196	PRO	N-CA-C	8.19	124.92	113.53
7	G	691	ILE	N-CA-C	8.20	123.69	111.89
6	F	411	SER	N-CA-CB	8.12	121.79	110.01
7	G	534	VAL	N-CA-C	-8.10	104.70	111.91
15	V	86	LYS	N-CA-C	-8.10	102.39	111.14
7	G	62	ARG	N-CA-C	8.10	121.59	108.32
9	I	201	ILE	N-CA-C	-8.01	102.63	110.72
2	B	110	PRO	N-CA-C	8.00	124.45	113.65
17	X	43	PHE	N-CA-C	-8.00	102.51	111.07
13	S	76	THR	N-CA-C	7.99	121.92	108.90
7	G	500	ILE	N-CA-CB	7.96	120.77	110.57
17	X	46	CYS	N-CA-C	-7.93	102.71	111.36
15	V	6	LYS	N-CA-C	-7.92	100.08	110.53
21	q	67	GLU	CB-CA-C	-7.91	99.64	112.06
8	H	271	LEU	N-CA-C	-7.91	102.60	111.14
7	G	651	PRO	CB-CA-C	-7.90	98.52	111.56
1	A	9	ILE	N-CA-C	-7.88	102.58	110.62
17	X	55	ARG	N-CA-CB	-7.85	97.22	110.49
7	G	270	VAL	N-CA-CB	-7.83	100.67	110.31
17	X	58	LYS	N-CA-C	-7.80	102.72	111.07
9	I	74	LEU	N-CA-C	-7.78	102.80	111.28
4	D	141	TYR	CA-C-N	7.78	130.21	120.72
4	D	141	TYR	C-N-CA	7.78	130.21	120.72
21	q	44	TYR	N-CA-C	-7.71	98.87	110.28
17	X	53	PRO	CB-CA-C	-7.69	98.92	111.31
6	F	334	THR	N-CA-C	-7.69	101.64	111.02
12	R	47	ARG	N-CA-C	7.67	120.61	111.33
21	q	89	TRP	N-CA-C	-7.67	102.86	111.14
7	G	569	GLN	N-CA-C	7.62	122.03	108.24
2	B	183	ARG	N-CA-C	-7.62	104.22	113.97
12	R	74	HIS	N-CA-C	7.60	121.22	110.50
5	E	68	ASN	N-CA-CB	7.59	121.01	110.01
9	I	119	CYS	N-CA-C	-7.59	103.09	111.36
14	T	141	PRO	N-CA-C	-7.56	103.02	113.53
6	F	295	PRO	CA-N-CD	7.52	122.53	112.00
9	I	158	CYS	N-CA-C	-7.52	103.08	111.28
4	D	361	ALA	N-CA-C	-7.51	103.22	112.38
8	H	223	PHE	CB-CA-C	-7.50	99.11	110.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	Z	73	PRO	N-CA-C	-7.46	103.15	113.53
6	F	125	CYS	N-CA-C	-7.44	103.77	112.92
4	D	350	LYS	CB-CA-C	-7.43	100.93	111.85
7	G	277	MET	N-CA-C	7.42	120.50	109.59
15	V	57	ASP	N-CA-CB	7.41	120.75	110.01
7	G	303	THR	N-CA-C	7.38	123.00	113.18
13	S	94	VAL	N-CA-C	7.38	117.50	110.42
7	G	510	TRP	N-CA-CB	7.38	120.84	109.85
7	G	374	THR	CB-CA-C	-7.33	99.70	111.28
6	F	430	GLY	N-CA-C	7.33	121.52	112.73
7	G	661	GLU	N-CA-C	7.32	118.94	110.97
14	T	105	MET	N-CA-C	7.30	119.32	111.36
12	R	39	ASP	N-CA-C	7.29	121.16	110.59
17	X	53	PRO	N-CD-CG	-7.28	92.28	103.20
21	q	24	LEU	N-CA-C	-7.28	103.35	111.28
7	G	384	ASN	N-CA-C	-7.27	103.39	111.82
15	V	68	LEU	N-CA-C	-7.24	103.39	111.28
3	C	195	HIS	CB-CA-C	7.22	117.31	110.17
6	F	295	PRO	N-CA-CB	-7.20	96.71	103.19
6	F	269	ARG	N-CA-C	7.19	118.76	111.07
8	H	50	ALA	N-CA-C	7.18	118.75	111.07
7	G	497	VAL	N-CA-C	-7.13	103.35	110.62
15	V	95	LEU	N-CA-C	-7.11	103.53	111.28
4	D	99	LEU	N-CA-C	7.08	121.07	109.24
11	Q	162	ALA	N-CA-C	7.08	119.00	111.28
6	F	246	GLU	N-CA-C	-7.07	103.58	111.28
7	G	150	ARG	N-CA-C	7.05	119.64	109.14
8	H	176	LEU	CA-C-N	-7.04	113.55	120.52
8	H	176	LEU	C-N-CA	-7.04	113.55	120.52
23	s	56	ARG	N-CA-C	7.00	120.58	108.76
6	F	428	GLY	N-CA-C	-6.99	103.82	112.77
6	F	455	GLN	N-CA-C	6.99	118.55	111.07
7	G	217	GLU	N-CA-C	-6.99	101.81	110.41
21	q	77	VAL	N-CA-C	-6.98	99.71	109.21
2	B	166	ASN	N-CA-C	-6.97	103.38	110.97
7	G	582	VAL	N-CA-C	6.96	118.51	108.48
7	G	294	TYR	N-CA-C	-6.95	104.61	113.23
6	F	418	GLN	N-CA-CB	6.94	120.14	110.07
12	R	45	ARG	N-CA-C	-6.94	104.68	113.01
6	F	103	ASN	N-CA-CB	6.92	121.06	110.61
18	Z	34	SER	N-CA-C	-6.91	103.67	111.07
14	T	145	VAL	N-CA-C	-6.87	103.78	110.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	X	53	PRO	N-CA-C	-6.87	104.63	114.18
7	G	268	GLY	N-CA-C	6.84	124.81	115.30
7	G	300	GLN	N-CA-CB	6.84	122.41	112.08
18	Z	28	ARG	N-CA-C	6.81	119.62	108.52
6	F	329	LYS	N-CA-C	6.80	119.56	111.33
7	G	133	GLN	N-CA-C	-6.77	101.27	110.68
22	r	11	LEU	N-CA-C	-6.76	103.99	111.36
15	V	114	TRP	N-CA-CB	6.76	120.37	110.30
8	H	8	THR	N-CA-C	-6.75	101.17	110.35
6	F	244	ASN	N-CA-C	-6.75	100.99	110.50
5	E	140	MET	N-CA-C	-6.73	103.86	111.07
15	V	8	THR	N-CA-C	6.71	119.05	108.79
9	I	208	ASP	N-CA-C	6.70	121.61	113.17
7	G	434	SER	N-CA-C	-6.69	101.06	110.29
4	D	184	ILE	N-CA-C	-6.66	103.82	110.62
10	P	371	PRO	CA-N-CD	-6.66	102.68	112.00
15	V	86	LYS	N-CA-CB	6.66	119.72	110.07
7	G	287	SER	N-CA-C	6.65	119.31	110.53
6	F	344	GLN	N-CA-C	-6.64	104.04	111.28
17	X	129	THR	N-CA-C	6.64	120.85	110.17
7	G	640	ASP	N-CA-CB	6.63	119.97	110.16
11	Q	141	ASN	N-CA-CB	6.62	120.86	110.46
7	G	601	GLY	N-CA-C	6.62	124.83	115.30
5	E	44	PRO	CA-N-CD	6.61	121.26	112.00
3	C	125	PHE	N-CA-CB	-6.61	100.65	110.17
8	H	223	PHE	N-CA-C	-6.61	104.00	111.07
6	F	196	PHE	N-CA-C	6.60	119.92	109.81
6	F	228	PRO	N-CA-C	-6.60	98.88	112.47
14	T	141	PRO	N-CA-CB	6.60	110.59	103.33
3	C	69	PRO	N-CA-C	-6.59	104.37	113.53
8	H	208	VAL	N-CA-CB	-6.59	104.15	111.66
7	G	435	PRO	N-CA-C	-6.58	100.17	110.50
8	H	182	ALA	N-CA-C	-6.58	104.03	111.07
8	H	267	SER	N-CA-C	-6.57	104.20	111.36
10	P	116	ILE	N-CA-C	-6.57	104.09	110.72
4	D	388	GLY	N-CA-C	6.56	119.70	110.38
6	F	336	LEU	N-CA-CB	-6.56	101.00	111.43
22	r	24	LEU	N-CA-C	6.53	119.71	110.50
18	Z	65	LEU	N-CA-C	-6.53	104.25	111.36
13	S	16	LEU	N-CA-C	-6.52	98.27	108.90
21	q	75	TRP	N-CA-C	6.52	121.51	112.45
17	X	98	ARG	N-CA-C	6.51	120.48	112.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	250	SER	N-CA-C	6.47	116.82	108.34
8	H	177	PRO	N-CA-C	-6.47	101.49	111.13
15	V	49	GLU	N-CA-C	-6.47	104.23	111.28
7	G	361	VAL	N-CA-C	-6.46	105.03	111.88
14	T	141	PRO	CA-N-CD	-6.46	102.95	112.00
21	q	28	PHE	N-CA-C	6.44	117.96	111.07
7	G	605	GLN	N-CA-C	6.43	119.00	108.52
12	R	81	GLY	N-CA-C	-6.43	106.85	115.21
3	C	125	PHE	N-CA-C	6.43	119.57	110.50
7	G	275	PRO	CB-CA-C	-6.42	102.57	110.98
6	F	370	LEU	N-CA-C	-6.40	104.38	111.36
7	G	95	PRO	N-CA-C	-6.40	101.14	110.80
7	G	275	PRO	CA-N-CD	6.40	120.95	112.00
11	Q	59	LEU	N-CA-C	-6.39	100.71	110.30
6	F	78	GLY	N-CA-C	-6.39	104.59	112.77
4	D	140	ASP	N-CA-C	-6.39	96.57	107.23
15	V	71	LEU	N-CA-C	6.36	118.22	111.28
5	E	141	LEU	N-CA-C	-6.35	101.72	110.35
7	G	273	ILE	N-CA-C	-6.34	98.38	107.77
9	I	205	ILE	N-CA-C	-6.33	104.33	110.72
22	r	8	ILE	N-CA-C	-6.32	104.34	110.72
6	F	415	ILE	N-CA-C	-6.32	104.34	110.72
19	a	26	ILE	N-CA-C	-6.31	104.48	113.07
8	H	271	LEU	N-CA-CB	6.30	119.21	110.07
15	V	91	ALA	N-CA-C	-6.30	104.42	111.28
7	G	176	CYS	N-CA-C	6.30	119.61	110.42
22	r	26	LEU	N-CA-CB	-6.29	100.97	110.35
10	P	315	THR	N-CA-C	6.27	118.95	109.23
4	D	233	HIS	N-CA-C	6.26	119.03	111.40
4	D	141	TYR	N-CA-C	6.26	120.92	113.16
17	X	99	HIS	N-CA-CB	6.25	119.41	110.16
8	H	52	ALA	N-CA-CB	6.24	119.06	110.01
6	F	416	SER	N-CA-C	6.24	117.75	111.07
7	G	383	SER	N-CA-C	-6.24	106.89	114.75
8	H	269	THR	N-CA-C	6.23	118.07	111.28
11	Q	141	ASN	N-CA-C	-6.22	105.69	113.28
21	q	69	ASN	N-CA-CB	6.22	121.37	111.66
5	E	64	ALA	N-CA-CB	6.21	119.19	109.94
18	Z	69	ILE	N-CA-CB	6.20	117.39	110.51
2	B	113	ASP	N-CA-CB	6.19	119.42	109.28
4	D	291	VAL	N-CA-C	-6.18	103.37	111.09
10	P	368	GLU	N-CA-CB	6.18	119.81	110.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	409	ILE	N-CA-C	6.16	116.34	110.42
8	H	101	GLY	N-CA-C	6.16	120.09	112.64
6	F	212	LEU	N-CA-C	-6.16	104.57	111.28
7	G	420	LYS	N-CA-C	6.15	118.77	111.33
17	X	51	LYS	N-CA-C	6.15	117.65	111.07
7	G	418	ILE	N-CA-C	-6.14	103.44	112.04
8	H	276	SER	N-CA-C	6.14	118.94	111.82
7	G	325	ARG	N-CA-CB	6.12	118.84	109.91
6	F	272	GLY	N-CA-C	6.09	122.33	111.01
13	S	61	VAL	N-CA-C	-6.08	99.73	108.42
7	G	638	THR	N-CA-C	-6.08	100.06	109.24
10	P	118	LYS	N-CA-C	6.08	118.87	111.82
18	Z	65	LEU	N-CA-CB	6.08	119.15	110.16
13	S	87	VAL	N-CA-C	-6.03	104.47	110.62
8	H	185	TRP	N-CA-C	-6.03	104.07	112.45
7	G	508	ALA	N-CA-C	6.03	117.85	111.28
8	H	24	GLU	N-CA-C	-6.03	104.07	112.45
7	G	532	PRO	N-CA-CB	-6.00	97.08	103.38
10	P	370	LYS	N-CA-C	5.99	119.20	108.47
9	I	160	GLU	N-CA-CB	-5.99	100.71	109.82
12	R	34	THR	N-CA-C	-5.99	106.62	112.97
2	B	196	PRO	N-CA-C	-5.99	101.81	111.03
7	G	353	ALA	N-CA-C	-5.98	104.70	112.23
9	I	66	LEU	N-CA-C	-5.96	104.36	111.69
5	E	66	VAL	N-CA-C	5.92	116.57	110.36
8	H	7	LEU	N-CA-C	-5.92	104.46	111.03
22	r	108	LYS	N-CA-C	5.89	117.78	111.36
22	r	92	LYS	N-CA-CB	-5.89	101.69	110.17
4	D	352	PRO	N-CA-CB	-5.88	97.38	103.08
8	H	208	VAL	N-CA-C	5.88	116.14	107.15
17	X	38	LYS	N-CA-C	-5.87	104.79	111.07
7	G	639	LEU	N-CA-C	5.87	118.63	111.82
7	G	480	ALA	N-CA-C	-5.86	104.97	111.36
13	S	86	GLU	N-CA-CB	5.86	118.84	110.16
21	q	5	GLU	N-CA-C	-5.86	104.98	111.36
11	Q	164	PHE	N-CA-CB	5.85	119.90	110.42
9	I	116	CYS	N-CA-C	-5.85	105.64	112.89
21	q	65	THR	N-CA-C	5.85	119.20	110.14
3	C	209	LEU	N-CA-CB	-5.84	100.67	110.83
10	P	330	THR	CB-CA-C	-5.84	109.83	116.54
10	P	122	HIS	N-CA-C	5.83	120.09	112.92
14	T	94	ASP	N-CA-CB	-5.83	105.19	111.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	P	367	GLU	CB-CA-C	-5.82	99.49	110.67
5	E	223	CYS	CB-CA-C	-5.82	109.32	117.23
7	G	672	ALA	N-CA-C	-5.82	104.94	111.28
7	G	289	LYS	N-CA-C	5.81	117.61	111.28
15	V	19	THR	N-CA-CB	5.81	120.70	110.37
6	F	393	ASN	N-CA-C	-5.80	104.86	111.07
17	X	36	CYS	CB-CA-C	-5.80	102.52	111.74
18	Z	44	ILE	N-CA-C	-5.78	104.87	110.42
17	X	97	PHE	N-CA-C	5.77	118.51	111.82
7	G	275	PRO	N-CA-CB	-5.76	97.97	103.33
4	D	414	ASP	N-CA-C	-5.75	101.45	110.36
5	E	137	THR	CA-C-N	-5.75	112.99	118.97
5	E	137	THR	C-N-CA	-5.75	112.99	118.97
4	D	258	VAL	N-CA-C	-5.74	104.08	110.62
10	P	119	ALA	N-CA-C	-5.73	104.95	111.14
19	a	3	PHE	N-CA-CB	5.73	118.66	110.06
13	S	73	GLN	N-CA-C	-5.71	100.39	109.59
10	P	272	LEU	N-CA-C	-5.69	101.86	110.28
12	R	35	GLY	N-CA-C	5.69	121.79	113.48
21	q	140	PRO	N-CA-C	-5.67	102.23	110.80
9	I	191	LEU	N-CA-C	-5.67	105.18	111.36
6	F	457	HIS	N-CA-CB	-5.66	100.87	110.50
17	X	56	CYS	N-CA-C	5.65	119.87	112.92
12	R	52	GLN	N-CA-C	5.65	117.98	110.53
11	Q	124	MET	CA-C-N	-5.64	114.98	122.98
11	Q	124	MET	C-N-CA	-5.64	114.98	122.98
2	B	112	TYR	N-CA-C	5.63	122.80	110.80
18	Z	64	ASP	N-CA-C	5.63	119.88	112.89
5	E	183	PRO	N-CA-C	-5.63	102.08	111.26
13	S	63	PRO	CA-N-CD	5.63	119.88	112.00
2	B	135	GLY	N-CA-C	5.62	118.60	111.85
4	D	352	PRO	N-CA-C	5.62	117.56	110.70
5	E	119	THR	N-CA-C	-5.59	105.96	112.89
6	F	268	GLU	CB-CA-C	-5.59	110.11	116.54
7	G	599	THR	CA-C-N	-5.58	114.23	122.83
7	G	599	THR	C-N-CA	-5.58	114.23	122.83
2	B	201	LEU	N-CA-C	-5.58	105.10	111.07
7	G	615	LEU	N-CA-C	-5.58	106.24	113.16
7	G	530	TYR	N-CA-C	-5.58	102.03	110.28
21	q	68	MET	N-CA-C	5.57	119.33	112.54
17	X	40	ASN	N-CA-C	-5.55	104.92	110.97
12	R	89	PRO	N-CA-CB	-5.54	98.28	103.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	163	PRO	N-CA-CB	-5.52	97.73	103.08
7	G	682	ASP	CA-C-N	-5.52	114.08	119.76
7	G	682	ASP	C-N-CA	-5.52	114.08	119.76
4	D	132	ALA	N-CA-C	-5.51	106.55	113.72
10	P	86	CYS	N-CA-C	-5.51	103.11	110.55
19	a	25	TYR	N-CA-C	-5.51	107.81	114.75
4	D	231	GLY	N-CA-C	-5.51	102.99	110.43
14	T	135	ALA	N-CA-CB	5.50	118.20	110.12
21	q	142	THR	N-CA-CB	5.50	119.74	109.68
22	r	111	PRO	N-CA-C	-5.49	106.38	113.57
7	G	127	ASP	CA-C-O	5.49	128.97	121.89
21	q	71	LYS	N-CA-C	5.47	119.94	113.16
7	G	404	GLY	N-CA-C	5.46	121.45	113.48
7	G	556	THR	N-CA-C	-5.45	101.48	109.81
4	D	201	PHE	N-CA-C	-5.43	105.44	111.36
17	X	27	ALA	N-CA-C	-5.43	105.01	111.69
22	r	94	ALA	N-CA-C	-5.42	101.82	109.96
7	G	420	LYS	N-CA-CB	-5.42	101.92	110.06
7	G	150	ARG	N-CA-CB	-5.42	102.84	111.62
12	R	88	HIS	CB-CA-C	5.41	117.36	109.08
11	Q	164	PHE	N-CA-C	-5.41	106.66	113.20
4	D	391	VAL	CA-C-N	-5.40	115.77	119.66
4	D	391	VAL	C-N-CA	-5.40	115.77	119.66
6	F	180	GLY	N-CA-C	-5.40	108.19	115.21
10	P	374	THR	N-CA-C	5.39	117.52	108.73
4	D	200	PHE	CA-CB-CG	5.38	119.18	113.80
5	E	74	GLN	N-CA-C	-5.37	107.38	114.04
2	B	101	ALA	N-CA-C	-5.37	105.43	111.28
4	D	109	CYS	N-CA-C	5.36	118.47	107.69
6	F	199	ARG	N-CA-C	5.36	117.47	109.59
18	Z	55	GLN	N-CA-C	-5.36	105.44	111.28
14	T	92	LYS	N-CA-C	-5.36	106.33	112.92
5	E	143	ASP	N-CA-C	5.35	119.01	111.52
11	Q	163	ASN	CB-CA-C	-5.35	99.30	109.95
18	Z	50	MET	N-CA-C	-5.34	105.46	111.28
4	D	141	TYR	N-CA-CB	-5.32	102.30	110.44
17	X	33	GLY	N-CA-C	-5.31	107.74	114.16
8	H	46	LEU	N-CA-C	-5.30	106.59	113.16
5	E	44	PRO	N-CA-CB	-5.30	97.67	103.39
8	H	103	LEU	N-CA-C	-5.29	105.41	111.07
10	P	68	TYR	N-CA-C	5.28	117.12	111.36
7	G	510	TRP	N-CA-C	-5.27	102.05	109.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	V	84	ALA	N-CA-C	5.27	116.71	111.07
8	H	146	MET	N-CA-C	-5.25	105.45	111.07
6	F	412	LEU	N-CA-C	-5.25	105.73	111.82
7	G	435	PRO	CB-CA-C	-5.24	105.84	111.56
4	D	363	VAL	N-CA-C	5.24	116.31	111.81
22	r	25	GLN	N-CA-C	5.22	118.91	112.54
9	I	160	GLU	CB-CA-C	5.22	119.22	110.92
7	G	277	MET	N-CA-CB	-5.21	101.69	109.71
10	P	204	SER	CA-C-O	-5.21	114.99	121.50
11	Q	72	ILE	N-CA-C	-5.20	108.44	113.53
22	r	107	SER	N-CA-C	-5.20	102.17	109.96
7	G	600	GLU	CB-CA-C	-5.19	103.01	111.06
8	H	305	ILE	N-CA-C	-5.19	106.08	111.58
17	X	54	ARG	CB-CA-C	5.19	119.46	110.84
9	I	95	PRO	N-CA-C	5.19	121.33	113.81
13	S	85	ASP	N-CA-C	5.18	117.83	111.82
7	G	569	GLN	CB-CA-C	-5.17	104.19	112.05
4	D	391	VAL	N-CA-C	5.16	113.82	109.02
7	G	713	ALA	N-CA-C	-5.16	105.54	111.07
4	D	91	ALA	CB-CA-C	-5.16	110.61	116.54
4	D	86	PRO	N-CA-C	-5.15	108.79	114.92
7	G	172	ILE	N-CA-C	-5.15	98.63	109.34
8	H	196	ALA	CA-C-N	-5.15	113.45	119.32
8	H	196	ALA	C-N-CA	-5.15	113.45	119.32
22	r	111	PRO	CA-N-CD	5.14	119.19	112.00
3	C	109	SER	N-CA-C	5.13	118.18	109.76
6	F	271	SER	N-CA-C	-5.13	99.93	108.34
3	C	156	VAL	N-CA-C	-5.13	104.09	111.17
6	F	337	MET	CB-CA-C	-5.13	103.06	111.68
8	H	277	TYR	N-CA-C	5.13	117.95	110.10
3	C	164	TRP	N-CA-C	5.11	116.93	111.36
3	C	221	GLU	N-CA-C	-5.11	102.32	108.25
7	G	393	GLY	N-CA-C	-5.11	107.68	115.66
20	b	82	LYS	N-CA-C	-5.09	103.81	110.53
10	P	376	ASN	CB-CA-C	-5.09	102.20	110.85
1	A	2	ASN	CA-C-N	-5.08	113.07	120.29
1	A	2	ASN	C-N-CA	-5.08	113.07	120.29
14	T	140	CYS	CB-CA-C	-5.08	104.06	109.85
5	E	181	ASN	N-CA-C	-5.07	99.53	108.20
6	F	293	SER	CB-CA-C	-5.06	104.41	111.80
4	D	224	ALA	N-CA-C	5.05	117.17	111.11
10	P	136	THR	N-CA-CB	-5.05	102.75	110.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	137	THR	N-CA-C	5.04	120.95	109.81
21	q	13	GLN	N-CA-C	-5.04	105.68	111.07
22	r	4	ALA	N-CA-C	-5.04	105.88	112.23
17	X	112	LEU	N-CA-CB	5.03	117.36	110.07
21	q	89	TRP	N-CA-CB	5.02	117.36	110.07
3	C	208	GLU	CA-C-O	-5.02	115.73	121.40
7	G	280	ASP	N-CA-CB	-5.02	102.74	110.12
18	Z	130	LYS	N-CA-C	-5.01	105.71	111.07
8	H	116	ILE	CB-CA-C	-5.01	105.38	112.14
12	R	65	ALA	N-CA-C	-5.00	105.96	111.71

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	737	0	800	67	0
2	B	1247	0	1256	136	0
3	C	1641	0	1596	116	0
4	D	3088	0	3059	312	0
5	E	1635	0	1626	173	0
6	F	3273	0	3231	307	0
7	G	5287	0	5323	526	0
8	H	2531	0	2619	320	0
9	I	1389	0	1352	139	0
10	P	2720	0	2740	227	0
11	Q	957	0	949	79	0
12	R	587	0	579	66	0
13	S	667	0	683	91	0
14	T	604	0	596	93	0
15	V	915	0	954	79	0
16	W	970	0	991	65	0
17	X	1164	0	1154	103	0
18	Z	1152	0	1148	77	0
19	a	548	0	562	63	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	b	620	0	617	74	0
21	q	1020	0	976	92	0
22	r	418	0	434	50	0
23	s	238	0	225	24	0
24	B	8	0	0	3	0
24	F	8	0	0	6	0
24	G	16	0	0	2	0
24	I	16	0	0	5	0
25	B	35	0	44	6	0
25	I	43	0	60	9	0
26	E	4	0	0	4	0
26	G	4	0	0	5	0
27	F	31	0	19	1	0
28	H	51	0	82	8	0
29	P	48	0	26	5	0
30	q	57	0	58	22	0
All	All	33729	0	33759	2794	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 41.

All (2794) 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:G:571:HIS:HD2	7:G:572:HIS:ND1	1.32	1.27
7:G:126:LEU:HD12	7:G:126:LEU:O	1.38	1.19
12:R:38:TYR:HE2	21:q:127:TYR:HB2	1.04	1.17
7:G:387:LEU:HA	7:G:514:ASN:HB2	1.22	1.16
4:D:145:MET:O	4:D:148:GLU:HG2	1.47	1.15
2:B:112:TYR:OH	9:I:91:GLY:HA3	1.47	1.13
5:E:174:GLU:HG2	6:F:369:ARG:HH12	1.12	1.12
9:I:54:THR:HG22	20:b:13:TRP:HE1	1.02	1.12
12:R:38:TYR:CE2	21:q:127:TYR:HB2	1.85	1.11
17:X:4:ILE:HG22	17:X:5:VAL:H	0.96	1.10
9:I:101:HIS:HB2	9:I:149:MET:HE1	1.33	1.09
2:B:112:TYR:CE1	9:I:84:ILE:HD11	1.88	1.09
9:I:85:ASN:HB2	9:I:89:GLU:OE1	1.53	1.08
15:V:84:ALA:O	15:V:87:GLU:HG2	1.53	1.08
7:G:571:HIS:CD2	7:G:572:HIS:ND1	2.22	1.08
8:H:172:MET:HE2	8:H:177:PRO:HD3	1.33	1.07
4:D:83:ASN:HA	4:D:98:VAL:HA	1.34	1.07

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:r:2:ALA:N	22:r:26:LEU:HD12	1.70	1.06
3:C:149:LEU:HD11	16:W:80:ARG:NH2	1.70	1.06
9:I:53:ALA:HB1	20:b:14:ALA:HB2	1.27	1.06
4:D:279:THR:HG23	15:V:13:GLY:HA3	1.34	1.06
6:F:270:ASN:OD1	6:F:270:ASN:O	1.70	1.06
13:S:23:LEU:HD12	13:S:23:LEU:O	1.54	1.06
8:H:24:GLU:HA	8:H:271:LEU:HD23	1.39	1.05
7:G:634:LEU:HD13	7:G:636:TYR:OH	1.57	1.04
14:T:138:LEU:HD12	14:T:138:LEU:O	1.55	1.04
2:B:149:TYR:HA	2:B:152:MET:HE2	1.35	1.04
13:S:79:LEU:HA	13:S:82:LEU:HD12	1.38	1.04
9:I:53:ALA:CB	20:b:14:ALA:HB2	1.88	1.02
17:X:90:ASP:OD2	19:a:62:VAL:HG11	1.59	1.02
8:H:186:PHE:CE1	8:H:270:PHE:CE1	2.48	1.02
9:I:208:ASP:O	9:I:208:ASP:OD1	1.75	1.02
6:F:392:MET:HE3	6:F:419:ILE:HD12	1.41	1.01
7:G:360:LYS:HB2	7:G:632:ILE:HD12	1.43	1.01
7:G:579:MET:O	7:G:579:MET:HG3	1.58	1.01
9:I:119:CYS:HG	24:I:303:SF4:FE2	0.75	1.01
15:V:72:LEU:HD11	15:V:80:VAL:HG21	1.40	1.00
3:C:124:ARG:NH1	3:C:125:PHE:CZ	2.30	1.00
2:B:202:LEU:HD12	9:I:86:TYR:CD2	1.95	1.00
21:q:66:THR:HG22	21:q:74:PHE:HB2	1.39	1.00
5:E:203:ILE:HG23	5:E:213:PRO:HG2	1.43	1.00
7:G:646:LEU:HD22	7:G:653:LEU:HD13	1.45	0.99
7:G:213:MET:HE2	7:G:215:MET:HB2	1.40	0.98
8:H:186:PHE:CE1	8:H:270:PHE:HE1	1.81	0.98
2:B:82:ILE:HG23	8:H:57:MET:SD	2.03	0.98
16:W:55:LEU:HB3	16:W:107:MET:CE	1.94	0.98
17:X:4:ILE:HG22	17:X:5:VAL:N	1.76	0.97
6:F:379:CYS:SG	24:F:502:SF4:FE1	1.56	0.97
6:F:382:CYS:HG	24:F:502:SF4:FE2	0.76	0.97
7:G:611:THR:HG21	11:Q:105:GLU:HA	1.47	0.97
7:G:597:VAL:HG12	7:G:603:ALA:HA	1.47	0.96
3:C:227:GLN:NE2	3:C:230:ARG:HH12	1.63	0.96
9:I:54:THR:HG22	20:b:13:TRP:NE1	1.80	0.96
10:P:376:ASN:OD1	10:P:377:TYR:N	1.98	0.96
7:G:557:ARG:HG3	7:G:579:MET:HE3	1.48	0.96
9:I:54:THR:CG2	20:b:13:TRP:HE1	1.77	0.96
6:F:345:ALA:O	6:F:346:GLN:HG2	1.66	0.96
5:E:57:GLU:HA	5:E:60:LYS:HE2	1.46	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:76:ARG:HH21	7:G:79:LEU:HD21	1.31	0.96
7:G:569:GLN:HE22	7:G:622:ILE:HG21	1.30	0.95
19:a:64:LYS:HE2	19:a:66:LEU:HD12	1.43	0.95
3:C:227:GLN:HE21	3:C:230:ARG:NH1	1.64	0.95
5:E:189:ASP:CG	6:F:163:TYR:HB3	1.92	0.95
7:G:78:CYS:SG	26:G:803:FES:FE2	1.59	0.95
9:I:94:SER:HB2	9:I:95:PRO:HD2	1.48	0.95
3:C:98:PHE:HA	15:V:90:LEU:HD11	1.47	0.94
4:D:302:LEU:HB2	4:D:401:GLU:HG2	1.48	0.94
13:S:16:LEU:HD11	13:S:51:LEU:HD11	1.46	0.94
7:G:64:CYS:HG	26:G:803:FES:FE1	0.71	0.94
3:C:85:ILE:CD1	3:C:140:ILE:HD11	1.98	0.94
9:I:162:CYS:SG	24:I:303:SF4:FE4	1.60	0.94
6:F:63:TYR:HB3	6:F:256:ARG:HE	1.29	0.93
8:H:90:PRO:HG3	8:H:162:LEU:HB3	1.48	0.93
4:D:145:MET:HG2	4:D:148:GLU:OE2	1.69	0.93
9:I:113:CYS:SG	24:I:303:SF4:FE3	1.60	0.93
4:D:359:ASP:HB3	7:G:150:ARG:HH22	1.34	0.93
7:G:176:CYS:SG	24:G:802:SF4:FE4	1.59	0.92
7:G:78:CYS:HG	26:G:803:FES:FE2	0.63	0.92
7:G:545:LEU:HB3	7:G:566:ILE:HG22	1.52	0.92
17:X:4:ILE:CG2	17:X:5:VAL:H	1.82	0.92
4:D:280:ALA:CB	15:V:11:LEU:HG	2.00	0.92
16:W:55:LEU:HB3	16:W:107:MET:HE1	1.52	0.92
5:E:179:CYS:SG	26:E:301:FES:FE2	1.63	0.91
6:F:225:LEU:HB2	11:Q:160:TYR:CE2	2.06	0.91
7:G:36:VAL:HG11	7:G:56:VAL:HG11	1.52	0.91
10:P:221:ARG:HD3	10:P:286:ARG:HD3	1.51	0.91
6:F:379:CYS:HG	24:F:502:SF4:FE1	0.88	0.90
7:G:262:VAL:HG23	7:G:276:ARG:HB3	1.51	0.90
5:E:39:VAL:HG22	7:G:205:GLN:HE22	1.34	0.90
7:G:362:ASP:HB2	13:S:71:PHE:CE1	2.06	0.90
7:G:283:GLU:O	7:G:283:GLU:HG2	1.71	0.90
4:D:84:PHE:HB3	4:D:97:LEU:HB3	1.50	0.90
9:I:80:GLU:HG3	19:a:1:MET:SD	2.11	0.90
7:G:617:ARG:HH11	16:W:129:HIS:HA	1.35	0.89
3:C:203:LEU:HD11	4:D:123:LEU:HD13	1.54	0.89
4:D:270:ASN:HB3	8:H:284:GLN:NE2	1.87	0.89
7:G:431:LEU:HD22	7:G:438:LEU:HD11	1.53	0.89
15:V:72:LEU:HD12	15:V:72:LEU:O	1.73	0.89
2:B:170:TYR:HB2	9:I:153:ILE:HG21	1.55	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Z:86:ILE:HG23	18:Z:128:ARG:HE	1.38	0.89
6:F:404:ALA:O	6:F:450:MET:SD	2.32	0.88
21:q:76:ASP:OD1	21:q:76:ASP:O	1.90	0.88
9:I:67:ILE:HG23	25:I:301:PC1:H381	1.53	0.88
1:A:55:PHE:CZ	8:H:282:TYR:HE2	1.92	0.88
10:P:344:PRO:HB2	10:P:347:LEU:HD13	1.56	0.88
25:B:302:PC1:H142	8:H:39:ILE:HD11	1.55	0.88
12:R:51:ARG:HH21	21:q:125:VAL:HG12	1.38	0.88
6:F:55:GLY:HA2	6:F:58:ARG:HD2	1.54	0.88
13:S:16:LEU:HD22	13:S:19:ILE:HD11	1.54	0.87
6:F:327:ILE:HD11	6:F:331:VAL:HG11	1.57	0.87
14:T:79:ILE:HB	14:T:145:VAL:HG13	1.55	0.87
3:C:217:ARG:HH12	16:W:112:GLU:HB2	1.38	0.87
10:P:122:HIS:HB2	12:R:46:VAL:HG12	1.55	0.87
7:G:546:PHE:HZ	7:G:569:GLN:HE21	1.16	0.87
6:F:41:ILE:HG21	6:F:250:VAL:HG12	1.53	0.87
8:H:24:GLU:HA	8:H:271:LEU:CD2	2.04	0.87
6:F:338:ASP:OD1	6:F:341:ALA:HB3	1.75	0.87
13:S:16:LEU:HD12	13:S:16:LEU:O	1.76	0.86
2:B:99:CYS:HB3	4:D:141:TYR:CD2	2.10	0.86
6:F:425:CYS:HG	24:F:502:SF4:FE4	0.56	0.86
9:I:153:ILE:HD11	9:I:155:CYS:HB3	1.56	0.86
14:T:138:LEU:HD13	14:T:144:ILE:HG12	1.56	0.86
22:r:2:ALA:N	22:r:26:LEU:CD1	2.37	0.86
7:G:387:LEU:CA	7:G:514:ASN:HB2	2.03	0.86
7:G:404:GLY:HA3	7:G:684:LEU:HD13	1.57	0.86
10:P:221:ARG:HD3	10:P:286:ARG:CD	2.05	0.86
5:E:147:ILE:HG23	5:E:200:ILE:HG12	1.58	0.86
25:B:302:PC1:H322	25:B:302:PC1:H232	1.55	0.86
7:G:617:ARG:NH1	16:W:129:HIS:HA	1.90	0.85
3:C:217:ARG:NH1	16:W:112:GLU:HB2	1.91	0.85
2:B:116:ARG:HA	8:H:37:PRO:HA	1.56	0.85
15:V:75:GLY:HA2	22:r:103:ARG:HD2	1.59	0.85
16:W:55:LEU:HD22	16:W:107:MET:HE2	1.58	0.85
9:I:78:PHE:HB3	22:r:8:ILE:CG2	2.07	0.85
21:q:42:ASP:OD2	21:q:83:PRO:HG2	1.77	0.85
3:C:114:THR:HG22	4:D:421:ARG:HH12	1.42	0.85
5:E:179:CYS:HG	26:E:301:FES:FE2	0.54	0.85
12:R:32:THR:HG22	12:R:36:GLN:H	1.39	0.85
14:T:110:LEU:HG	14:T:114:ASP:HB2	1.59	0.85
2:B:152:MET:HB3	2:B:153:PRO:HD2	1.57	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:571:HIS:HD2	7:G:572:HIS:CE1	1.96	0.84
7:G:404:GLY:CA	7:G:684:LEU:HD13	2.08	0.84
10:P:94:LEU:HA	10:P:97:MET:HE2	1.59	0.84
15:V:84:ALA:O	15:V:87:GLU:CG	2.25	0.84
10:P:275:HIS:HA	10:P:278:LYS:HE2	1.60	0.84
21:q:85:GLU:HG2	21:q:98:PRO:HB3	1.59	0.84
2:B:82:ILE:HG12	8:H:57:MET:CE	2.06	0.84
8:H:142:TYR:HA	8:H:289:LEU:CD1	2.06	0.84
15:V:56:LEU:HD12	15:V:57:ASP:N	1.92	0.84
8:H:172:MET:CE	8:H:176:LEU:HB2	2.07	0.83
22:r:4:ALA:HB1	22:r:9:GLN:HB2	1.60	0.83
7:G:674:LEU:HD11	13:S:46:LYS:HE2	1.60	0.83
3:C:114:THR:HG22	4:D:421:ARG:NH1	1.93	0.83
3:C:172:MET:CE	3:C:187:LEU:HB2	2.08	0.83
7:G:176:CYS:HG	24:G:802:SF4:FE4	0.53	0.83
3:C:168:GLU:HB2	3:C:186:ILE:HD11	1.59	0.83
7:G:304:GLU:HG2	7:G:615:LEU:HD12	1.60	0.83
17:X:50:GLU:HG2	17:X:138:PRO:HG3	1.59	0.83
2:B:92:PRO:HD2	2:B:121:PHE:H	1.44	0.83
3:C:172:MET:HE1	3:C:187:LEU:HB2	1.60	0.83
6:F:278:ILE:HD11	6:F:299:LEU:HD21	1.61	0.82
13:S:48:HIS:CE1	13:S:95:LEU:HD22	2.13	0.82
4:D:329:ARG:HD2	4:D:453:THR:HB	1.62	0.82
7:G:130:ILE:HG22	7:G:175:ARG:HH22	1.43	0.82
10:P:122:HIS:CB	12:R:46:VAL:HG12	2.08	0.82
4:D:254:ARG:HH11	22:r:25:GLN:HB2	1.44	0.82
10:P:141:PHE:HD2	10:P:179:LYS:HD2	1.43	0.82
11:Q:146:ASP:OD1	11:Q:146:ASP:O	1.97	0.82
16:W:55:LEU:CD2	16:W:107:MET:HE2	2.09	0.82
10:P:221:ARG:CD	10:P:286:ARG:HD3	2.10	0.81
5:E:174:GLU:OE2	6:F:373:PHE:CD1	2.33	0.81
6:F:422:HIS:HD2	7:G:79:LEU:HD12	1.45	0.81
7:G:64:CYS:SG	26:G:803:FES:FE1	1.72	0.81
7:G:404:GLY:HA2	7:G:684:LEU:CD1	2.09	0.81
3:C:85:ILE:HG13	3:C:140:ILE:HD11	1.60	0.81
7:G:425:ASN:OD1	7:G:426:ASP:N	2.12	0.81
8:H:172:MET:CE	8:H:177:PRO:HD3	2.09	0.81
21:q:71:LYS:O	21:q:72:ASN:OD1	1.99	0.81
7:G:652:ASN:OD1	7:G:653:LEU:N	2.14	0.81
8:H:97:ASN:HD22	19:a:38:VAL:HG13	1.46	0.81
8:H:187:ILE:HD12	28:H:401:3PE:H242	1.62	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:b:67:PRO:HD3	20:b:74:LEU:HB2	1.60	0.81
2:B:99:CYS:HB3	4:D:141:TYR:CE2	2.16	0.80
4:D:145:MET:CG	4:D:148:GLU:OE2	2.30	0.80
10:P:163:ARG:HD2	10:P:253:THR:HA	1.62	0.80
14:T:93:ILE:HG21	14:T:110:LEU:HD22	1.63	0.80
3:C:227:GLN:NE2	3:C:230:ARG:NH1	2.25	0.80
7:G:385:TYR:HA	7:G:515:ILE:HD11	1.63	0.80
6:F:422:HIS:HD2	7:G:79:LEU:CD1	1.95	0.80
6:F:422:HIS:NE2	7:G:112:ALA:HA	1.95	0.80
8:H:51:ASP:OD1	8:H:52:ALA:N	2.15	0.80
8:H:235:ASN:ND2	8:H:270:PHE:CE2	2.50	0.80
13:S:36:PHE:HZ	13:S:44:LEU:HD11	1.45	0.80
15:V:95:LEU:HA	15:V:100:TRP:HH2	1.46	0.80
3:C:85:ILE:CG1	3:C:140:ILE:HD11	2.12	0.80
7:G:334:GLU:OE1	13:S:71:PHE:HE1	1.64	0.80
9:I:162:CYS:HG	24:I:303:SF4:FE4	0.50	0.80
17:X:120:PRO:CB	17:X:125:LEU:HD11	2.13	0.79
4:D:127:LYS:HB3	4:D:131:GLN:HG3	1.65	0.79
6:F:338:ASP:OD1	6:F:341:ALA:CB	2.30	0.79
7:G:432:ILE:HG23	7:G:451:ILE:HD11	1.63	0.79
8:H:17:MET:SD	8:H:229:THR:OG1	2.41	0.79
5:E:78:VAL:HG23	5:E:79:LEU:HD12	1.63	0.79
6:F:392:MET:CE	6:F:416:SER:HA	2.12	0.79
10:P:208:GLY:H	10:P:211:ASP:HB3	1.48	0.79
7:G:213:MET:HE2	7:G:215:MET:CB	2.13	0.79
14:T:87:LEU:HD21	14:T:104:PHE:HZ	1.47	0.79
7:G:404:GLY:CA	7:G:684:LEU:CD1	2.61	0.79
9:I:113:CYS:HG	24:I:303:SF4:FE3	0.48	0.79
7:G:169:VAL:HG22	7:G:223:ILE:HD11	1.64	0.79
8:H:27:ILE:HG23	8:H:31:MET:HE3	1.65	0.79
9:I:68:ARG:NH2	18:Z:26:PRO:HD2	1.97	0.79
2:B:82:ILE:HG12	8:H:57:MET:HE1	1.64	0.78
4:D:359:ASP:HB3	7:G:150:ARG:NH2	1.97	0.78
6:F:425:CYS:SG	24:F:502:SF4:FE4	1.74	0.78
7:G:272:ARG:HD2	7:G:274:LEU:HD23	1.63	0.78
7:G:454:ASP:HA	7:G:459:ARG:HH21	1.48	0.78
8:H:20:LEU:HD22	8:H:228:TYR:HD2	1.48	0.78
4:D:198:THR:HG22	8:H:32:GLN:HE21	1.49	0.78
13:S:20:ARG:HG3	13:S:54:LEU:HB2	1.64	0.78
19:a:3:PHE:HE2	30:q:201:CDL:HA4	1.47	0.78
11:Q:81:VAL:HG21	11:Q:150:LYS:HG3	1.65	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:86:TRP:CZ2	19:a:64:LYS:HB3	2.18	0.78
4:D:254:ARG:HE	22:r:25:GLN:NE2	1.81	0.78
6:F:422:HIS:CD2	7:G:79:LEU:CD1	2.66	0.78
8:H:151:LEU:HA	8:H:154:LEU:HD12	1.66	0.78
2:B:82:ILE:HA	8:H:57:MET:HE1	1.64	0.77
14:T:87:LEU:HD22	14:T:104:PHE:CE1	2.19	0.77
7:G:667:GLN:HE21	13:S:38:VAL:HA	1.49	0.77
4:D:128:THR:H	4:D:131:GLN:HE21	1.32	0.77
4:D:280:ALA:HB1	15:V:11:LEU:HG	1.66	0.77
7:G:126:LEU:O	7:G:126:LEU:CD1	2.26	0.77
7:G:664:TYR:OH	13:S:23:LEU:HD11	1.84	0.77
6:F:424:ILE:HD11	7:G:73:GLY:O	1.85	0.77
7:G:600:GLU:HG3	7:G:659:ILE:HD12	1.66	0.77
8:H:196:ALA:HB2	8:H:274:ARG:HG3	1.65	0.77
17:X:124:GLN:O	17:X:125:LEU:HD12	1.85	0.77
18:Z:144:THR:HA	19:a:45:TRP:HZ3	1.50	0.77
7:G:357:LEU:HD12	7:G:632:ILE:HD11	1.65	0.77
14:T:83:VAL:CG2	14:T:126:PHE:HZ	1.97	0.77
7:G:377:ALA:HB2	7:G:671:LEU:HD22	1.67	0.77
7:G:506:VAL:HG21	7:G:510:TRP:CD1	2.20	0.77
21:q:56:PHE:HA	21:q:59:HIS:HD2	1.50	0.77
7:G:632:ILE:HG13	7:G:632:ILE:O	1.85	0.77
2:B:112:TYR:OH	9:I:91:GLY:CA	2.31	0.76
12:R:95:LEU:HD21	12:R:111:PHE:HB3	1.66	0.76
7:G:355:LYS:HA	7:G:366:LEU:HD11	1.65	0.76
7:G:655:ARG:NH1	13:S:59:SER:HB3	2.01	0.76
4:D:456:ILE:HG23	4:D:461:ILE:HD11	1.67	0.76
7:G:406:ASN:ND2	7:G:436:VAL:HG21	2.01	0.76
4:D:271:ARG:HD2	8:H:279:ARG:O	1.85	0.76
14:T:119:ILE:HD12	14:T:138:LEU:HD11	1.67	0.76
17:X:20:VAL:HG22	17:X:24:VAL:HG21	1.66	0.76
6:F:423:THR:HG21	6:F:428:GLY:HA3	1.67	0.76
8:H:85:LEU:HD21	8:H:108:THR:HB	1.68	0.76
8:H:228:TYR:HA	8:H:231:ILE:HD12	1.68	0.76
9:I:184:LEU:HD23	11:Q:112:MET:HG3	1.68	0.76
2:B:93:MET:HE1	2:B:131:MET:HE2	1.68	0.76
4:D:270:ASN:HB3	8:H:284:GLN:HE22	1.51	0.76
6:F:163:TYR:HA	6:F:199:ARG:HH12	1.51	0.76
6:F:392:MET:HE1	6:F:416:SER:HA	1.66	0.76
4:D:174:PHE:CZ	4:D:217:VAL:HG11	2.21	0.76
10:P:348:LYS:O	10:P:351:GLU:HG2	1.86	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:q:96:ASP:OD1	21:q:97:PRO:HD2	1.85	0.75
4:D:371:MET:SD	4:D:381:HIS:CD2	2.80	0.75
7:G:667:GLN:NE2	13:S:38:VAL:HA	2.00	0.75
10:P:143:ASP:HA	10:P:147:ASN:HB2	1.67	0.75
7:G:360:LYS:HE3	7:G:632:ILE:HB	1.68	0.75
7:G:506:VAL:HG21	7:G:510:TRP:HD1	1.50	0.75
10:P:170:LEU:HA	10:P:202:ARG:HB3	1.68	0.75
14:T:93:ILE:HG23	14:T:110:LEU:HD13	1.66	0.75
8:H:35:LYS:HG3	9:I:83:THR:HG22	1.68	0.75
10:P:214:LEU:HG	10:P:353:LEU:HD21	1.68	0.75
11:Q:61:ILE:O	11:Q:61:ILE:HD12	1.86	0.75
8:H:215:TYR:HD2	8:H:219:PRO:HB2	1.50	0.75
11:Q:167:ASN:O	11:Q:168:LYS:CD	2.35	0.75
6:F:409:ILE:HG12	6:F:446:LEU:CD2	2.17	0.74
7:G:76:ARG:NH2	7:G:79:LEU:HD21	2.02	0.74
12:R:104:CYS:SG	12:R:107:CYS:HB2	2.27	0.74
6:F:203:ALA:HB3	6:F:206:CYS:SG	2.27	0.74
7:G:261:ILE:HG22	7:G:286:ILE:HG21	1.68	0.74
7:G:608:VAL:HG23	11:Q:103:THR:OG1	1.88	0.74
4:D:249:LYS:HA	18:Z:19:ILE:HG23	1.68	0.74
9:I:64:THR:HG22	25:I:301:PC1:H231	1.68	0.74
20:b:35:ILE:HD12	20:b:35:ILE:O	1.87	0.74
7:G:283:GLU:O	7:G:285:TRP:CE3	2.41	0.74
17:X:29:ALA:HB2	18:Z:71:LEU:HD11	1.69	0.74
2:B:147:LYS:HE3	2:B:151:GLN:HE21	1.51	0.74
8:H:116:ILE:HG13	8:H:117:LEU:N	2.00	0.74
10:P:235:THR:OG1	10:P:273:LEU:HB3	1.87	0.74
14:T:103:HIS:CG	14:T:106:LYS:HD2	2.23	0.74
14:T:88:LYS:HG3	14:T:98:LEU:HD22	1.70	0.74
21:q:68:MET:SD	21:q:81:MET:HB3	2.28	0.74
4:D:383:LYS:HD3	7:G:140:GLN:NE2	2.03	0.74
6:F:213:ILE:HG23	6:F:235:VAL:HA	1.68	0.73
14:T:117:GLU:HA	14:T:120:MET:HE3	1.68	0.73
5:E:135:THR:CG2	5:E:172:GLU:HG3	2.18	0.73
7:G:275:PRO:HG3	7:G:286:ILE:HG12	1.70	0.73
9:I:171:PRO:HB3	21:q:93:MET:HE1	1.69	0.73
14:T:94:ASP:HB3	14:T:98:LEU:HB2	1.68	0.73
10:P:350:ILE:HB	10:P:366:ILE:HG23	1.70	0.73
16:W:55:LEU:HB3	16:W:107:MET:HE2	1.66	0.73
21:q:56:PHE:HD1	21:q:59:HIS:HE2	1.35	0.73
7:G:33:GLU:HB3	7:G:98:LYS:HE2	1.70	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:206:GLU:OE1	22:r:25:GLN:NE2	2.22	0.73
6:F:392:MET:CE	6:F:419:ILE:HD12	2.18	0.73
7:G:183:ILE:HD11	7:G:206:VAL:HG13	1.69	0.73
5:E:78:VAL:HA	5:E:104:LEU:HD13	1.69	0.73
15:V:54:GLU:HG2	15:V:58:MET:HE2	1.70	0.73
6:F:222:LYS:HB3	6:F:381:GLN:OE1	1.89	0.73
18:Z:93:GLU:O	18:Z:97:ILE:HG13	1.88	0.73
1:A:73:LEU:O	1:A:76:PRO:HD2	1.88	0.73
6:F:409:ILE:HG12	6:F:446:LEU:HD21	1.70	0.73
8:H:64:LEU:H	8:H:64:LEU:HD23	1.51	0.73
8:H:172:MET:HE3	8:H:176:LEU:HB2	1.71	0.73
17:X:23:ALA:HB2	17:X:95:GLN:NE2	2.03	0.73
2:B:92:PRO:HD3	2:B:119:VAL:HG13	1.71	0.73
1:A:21:ALA:O	1:A:25:PRO:HD3	1.88	0.72
15:V:12:VAL:HG13	15:V:13:GLY:N	2.04	0.72
17:X:44:MET:HE3	17:X:48:TRP:HE1	1.53	0.72
21:q:56:PHE:HA	21:q:59:HIS:CD2	2.24	0.72
7:G:89:VAL:HB	7:G:94:MET:HG3	1.71	0.72
13:S:69:TYR:CE2	13:S:75:LYS:HG3	2.24	0.72
18:Z:65:LEU:O	18:Z:69:ILE:HG12	1.90	0.72
20:b:31:ILE:HA	20:b:34:MET:HE2	1.71	0.72
9:I:93:LEU:O	21:q:93:MET:HG2	1.89	0.72
4:D:88:HIS:CD2	4:D:90:ALA:HB3	2.25	0.72
6:F:42:PHE:HA	6:F:137:LYS:NZ	2.04	0.72
6:F:127:ASP:HB3	6:F:245:VAL:HG21	1.70	0.72
8:H:142:TYR:HA	8:H:289:LEU:HD11	1.71	0.72
8:H:175:LEU:HD21	25:I:301:PC1:H2C2	1.71	0.72
3:C:93:ILE:HB	3:C:94:PRO:HD3	1.71	0.72
6:F:327:ILE:HG23	6:F:332:CYS:SG	2.29	0.72
7:G:394:VAL:HB	7:G:417:ARG:CG	2.20	0.72
10:P:317:ASP:HB3	10:P:321:ARG:NH2	2.04	0.72
4:D:90:ALA:HB2	8:H:205:SER:HA	1.70	0.72
5:E:128:LYS:HB3	5:E:167:LEU:HA	1.71	0.72
8:H:85:LEU:HB3	8:H:233:LEU:HD21	1.72	0.72
11:Q:167:ASN:O	11:Q:168:LYS:HD2	1.88	0.72
6:F:278:ILE:HD11	6:F:299:LEU:CD2	2.19	0.72
8:H:35:LYS:HG3	9:I:83:THR:CG2	2.20	0.72
6:F:225:LEU:HB3	6:F:227:PRO:HD2	1.72	0.72
10:P:166:HIS:HB3	10:P:200:ILE:HD13	1.72	0.72
5:E:151:LEU:HD12	5:E:204:ILE:HD11	1.72	0.71
5:E:174:GLU:HG2	6:F:369:ARG:NH1	1.96	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:126:LEU:HD11	12:R:89:PRO:CB	2.20	0.71
3:C:160:ILE:HD12	4:D:286:TYR:HE1	1.55	0.71
3:C:172:MET:HE3	3:C:187:LEU:HD12	1.71	0.71
7:G:597:VAL:HG12	7:G:603:ALA:CA	2.19	0.71
3:C:70:LYS:O	15:V:103:LEU:HD12	1.90	0.71
2:B:199:GLU:HB3	9:I:86:TYR:HE1	1.56	0.71
5:E:222:PHE:H	5:E:225:GLU:HG2	1.55	0.71
8:H:172:MET:HE3	8:H:176:LEU:HD12	1.73	0.71
2:B:194:CYS:HB3	2:B:195:PRO:HD3	1.72	0.71
4:D:439:SER:HB3	4:D:450:ILE:HD12	1.72	0.71
8:H:307:LEU:HA	8:H:310:PHE:CE2	2.25	0.71
3:C:67:ILE:HG21	3:C:98:PHE:CZ	2.26	0.71
6:F:371:ILE:HD11	6:F:435:VAL:HG22	1.71	0.71
7:G:286:ILE:HA	7:G:413:LEU:HD11	1.73	0.71
12:R:67:GLN:HG2	12:R:109:LEU:CD2	2.21	0.71
6:F:422:HIS:CD2	7:G:79:LEU:HD13	2.25	0.71
4:D:254:ARG:NH1	22:r:25:GLN:HB2	2.06	0.71
4:D:140:ASP:HB3	4:D:147:ASN:HD21	1.56	0.71
7:G:283:GLU:HG2	7:G:285:TRP:CZ3	2.25	0.71
8:H:23:VAL:HG11	19:a:9:LEU:HD21	1.72	0.71
2:B:108:ALA:HA	2:B:114:MET:HG2	1.71	0.70
3:C:124:ARG:NH1	3:C:125:PHE:CE1	2.59	0.70
17:X:93:ASN:OD1	17:X:94:MET:N	2.24	0.70
4:D:141:TYR:O	4:D:144:MET:SD	2.49	0.70
6:F:63:TYR:HB3	6:F:256:ARG:NE	2.04	0.70
12:R:70:ASN:HB2	12:R:111:PHE:HD1	1.55	0.70
17:X:124:GLN:O	20:b:70:PRO:HB2	1.91	0.70
7:G:541:PRO:HB2	7:G:561:PRO:HG3	1.72	0.70
6:F:41:ILE:HD11	6:F:262:PHE:HE1	1.56	0.70
8:H:33:LEU:CD2	22:r:25:GLN:HG2	2.21	0.70
8:H:169:GLN:HE21	8:H:174:LEU:H	1.38	0.70
7:G:463:CYS:O	7:G:467:LYS:HG2	1.92	0.70
8:H:116:ILE:HA	8:H:211:PHE:CE1	2.27	0.70
6:F:37:ASP:HA	6:F:40:ARG:HD2	1.71	0.70
8:H:61:MET:HE3	8:H:63:PRO:HA	1.72	0.70
18:Z:12:PRO:HD3	18:Z:16:TYR:CZ	2.25	0.70
4:D:271:ARG:HG2	8:H:281:ARG:HG3	1.71	0.70
7:G:117:MET:HE3	7:G:143:SER:HA	1.74	0.70
3:C:85:ILE:CD1	3:C:140:ILE:CD1	2.70	0.70
3:C:168:GLU:CB	3:C:186:ILE:HD11	2.22	0.70
8:H:92:PRO:HD3	8:H:255:TYR:CD2	2.27	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:235:VAL:HG22	6:F:236:PHE:CD2	2.26	0.69
9:I:62:MET:HE2	9:I:62:MET:HA	1.72	0.69
8:H:90:PRO:HD3	8:H:162:LEU:HD23	1.75	0.69
8:H:102:ILE:HG13	8:H:162:LEU:HD12	1.74	0.69
10:P:172:ALA:O	10:P:185:ALA:HB2	1.91	0.69
2:B:92:PRO:HG3	2:B:119:VAL:HG13	1.73	0.69
8:H:93:HIS:HB3	19:a:27:HIS:ND1	2.06	0.69
17:X:18:VAL:HG21	18:Z:74:LEU:HD11	1.74	0.69
7:G:362:ASP:HB2	13:S:71:PHE:CD1	2.26	0.69
10:P:69:VAL:HG21	10:P:129:LEU:HD11	1.75	0.69
8:H:196:ALA:HB3	8:H:274:ARG:HA	1.75	0.69
14:T:100:VAL:HB	14:T:142:GLN:HB2	1.74	0.69
15:V:35:LEU:HA	15:V:38:PHE:CD1	2.27	0.69
4:D:174:PHE:HZ	4:D:217:VAL:HG11	1.58	0.69
4:D:339:GLN:NE2	9:I:37:LYS:NZ	2.41	0.69
7:G:335:GLY:HA2	7:G:362:ASP:O	1.93	0.69
15:V:56:LEU:HD12	15:V:56:LEU:C	2.16	0.69
5:E:134:CYS:HG	26:E:301:FES:FE1	1.09	0.69
6:F:81:LYS:HE2	6:F:97:LEU:HD23	1.75	0.69
13:S:51:LEU:HD13	13:S:95:LEU:HD12	1.75	0.69
15:V:12:VAL:HG13	15:V:13:GLY:H	1.56	0.69
7:G:341:ILE:HG13	7:G:545:LEU:HD11	1.74	0.69
10:P:55:VAL:HG12	10:P:123:SER:HA	1.74	0.69
10:P:148:ILE:HB	10:P:149:PRO:HD3	1.74	0.69
6:F:204:TYR:HB3	6:F:377:GLU:HG3	1.74	0.69
6:F:345:ALA:O	6:F:346:GLN:CG	2.40	0.69
6:F:383:THR:HG21	7:G:120:LEU:CD2	2.23	0.69
10:P:320:GLU:O	10:P:324:ILE:HG12	1.93	0.69
22:r:20:LEU:C	22:r:20:LEU:HD12	2.18	0.69
2:B:99:CYS:HB2	4:D:141:TYR:CG	2.28	0.68
2:B:131:MET:HE3	2:B:152:MET:CE	2.23	0.68
4:D:254:ARG:HH11	22:r:25:GLN:CB	2.06	0.68
4:D:375:MET:HE1	7:G:126:LEU:HA	1.75	0.68
7:G:476:LEU:HB3	7:G:515:ILE:HG22	1.75	0.68
14:T:87:LEU:HD22	14:T:104:PHE:HE1	1.58	0.68
19:a:31:ASN:ND2	19:a:36:LYS:HB2	2.08	0.68
4:D:194:ILE:HG23	4:D:271:ARG:HE	1.58	0.68
17:X:44:MET:HE3	17:X:48:TRP:NE1	2.08	0.68
5:E:70:PRO:HB2	5:E:73:HIS:CD2	2.28	0.68
5:E:151:LEU:HD23	5:E:170:LEU:HD13	1.73	0.68
14:T:138:LEU:HD13	14:T:144:ILE:CG1	2.22	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:141:ARG:NH1	4:D:410:TYR:HE1	1.90	0.68
7:G:304:GLU:OE2	10:P:41:ILE:HG12	1.94	0.68
8:H:42:PRO:HB3	21:q:27:PHE:CE2	2.28	0.68
10:P:141:PHE:CD2	10:P:179:LYS:HD2	2.29	0.68
10:P:344:PRO:HD2	10:P:347:LEU:HD22	1.74	0.68
14:T:116:VAL:HG12	14:T:120:MET:HE2	1.75	0.68
4:D:148:GLU:CD	4:D:227:ILE:HB	2.19	0.68
8:H:5:ASN:HD21	19:a:23:THR:HG23	1.58	0.68
2:B:217:LYS:O	2:B:220:ILE:HG12	1.94	0.68
4:D:145:MET:CB	4:D:148:GLU:OE2	2.42	0.68
7:G:171:THR:HG22	7:G:231:LEU:HB3	1.75	0.68
13:S:19:ILE:HD12	13:S:94:VAL:HG11	1.76	0.68
2:B:92:PRO:HG2	2:B:121:PHE:HA	1.75	0.68
8:H:175:LEU:O	8:H:179:TRP:HB3	1.93	0.68
6:F:41:ILE:HD11	6:F:262:PHE:CE1	2.28	0.68
7:G:283:GLU:HG2	7:G:285:TRP:HZ3	1.56	0.68
8:H:30:TYR:CE1	19:a:1:MET:O	2.47	0.68
9:I:78:PHE:HB3	22:r:8:ILE:HG22	1.76	0.68
6:F:42:PHE:HA	6:F:137:LYS:HZ2	1.57	0.68
7:G:371:ILE:HG12	7:G:533:GLY:HA2	1.74	0.68
8:H:186:PHE:CZ	8:H:270:PHE:CE1	2.81	0.68
15:V:116:ILE:HG23	15:V:116:ILE:O	1.92	0.68
5:E:192:TYR:HB3	5:E:195:LEU:HD11	1.76	0.68
5:E:206:GLU:HB2	5:E:213:PRO:HG3	1.76	0.68
7:G:43:VAL:HG12	7:G:55:LYS:HD3	1.75	0.68
10:P:317:ASP:HB3	10:P:321:ARG:HH22	1.58	0.68
13:S:16:LEU:HB3	13:S:69:TYR:HD1	1.58	0.68
6:F:39:ASP:HB3	6:F:265:PHE:CZ	2.29	0.67
4:D:279:THR:HA	15:V:12:VAL:CG1	2.24	0.67
10:P:185:ALA:O	10:P:188:GLU:HG2	1.94	0.67
15:V:84:ALA:C	15:V:87:GLU:HG2	2.19	0.67
2:B:110:PRO:HB3	8:H:33:LEU:O	1.93	0.67
7:G:126:LEU:CD1	12:R:89:PRO:CB	2.73	0.67
7:G:301:ARG:NH2	7:G:591:GLU:OE1	2.28	0.67
7:G:557:ARG:HD2	7:G:579:MET:HB2	1.76	0.67
6:F:225:LEU:H	11:Q:160:TYR:HE2	1.43	0.67
6:F:375:LYS:HD2	6:F:390:ASP:OD1	1.95	0.67
8:H:92:PRO:HD3	8:H:255:TYR:HD2	1.58	0.67
12:R:48:PHE:CD2	21:q:125:VAL:HG21	2.29	0.67
6:F:426:ALA:O	6:F:429:ASP:HB2	1.95	0.67
7:G:617:ARG:HH12	16:W:129:HIS:N	1.93	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:54:LYS:HG3	8:H:55:LEU:N	2.07	0.67
10:P:288:PHE:CZ	10:P:290:PRO:HB3	2.30	0.67
4:D:279:THR:HA	15:V:12:VAL:HG13	1.75	0.67
8:H:33:LEU:HD21	22:r:25:GLN:HG2	1.74	0.67
15:V:72:LEU:HD11	15:V:80:VAL:CG2	2.19	0.67
3:C:149:LEU:CD1	16:W:80:ARG:NH2	2.56	0.67
5:E:39:VAL:HG22	7:G:205:GLN:NE2	2.09	0.67
8:H:90:PRO:HG2	8:H:240:ILE:HG21	1.77	0.67
8:H:102:ILE:CG2	8:H:150:LEU:HD13	2.25	0.67
8:H:196:ALA:O	8:H:197:PRO:C	2.37	0.67
2:B:92:PRO:CD	2:B:119:VAL:HG13	2.26	0.66
7:G:175:ARG:HB2	7:G:230:ALA:HA	1.74	0.66
17:X:132:LYS:HB3	20:b:59:ASP:HB3	1.76	0.66
7:G:569:GLN:OE1	7:G:622:ILE:HD13	1.96	0.66
7:G:651:PRO:HG3	13:S:57:GLU:H	1.58	0.66
9:I:68:ARG:HH22	18:Z:26:PRO:HD2	1.60	0.66
9:I:92:PRO:HA	21:q:91:HIS:O	1.95	0.66
3:C:172:MET:CE	3:C:187:LEU:HD12	2.26	0.66
6:F:296:LEU:HD23	6:F:332:CYS:HB3	1.75	0.66
14:T:87:LEU:CD2	14:T:104:PHE:CZ	2.78	0.66
10:P:263:PHE:HD1	10:P:333:PRO:HB2	1.60	0.66
4:D:207:ARG:HA	4:D:210:MET:HE3	1.78	0.66
5:E:147:ILE:HD11	5:E:183:PRO:HB3	1.78	0.66
12:R:42:ASP:HB3	12:R:44:ARG:HH11	1.61	0.66
16:W:121:PHE:HA	16:W:124:LYS:HE2	1.75	0.66
2:B:98:ALA:HB2	2:B:136:THR:H	1.61	0.66
7:G:374:THR:O	7:G:374:THR:OG1	2.08	0.66
14:T:83:VAL:HG22	14:T:126:PHE:CZ	2.31	0.66
17:X:56:CYS:HA	17:X:135:ARG:HH12	1.60	0.66
4:D:84:PHE:CB	4:D:97:LEU:HB3	2.23	0.66
7:G:218:LEU:HD21	7:G:413:LEU:HD23	1.77	0.66
10:P:268:PRO:HG2	10:P:344:PRO:HA	1.77	0.66
12:R:97:LYS:HE3	12:R:100:LYS:HD3	1.77	0.66
2:B:199:GLU:HB3	9:I:86:TYR:CE1	2.31	0.66
15:V:72:LEU:HD12	15:V:72:LEU:C	2.19	0.66
21:q:13:GLN:HE22	30:q:201:CDL:HA31	1.60	0.66
7:G:301:ARG:HE	7:G:613:PRO:HG3	1.59	0.66
7:G:382:ARG:HD2	13:S:56:ARG:CD	2.25	0.66
13:S:24:CYS:SG	13:S:61:VAL:O	2.53	0.66
14:T:130:ILE:HG23	14:T:131:PRO:HD2	1.77	0.66
4:D:101:LEU:HD11	4:D:106:VAL:HG22	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:138:PRO:HD2	26:E:301:FES:S2	2.36	0.65
7:G:246:ARG:NH2	11:Q:123:ASN:OD1	2.28	0.65
7:G:655:ARG:NH1	13:S:59:SER:CB	2.58	0.65
9:I:200:GLU:OE2	21:q:93:MET:SD	2.54	0.65
15:V:72:LEU:O	15:V:72:LEU:CD1	2.42	0.65
7:G:388:ASN:H	7:G:514:ASN:HB3	1.61	0.65
7:G:617:ARG:NH1	16:W:129:HIS:CA	2.59	0.65
2:B:82:ILE:HG12	8:H:57:MET:HE2	1.78	0.65
2:B:170:TYR:CE1	9:I:124:PRO:HB2	2.32	0.65
7:G:126:LEU:CD1	12:R:89:PRO:HB3	2.25	0.65
16:W:65:LYS:HE2	16:W:110:PHE:HA	1.78	0.65
12:R:76:ILE:HD11	12:R:92:TYR:HB3	1.77	0.65
13:S:48:HIS:CE1	13:S:95:LEU:CD2	2.80	0.65
13:S:58:CYS:HB2	13:S:61:VAL:HG12	1.78	0.65
15:V:38:PHE:CD1	15:V:95:LEU:HD21	2.31	0.65
4:D:230:GLY:O	4:D:358:VAL:HG23	1.96	0.65
5:E:43:THR:OG1	5:E:44:PRO:HD2	1.96	0.65
2:B:98:ALA:CB	2:B:136:THR:H	2.10	0.65
13:S:16:LEU:HB3	13:S:69:TYR:CD1	2.32	0.65
4:D:237:PRO:HG2	4:D:240:LEU:HB2	1.78	0.65
7:G:421:SER:HB2	7:G:427:LEU:CD1	2.26	0.65
7:G:639:LEU:HD21	7:G:643:ARG:NE	2.11	0.65
3:C:63:TYR:OH	3:C:102:HIS:NE2	2.27	0.65
3:C:85:ILE:HD11	3:C:140:ILE:HD11	1.76	0.65
7:G:76:ARG:HH21	7:G:79:LEU:CD2	2.07	0.65
7:G:634:LEU:HB3	7:G:636:TYR:CZ	2.31	0.65
14:T:118:ILE:HG23	14:T:122:MET:HE3	1.78	0.65
3:C:114:THR:CG2	4:D:421:ARG:NH1	2.58	0.65
4:D:217:VAL:HG12	4:D:240:LEU:HD22	1.78	0.65
4:D:378:LEU:HD22	7:G:126:LEU:HD13	1.78	0.65
6:F:339:PHE:CD1	6:F:349:LEU:HB3	2.32	0.65
2:B:99:CYS:CB	4:D:141:TYR:CG	2.80	0.65
8:H:90:PRO:HD3	8:H:162:LEU:CD2	2.27	0.65
8:H:145:THR:HG22	8:H:289:LEU:HD11	1.78	0.65
12:R:70:ASN:HB2	12:R:111:PHE:CD1	2.31	0.65
14:T:120:MET:HG2	16:W:44:ARG:HH11	1.61	0.65
9:I:93:LEU:HD13	9:I:97:PHE:CD2	2.32	0.64
5:E:79:LEU:HB2	5:E:80:PRO:HD3	1.78	0.64
5:E:135:THR:HG21	5:E:172:GLU:HG3	1.80	0.64
10:P:169:HIS:H	10:P:184:LYS:HE3	1.63	0.64
5:E:136:THR:HG22	5:E:137:THR:H	1.62	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:110:PRO:HB3	6:F:152:ARG:HH12	1.62	0.64
8:H:138:GLN:HG3	8:H:139:THR:N	2.11	0.64
10:P:88:VAL:HG12	10:P:92:MET:HE2	1.80	0.64
12:R:52:GLN:HE21	21:q:122:GLU:C	2.04	0.64
12:R:112:LYS:O	12:R:113:GLN:C	2.40	0.64
3:C:67:ILE:HG21	3:C:98:PHE:CE1	2.33	0.64
6:F:152:ARG:NH2	23:s:60:PRO:HG3	2.13	0.64
12:R:32:THR:HG22	12:R:36:GLN:N	2.09	0.64
14:T:87:LEU:HD21	14:T:104:PHE:CZ	2.32	0.64
4:D:97:LEU:O	4:D:99:LEU:HG	1.98	0.64
10:P:135:GLU:HB2	10:P:140:ASP:HA	1.78	0.64
11:Q:163:ASN:OD1	11:Q:164:PHE:N	2.31	0.64
17:X:37:ASP:OD1	17:X:38:LYS:N	2.31	0.64
1:A:52:SER:HB3	1:A:55:PHE:HB2	1.80	0.64
7:G:370:GLU:OE2	7:G:478:SER:HB3	1.97	0.64
13:S:15:GLY:HA3	13:S:17:ARG:HH22	1.62	0.64
13:S:69:TYR:CD2	13:S:75:LYS:HG3	2.33	0.64
3:C:73:GLN:NE2	15:V:112:TRP:HE1	1.95	0.64
3:C:125:PHE:HE2	3:C:148:GLU:HA	1.62	0.64
6:F:388:GLY:HA3	6:F:419:ILE:HD11	1.80	0.64
7:G:386:LEU:HD21	7:G:523:VAL:CG1	2.28	0.64
7:G:394:VAL:HB	7:G:417:ARG:HG3	1.80	0.64
7:G:579:MET:O	7:G:579:MET:CG	2.35	0.64
10:P:166:HIS:HB3	10:P:200:ILE:CD1	2.27	0.64
14:T:83:VAL:HG23	14:T:126:PHE:HZ	1.62	0.64
30:q:201:CDL:H1	22:r:3:SER:HB2	1.80	0.64
5:E:245:GLN:HB2	6:F:257:ARG:C	2.23	0.64
6:F:113:LEU:HD23	6:F:154:ALA:HB2	1.79	0.64
6:F:424:ILE:HA	7:G:76:ARG:NH1	2.13	0.64
8:H:316:PRO:HG3	18:Z:57:ARG:HB3	1.80	0.64
9:I:105:ARG:HG2	9:I:111:GLU:HA	1.79	0.64
25:I:301:PC1:H361	25:I:301:PC1:H322	1.79	0.64
10:P:166:HIS:HE1	10:P:168:SER:HB2	1.63	0.64
4:D:260:GLU:HG3	18:Z:25:LEU:HD22	1.78	0.64
5:E:176:LEU:HB2	5:E:184:MET:CE	2.28	0.64
6:F:326:LEU:HD23	6:F:367:ILE:HD11	1.80	0.64
13:S:16:LEU:HD12	13:S:16:LEU:C	2.22	0.64
17:X:65:GLY:HA2	17:X:68:LEU:HD12	1.78	0.64
18:Z:65:LEU:O	18:Z:68:ARG:HG2	1.98	0.64
4:D:339:GLN:NE2	9:I:37:LYS:HZ1	1.95	0.63
8:H:35:LYS:HE3	8:H:38:ASN:ND2	2.12	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:S:16:LEU:HA	13:S:69:TYR:HA	1.79	0.63
16:W:55:LEU:CB	16:W:107:MET:CE	2.75	0.63
10:P:163:ARG:CD	10:P:253:THR:HA	2.27	0.63
3:C:212:ASP:HB3	3:C:215:VAL:HG22	1.80	0.63
4:D:279:THR:HG23	15:V:13:GLY:CA	2.19	0.63
6:F:35:LEU:HD11	6:F:39:ASP:O	1.99	0.63
6:F:278:ILE:HG22	6:F:282:VAL:HG21	1.80	0.63
15:V:38:PHE:CE1	15:V:95:LEU:HD21	2.33	0.63
8:H:196:ALA:CB	8:H:274:ARG:HA	2.28	0.63
3:C:186:ILE:HG13	3:C:187:LEU:H	1.64	0.63
7:G:127:ASP:HA	12:R:106:TYR:OH	1.99	0.63
10:P:284:THR:HG23	10:P:356:HIS:HB2	1.79	0.63
4:D:253:LEU:HD22	22:r:23:LYS:HB2	1.81	0.63
10:P:165:ILE:HA	10:P:199:ILE:O	1.99	0.63
11:Q:112:MET:SD	21:q:126:PRO:HB2	2.38	0.63
12:R:98:GLU:CD	12:R:98:GLU:H	2.07	0.63
2:B:92:PRO:HD2	2:B:121:PHE:N	2.13	0.63
4:D:142:VAL:HG13	4:D:207:ARG:NH1	2.14	0.63
4:D:257:GLU:O	4:D:258:VAL:C	2.40	0.63
7:G:475:VAL:HG21	7:G:516:LEU:HD23	1.78	0.63
22:r:109:ASP:O	22:r:110:GLN:HG2	1.99	0.63
4:D:348:LEU:O	18:Z:11:PRO:HB3	1.98	0.63
7:G:117:MET:HE3	7:G:143:SER:CA	2.29	0.63
17:X:25:LEU:HD11	19:a:50:ARG:NH2	2.13	0.63
17:X:130:LYS:NZ	20:b:63:MET:HB2	2.14	0.63
4:D:145:MET:C	4:D:148:GLU:HG2	2.22	0.62
14:T:93:ILE:CG2	14:T:110:LEU:HD13	2.28	0.62
15:V:84:ALA:HA	15:V:87:GLU:OE2	1.99	0.62
17:X:83:THR:HA	17:X:86:TRP:CD1	2.34	0.62
20:b:48:ALA:O	20:b:49:THR:C	2.40	0.62
4:D:109:CYS:O	4:D:111:PRO:HD3	1.99	0.62
5:E:118:TYR:CD2	6:F:201:ALA:HB3	2.34	0.62
7:G:394:VAL:HB	7:G:417:ARG:HG2	1.81	0.62
8:H:289:LEU:O	8:H:289:LEU:HD23	1.99	0.62
18:Z:70:ALA:O	18:Z:73:PRO:HD2	1.99	0.62
2:B:70:ARG:HG3	2:B:73:TYR:H	1.63	0.62
8:H:289:LEU:HD23	8:H:289:LEU:C	2.25	0.62
10:P:297:VAL:O	10:P:300:TRP:HB3	1.98	0.62
5:E:48:PRO:HA	5:E:95:SER:HB2	1.81	0.62
7:G:222:VAL:HG12	7:G:231:LEU:HD11	1.81	0.62
10:P:43:HIS:H	10:P:51:VAL:HG13	1.64	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:W:55:LEU:CB	16:W:107:MET:HE2	2.30	0.62
2:B:154:GLU:HB3	2:B:155:PRO:HD3	1.81	0.62
4:D:181:LEU:HD22	4:D:207:ARG:HG3	1.81	0.62
7:G:311:LYS:HE3	7:G:313:LEU:HD13	1.82	0.62
8:H:153:VAL:O	8:H:156:MET:HG2	2.00	0.62
10:P:156:SER:HB2	10:P:161:VAL:HG21	1.81	0.62
10:P:164:PHE:HE2	10:P:166:HIS:HB2	1.63	0.62
17:X:69:ASN:O	17:X:73:GLN:HG3	2.00	0.62
2:B:99:CYS:HB2	4:D:141:TYR:CD1	2.35	0.62
2:B:99:CYS:CB	4:D:141:TYR:CD2	2.82	0.62
3:C:73:GLN:HE21	15:V:112:TRP:HE1	1.47	0.62
7:G:445:LEU:HD21	7:G:462:PHE:HB2	1.81	0.62
7:G:488:ALA:HB2	7:G:677:GLN:HB3	1.80	0.62
10:P:217:PHE:HA	10:P:220:TYR:HD2	1.63	0.62
14:T:103:HIS:CD2	14:T:106:LYS:HD2	2.34	0.62
20:b:66:VAL:HG22	20:b:75:GLY:HA3	1.81	0.62
6:F:71:LYS:HE2	6:F:71:LYS:HA	1.82	0.62
6:F:346:GLN:HE22	6:F:440:ARG:HD3	1.64	0.62
8:H:81:LEU:HD22	8:H:108:THR:HG23	1.82	0.62
9:I:135:ARG:HE	9:I:141:ARG:HG3	1.64	0.62
5:E:70:PRO:HB2	5:E:73:HIS:HD2	1.63	0.62
5:E:176:LEU:HB2	5:E:184:MET:HE3	1.80	0.62
7:G:260:ASN:H	7:G:281:ILE:HD11	1.65	0.62
7:G:476:LEU:HD21	7:G:481:LEU:HD21	1.82	0.62
10:P:239:PRO:HG2	10:P:345:LEU:HD12	1.81	0.62
13:S:48:HIS:HE1	13:S:95:LEU:HD22	1.63	0.62
17:X:129:THR:HG23	20:b:68:SER:HA	1.81	0.62
21:q:10:GLY:HA2	30:q:201:CDL:OA6	2.00	0.62
2:B:202:LEU:CD1	9:I:86:TYR:CD2	2.77	0.62
4:D:283:ALA:HB1	4:D:293:LEU:HD23	1.82	0.62
7:G:557:ARG:HA	7:G:560:LEU:HD12	1.81	0.62
3:C:149:LEU:HD11	16:W:80:ARG:HH21	1.58	0.62
3:C:206:TYR:C	3:C:223:VAL:HG23	2.24	0.62
4:D:333:ARG:NH1	4:D:455:ASP:OD1	2.33	0.62
5:E:65:ILE:HG21	5:E:80:PRO:HB2	1.80	0.62
5:E:140:MET:HE1	6:F:366:ALA:HA	1.81	0.62
6:F:424:ILE:HA	7:G:76:ARG:HH12	1.65	0.62
8:H:51:ASP:HA	8:H:54:LYS:HG2	1.80	0.62
14:T:103:HIS:ND1	14:T:140:CYS:SG	2.73	0.62
17:X:115:LEU:HD13	17:X:117:TRP:CH2	2.34	0.62
20:b:67:PRO:HD2	20:b:72:ASP:HB2	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:98:PHE:HA	15:V:90:LEU:CD1	2.28	0.61
7:G:68:ARG:HD3	7:G:285:TRP:CZ3	2.34	0.61
10:P:41:ILE:HB	10:P:43:HIS:CE1	2.35	0.61
12:R:51:ARG:NH2	21:q:125:VAL:HG12	2.14	0.61
13:S:16:LEU:CD2	13:S:19:ILE:HD11	2.28	0.61
21:q:71:LYS:O	21:q:72:ASN:CG	2.43	0.61
1:A:73:LEU:N	1:A:74:PRO:HD2	2.15	0.61
5:E:193:GLU:HB2	5:E:217:PRO:HG3	1.82	0.61
7:G:370:GLU:HB3	7:G:522:GLN:OE1	2.00	0.61
7:G:421:SER:CB	7:G:427:LEU:CD1	2.78	0.61
8:H:33:LEU:HD11	9:I:76:TYR:CD1	2.35	0.61
8:H:248:TYR:HB3	8:H:250:ASN:OD1	2.00	0.61
10:P:172:ALA:H	10:P:202:ARG:HH21	1.45	0.61
9:I:209:TYR:HA	9:I:212:ARG:HG2	1.82	0.61
17:X:53:PRO:HD2	17:X:54:ARG:H	1.65	0.61
18:Z:28:ARG:HG3	18:Z:28:ARG:O	1.99	0.61
21:q:74:PHE:CD2	21:q:75:TRP:CD1	2.89	0.61
22:r:20:LEU:HD12	22:r:21:GLN:N	2.14	0.61
4:D:94:VAL:O	4:D:94:VAL:HG23	1.99	0.61
4:D:188:THR:HB	4:D:200:PHE:HA	1.81	0.61
6:F:357:MET:HE1	6:F:363:ILE:HG13	1.82	0.61
11:Q:167:ASN:O	11:Q:168:LYS:CG	2.48	0.61
14:T:138:LEU:HD12	14:T:138:LEU:C	2.24	0.61
6:F:392:MET:HG2	6:F:412:LEU:HD11	1.82	0.61
8:H:301:CYS:O	8:H:305:ILE:HG13	2.01	0.61
14:T:138:LEU:O	14:T:138:LEU:CD1	2.40	0.61
4:D:202:TRP:CZ3	4:D:261:MET:HG3	2.36	0.61
7:G:666:GLN:HE21	7:G:667:GLN:NE2	1.99	0.61
15:V:82:LEU:O	15:V:86:LYS:HG3	2.00	0.61
2:B:98:ALA:O	24:B:301:SF4:S3	2.59	0.61
2:B:142:ALA:HB3	2:B:143:PRO:HD3	1.82	0.61
4:D:141:TYR:HB3	4:D:223:HIS:HE1	1.66	0.61
5:E:222:PHE:CE1	6:F:48:ARG:HG3	2.36	0.61
7:G:339:ALA:C	7:G:545:LEU:HD12	2.25	0.61
7:G:373:PRO:HG2	7:G:481:LEU:HD22	1.81	0.61
7:G:515:ILE:O	7:G:515:ILE:HG13	1.98	0.61
19:a:3:PHE:CE2	30:q:201:CDL:HA4	2.34	0.61
4:D:456:ILE:HG23	4:D:461:ILE:CD1	2.31	0.61
5:E:222:PHE:N	5:E:225:GLU:HG2	2.15	0.61
6:F:266:GLY:HA3	6:F:271:SER:HA	1.82	0.61
2:B:112:TYR:CE1	2:B:199:GLU:HG2	2.36	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:162:PHE:HB3	6:F:165:GLU:HB2	1.83	0.61
7:G:343:GLY:HA3	7:G:550:ALA:HA	1.82	0.61
7:G:391:ILE:HG22	7:G:417:ARG:HE	1.66	0.61
7:G:545:LEU:HB3	7:G:566:ILE:CG2	2.29	0.61
8:H:87:VAL:HG13	8:H:95:LEU:HD23	1.83	0.61
21:q:34:ARG:NE	21:q:58:ARG:NH2	2.48	0.61
4:D:148:GLU:CG	4:D:227:ILE:HB	2.31	0.61
6:F:375:LYS:CD	6:F:390:ASP:OD1	2.48	0.61
8:H:106:LEU:HD21	8:H:150:LEU:HD12	1.82	0.61
8:H:116:ILE:HD12	8:H:135:ALA:CB	2.30	0.61
4:D:279:THR:CG2	15:V:13:GLY:HA3	2.22	0.60
7:G:421:SER:CB	7:G:427:LEU:HD11	2.31	0.60
7:G:35:PHE:O	7:G:101:ASN:HA	2.01	0.60
7:G:172:ILE:N	7:G:230:ALA:O	2.31	0.60
4:D:90:ALA:HA	4:D:193:ASP:OD1	2.01	0.60
6:F:90:GLY:O	6:F:350:GLY:HA2	2.02	0.60
7:G:395:GLU:HA	7:G:421:SER:OG	2.00	0.60
7:G:569:GLN:NE2	7:G:622:ILE:HG21	2.10	0.60
17:X:127:LYS:HD3	20:b:66:VAL:HG21	1.83	0.60
4:D:186:ALA:HB1	4:D:455:ASP:OD1	2.02	0.60
5:E:225:GLU:HG3	5:E:226:PRO:O	2.02	0.60
7:G:130:ILE:HG22	7:G:175:ARG:NH2	2.15	0.60
7:G:306:MET:HG2	7:G:316:TYR:HA	1.84	0.60
7:G:421:SER:HB2	7:G:427:LEU:HD12	1.83	0.60
10:P:146:VAL:HG23	10:P:187:GLY:HA2	1.83	0.60
12:R:38:TYR:HE2	21:q:127:TYR:CB	1.97	0.60
3:C:242:PRO:O	3:C:243:ALA:C	2.44	0.60
4:D:202:TRP:CH2	4:D:261:MET:HG3	2.37	0.60
5:E:131:ILE:HD11	5:E:168:PHE:HD2	1.65	0.60
5:E:204:ILE:HG22	5:E:208:LYS:HG3	1.82	0.60
6:F:447:GLU:O	6:F:450:MET:HB2	2.01	0.60
7:G:68:ARG:CD	7:G:285:TRP:CZ3	2.84	0.60
7:G:126:LEU:HD11	12:R:89:PRO:HB3	1.82	0.60
8:H:17:MET:HE1	8:H:225:MET:HB3	1.84	0.60
13:S:23:LEU:O	13:S:23:LEU:CD1	2.41	0.60
14:T:79:ILE:CB	14:T:145:VAL:HG13	2.28	0.60
14:T:83:VAL:HG22	14:T:126:PHE:HZ	1.66	0.60
4:D:80:MET:O	4:D:100:GLU:HA	2.02	0.60
6:F:158:ILE:CD1	6:F:166:ALA:HB2	2.31	0.60
13:S:16:LEU:CB	13:S:69:TYR:HD1	2.15	0.60
22:r:12:ARG:HB3	22:r:20:LEU:HD21	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:84:GLU:OE2	3:C:141:ARG:NH1	2.35	0.60
3:C:164:TRP:CZ3	4:D:113:ILE:HD13	2.37	0.60
3:C:167:ARG:NH2	3:C:186:ILE:HG22	2.17	0.60
6:F:44:ASN:OD1	6:F:49:HIS:HB2	2.02	0.60
8:H:127:TYR:CD2	8:H:207:LEU:HG	2.36	0.60
8:H:195:ARG:O	8:H:199:ASP:HB2	2.02	0.60
10:P:55:VAL:CG1	10:P:123:SER:HA	2.31	0.60
2:B:170:TYR:CB	9:I:153:ILE:HG21	2.31	0.60
6:F:191:TYR:HE2	6:F:193:PHE:HD2	1.50	0.60
10:P:136:THR:CG2	10:P:139:PHE:HB2	2.31	0.60
10:P:229:VAL:HB	10:P:323:HIS:CD2	2.37	0.60
10:P:268:PRO:CG	10:P:344:PRO:HA	2.31	0.60
12:R:42:ASP:HB3	12:R:44:ARG:NH1	2.17	0.60
4:D:304:LYS:HE2	9:I:35:THR:N	2.16	0.60
5:E:175:CYS:SG	6:F:122:PRO:HA	2.42	0.60
17:X:124:GLN:HA	17:X:127:LYS:HE3	1.83	0.60
18:Z:143:TYR:O	18:Z:144:THR:C	2.45	0.60
2:B:92:PRO:CG	2:B:119:VAL:HG13	2.31	0.60
2:B:141:MET:HE2	4:D:115:LEU:HD23	1.84	0.60
3:C:160:ILE:HD12	4:D:286:TYR:CE1	2.37	0.60
4:D:156:GLU:HG3	4:D:229:PRO:O	2.01	0.60
7:G:281:ILE:CG2	7:G:602:ARG:NH1	2.65	0.60
7:G:373:PRO:HB3	7:G:487:ALA:HA	1.84	0.60
8:H:102:ILE:HD12	8:H:154:LEU:CD2	2.32	0.60
18:Z:86:ILE:HG23	18:Z:128:ARG:NE	2.15	0.60
18:Z:122:GLY:O	18:Z:126:GLY:N	2.34	0.60
2:B:115:ASP:HA	2:B:119:VAL:O	2.02	0.59
6:F:398:ARG:NH2	7:G:155:GLU:HG3	2.17	0.59
7:G:131:CYS:HA	7:G:175:ARG:NH1	2.18	0.59
7:G:197:THR:HG22	7:G:206:VAL:HG22	1.82	0.59
14:T:103:HIS:HB2	14:T:106:LYS:HB2	1.83	0.59
17:X:37:ASP:HA	17:X:40:ASN:HB2	1.84	0.59
21:q:98:PRO:O	21:q:99:THR:C	2.45	0.59
2:B:112:TYR:HH	9:I:91:GLY:HA3	1.62	0.59
4:D:148:GLU:HG3	4:D:227:ILE:HB	1.83	0.59
4:D:256:ASP:O	4:D:259:GLU:HB2	2.02	0.59
17:X:78:CYS:SG	17:X:110:CYS:HB3	2.42	0.59
4:D:404:LYS:HZ2	4:D:455:ASP:HB3	1.67	0.59
7:G:388:ASN:H	7:G:514:ASN:CB	2.15	0.59
15:V:35:LEU:HA	15:V:38:PHE:HD1	1.66	0.59
16:W:64:ASP:O	16:W:68:GLU:HG3	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:20:VAL:HG12	17:X:25:LEU:HD21	1.84	0.59
18:Z:98:MET:HB2	18:Z:104:TRP:NE1	2.18	0.59
4:D:82:LEU:HD13	8:H:126:LYS:HD2	1.83	0.59
6:F:157:TYR:CZ	6:F:200:GLY:HA2	2.37	0.59
7:G:334:GLU:OE1	13:S:71:PHE:CE1	2.51	0.59
9:I:64:THR:HG21	25:I:301:PC1:H121	1.83	0.59
15:V:90:LEU:HD21	15:V:94:MET:CE	2.33	0.59
4:D:376:GLU:HG3	7:G:151:SER:HB2	1.83	0.59
8:H:239:THR:O	8:H:239:THR:HG22	2.01	0.59
30:q:201:CDL:H722	30:q:201:CDL:H512	1.84	0.59
4:D:253:LEU:HB2	22:r:23:LYS:CD	2.31	0.59
7:G:68:ARG:HD3	7:G:285:TRP:HZ3	1.67	0.59
17:X:120:PRO:HB2	17:X:125:LEU:HD11	1.85	0.59
20:b:6:SER:O	20:b:9:LEU:HB3	2.02	0.59
2:B:94:THR:HG21	4:D:88:HIS:C	2.28	0.59
17:X:50:GLU:CG	17:X:138:PRO:HG3	2.30	0.59
7:G:387:LEU:HD21	7:G:516:LEU:HB3	1.85	0.59
10:P:164:PHE:HB3	10:P:198:ALA:HB1	1.83	0.59
20:b:8:PHE:HA	20:b:11:ASN:ND2	2.17	0.59
20:b:27:GLY:O	20:b:30:ILE:HG22	2.02	0.59
21:q:96:ASP:OD1	21:q:97:PRO:CD	2.50	0.59
2:B:98:ALA:HB3	2:B:135:GLY:HA2	1.85	0.59
7:G:337:ALA:O	7:G:543:LYS:N	2.36	0.59
8:H:11:VAL:HB	8:H:12:PRO:HD3	1.84	0.59
8:H:116:ILE:HD12	8:H:135:ALA:HB1	1.85	0.59
8:H:183:MET:HE2	25:I:301:PC1:H291	1.85	0.59
11:Q:167:ASN:HB3	23:s:64:ARG:HE	1.67	0.59
15:V:31:THR:HG22	15:V:88:LEU:HD13	1.85	0.59
18:Z:105:LYS:O	18:Z:106:VAL:C	2.46	0.59
3:C:227:GLN:NE2	9:I:129:THR:OG1	2.36	0.59
6:F:410:ASP:OD1	6:F:411:SER:N	2.36	0.59
7:G:517:HIS:H	7:G:599:THR:HG21	1.68	0.59
9:I:114:ILE:HG22	9:I:141:ARG:HH12	1.66	0.59
10:P:350:ILE:HB	10:P:366:ILE:CG2	2.32	0.59
10:P:357:ARG:HD3	10:P:361:TRP:O	2.03	0.59
18:Z:144:THR:HA	19:a:45:TRP:CZ3	2.34	0.59
4:D:191:ALA:HB1	4:D:196:ALA:HB3	1.85	0.58
6:F:387:GLU:HG3	7:G:123:ASN:OD1	2.03	0.58
7:G:259:SER:HA	7:G:281:ILE:CD1	2.32	0.58
7:G:611:THR:HG21	11:Q:105:GLU:CA	2.30	0.58
8:H:172:MET:HE1	18:Z:46:GLY:CA	2.33	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:180:SER:O	10:P:184:LYS:HG3	2.03	0.58
13:S:47:ALA:O	13:S:49:PRO:HD3	2.03	0.58
16:W:104:THR:O	16:W:108:ARG:HG3	2.02	0.58
20:b:11:ASN:O	20:b:15:LYS:N	2.31	0.58
4:D:388:GLY:HA3	4:D:417:SER:OG	2.03	0.58
7:G:592:LYS:CA	7:G:608:VAL:HG12	2.33	0.58
10:P:318:LYS:O	10:P:322:ILE:HG13	2.03	0.58
3:C:80:LEU:HD13	4:D:396:THR:HG22	1.85	0.58
11:Q:166:TRP:CE3	23:s:67:PRO:HG3	2.38	0.58
13:S:63:PRO:HB2	13:S:79:LEU:HB2	1.85	0.58
17:X:127:LYS:HD3	20:b:66:VAL:CG2	2.34	0.58
21:q:51:ASP:O	21:q:59:HIS:HB2	2.03	0.58
4:D:404:LYS:NZ	4:D:455:ASP:HB3	2.18	0.58
6:F:422:HIS:CD2	7:G:79:LEU:HD12	2.31	0.58
9:I:93:LEU:HD13	9:I:97:PHE:CE2	2.38	0.58
10:P:328:MET:HG3	10:P:330:THR:H	1.67	0.58
12:R:40:GLU:HA	12:R:45:ARG:CZ	2.33	0.58
13:S:16:LEU:HD11	13:S:51:LEU:CD1	2.29	0.58
21:q:137:TRP:CZ2	21:q:140:PRO:HD3	2.38	0.58
1:A:55:PHE:O	1:A:56:PHE:C	2.46	0.58
4:D:266:ARG:NH2	9:I:65:GLU:HG2	2.19	0.58
5:E:150:THR:O	5:E:154:LYS:HG2	2.02	0.58
6:F:326:LEU:HD21	6:F:363:ILE:HD11	1.85	0.58
6:F:392:MET:HG2	6:F:412:LEU:CD1	2.34	0.58
7:G:171:THR:HA	7:G:231:LEU:HA	1.86	0.58
9:I:208:ASP:O	9:I:208:ASP:CG	2.44	0.58
4:D:233:HIS:CE1	4:D:234:GLN:HE21	2.21	0.58
6:F:326:LEU:C	6:F:326:LEU:HD12	2.28	0.58
6:F:346:GLN:HE22	6:F:440:ARG:CD	2.17	0.58
18:Z:54:ASN:O	18:Z:58:ARG:HG2	2.02	0.58
4:D:128:THR:H	4:D:131:GLN:NE2	2.00	0.58
4:D:375:MET:HE1	7:G:126:LEU:CA	2.34	0.58
7:G:571:HIS:CD2	7:G:572:HIS:CE1	2.82	0.58
11:Q:77:VAL:HG12	11:Q:101:PHE:HA	1.86	0.58
17:X:20:VAL:C	19:a:54:ILE:HD13	2.29	0.58
18:Z:135:ASN:O	18:Z:139:GLY:HA3	2.04	0.58
1:A:25:PRO:HG3	8:H:60:PRO:HD3	1.85	0.58
8:H:20:LEU:HD22	8:H:228:TYR:CD2	2.33	0.58
8:H:90:PRO:HA	8:H:94:PRO:HB3	1.86	0.58
8:H:197:PRO:HD3	8:H:273:ILE:HG22	1.85	0.58
10:P:56:ALA:HA	10:P:125:VAL:O	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:85:ILE:HD11	3:C:140:ILE:CD1	2.34	0.58
7:G:548:LEU:HA	7:G:569:GLN:HB3	1.86	0.58
13:S:16:LEU:O	13:S:16:LEU:CD1	2.51	0.58
13:S:65:LEU:HB2	13:S:79:LEU:HD11	1.84	0.58
18:Z:129:THR:HB	18:Z:132:GLU:HG3	1.86	0.58
3:C:186:ILE:HG13	3:C:187:LEU:N	2.17	0.58
5:E:182:ALA:O	5:E:183:PRO:C	2.43	0.58
7:G:567:VAL:HG12	7:G:582:VAL:HB	1.85	0.58
10:P:275:HIS:HB3	10:P:372:ALA:HB1	1.86	0.58
14:T:90:TYR:CE2	14:T:92:LYS:HB3	2.39	0.58
6:F:116:ASN:OD1	6:F:244:ASN:HA	2.03	0.57
7:G:528:LEU:HD22	7:G:649:VAL:HG21	1.86	0.57
7:G:569:GLN:HE22	7:G:622:ILE:CG2	2.09	0.57
8:H:288:LEU:HA	8:H:292:ASN:HB2	1.86	0.57
10:P:211:ASP:OD1	10:P:214:LEU:HB3	2.04	0.57
2:B:202:LEU:HD13	2:B:202:LEU:C	2.29	0.57
3:C:120:THR:OG1	11:Q:128:PHE:HA	2.04	0.57
7:G:546:PHE:CD1	7:G:567:VAL:HG23	2.40	0.57
4:D:375:MET:HE3	7:G:124:HIS:HB3	1.86	0.57
5:E:135:THR:OG1	5:E:172:GLU:CG	2.52	0.57
6:F:391:TRP:CH2	7:G:118:GLU:OE2	2.57	0.57
6:F:424:ILE:CG1	7:G:76:ARG:HH11	2.16	0.57
7:G:171:THR:HG22	7:G:231:LEU:CB	2.34	0.57
8:H:227:GLU:O	8:H:231:ILE:HG13	2.04	0.57
11:Q:166:TRP:HE3	23:s:67:PRO:HG3	1.67	0.57
19:a:36:LYS:HA	19:a:59:ARG:HH22	1.68	0.57
6:F:336:LEU:C	6:F:336:LEU:HD12	2.30	0.57
8:H:86:TRP:NE1	8:H:233:LEU:HB2	2.20	0.57
8:H:102:ILE:HD12	8:H:154:LEU:HD21	1.86	0.57
8:H:152:SER:HB3	8:H:181:MET:HE1	1.87	0.57
10:P:214:LEU:HD23	10:P:352:VAL:CG1	2.34	0.57
4:D:88:HIS:CG	4:D:90:ALA:HB3	2.39	0.57
4:D:166:ARG:HH22	18:Z:10:MET:HG2	1.68	0.57
4:D:198:THR:N	4:D:199:PRO:HD2	2.19	0.57
4:D:326:CYS:SG	4:D:453:THR:HG21	2.44	0.57
6:F:109:ARG:NH2	6:F:232:ASP:O	2.36	0.57
7:G:267:THR:HB	11:Q:115:ALA:HB2	1.86	0.57
7:G:572:HIS:HB2	7:G:699:SER:OG	2.03	0.57
17:X:130:LYS:HZ2	20:b:63:MET:HB2	1.69	0.57
25:B:302:PC1:H143	21:q:29:ARG:O	2.05	0.57
8:H:64:LEU:HD12	10:P:362:LEU:HD11	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Q:125:VAL:HG23	11:Q:125:VAL:O	2.05	0.57
3:C:80:LEU:HD13	4:D:396:THR:CG2	2.34	0.57
5:E:56:PRO:O	5:E:60:LYS:HG3	2.04	0.57
7:G:73:GLY:HA2	26:G:803:FES:S1	2.45	0.57
8:H:102:ILE:HG23	8:H:150:LEU:HD13	1.86	0.57
14:T:90:TYR:CE2	14:T:92:LYS:CB	2.87	0.57
4:D:212:GLU:O	4:D:216:ARG:HG2	2.05	0.57
4:D:363:VAL:O	4:D:389:TYR:CE1	2.57	0.57
5:E:126:VAL:HG21	5:E:130:HIS:ND1	2.19	0.57
6:F:110:PRO:HB3	6:F:152:ARG:NH1	2.19	0.57
7:G:102:ILE:H	7:G:102:ILE:HD12	1.70	0.57
7:G:136:GLU:CD	11:Q:87:MET:HG3	2.29	0.57
7:G:137:CYS:HB3	7:G:140:GLN:HG2	1.87	0.57
11:Q:166:TRP:CE3	23:s:67:PRO:CG	2.88	0.57
12:R:37:VAL:O	12:R:38:TYR:C	2.44	0.57
15:V:31:THR:O	15:V:35:LEU:HG	2.04	0.57
3:C:104:ASN:O	22:r:97:PRO:HD3	2.04	0.57
4:D:259:GLU:O	4:D:263:THR:HG22	2.05	0.57
7:G:49:VAL:HB	7:G:91:ALA:HA	1.86	0.57
8:H:19:PHE:CE1	19:a:11:ILE:HD12	2.40	0.57
10:P:168:SER:HA	10:P:184:LYS:HE3	1.87	0.57
14:T:83:VAL:CG2	14:T:126:PHE:CZ	2.83	0.57
21:q:129:THR:O	21:q:129:THR:HG22	2.03	0.57
5:E:185:VAL:HG22	5:E:195:LEU:HD12	1.86	0.57
6:F:346:GLN:NE2	6:F:440:ARG:CD	2.67	0.57
8:H:8:THR:O	8:H:9:LEU:HB3	2.05	0.57
15:V:28:TYR:HE2	15:V:59:VAL:HG21	1.69	0.57
2:B:98:ALA:H	2:B:135:GLY:HA3	1.69	0.56
4:D:359:ASP:O	7:G:150:ARG:NH2	2.38	0.56
6:F:76:ILE:HG23	6:F:255:CYS:SG	2.45	0.56
7:G:171:THR:HB	7:G:173:MET:HG3	1.87	0.56
7:G:372:PHE:H	7:G:532:PRO:HB2	1.69	0.56
8:H:113:VAL:O	8:H:116:ILE:HG12	2.05	0.56
18:Z:7:LYS:HB2	18:Z:7:LYS:NZ	2.20	0.56
21:q:14:VAL:HG13	21:q:23:LEU:CD2	2.35	0.56
2:B:166:ASN:HB3	9:I:150:THR:HG22	1.87	0.56
7:G:425:ASN:CG	7:G:426:ASP:H	2.11	0.56
14:T:134:ASP:OD1	14:T:134:ASP:O	2.23	0.56
18:Z:120:LEU:HB2	18:Z:123:GLU:HG3	1.87	0.56
21:q:65:THR:HG22	21:q:66:THR:N	2.20	0.56
2:B:161:MET:SD	2:B:201:LEU:HD22	2.45	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:170:LEU:HD12	5:E:171:ILE:N	2.20	0.56
10:P:208:GLY:O	10:P:209:ARG:C	2.48	0.56
18:Z:92:GLU:O	18:Z:96:ILE:HG13	2.05	0.56
3:C:65:ALA:HA	3:C:72:VAL:HG21	1.87	0.56
8:H:142:TYR:HE1	8:H:285:LEU:HD23	1.71	0.56
9:I:53:ALA:CA	20:b:14:ALA:HB2	2.35	0.56
14:T:90:TYR:HE2	14:T:92:LYS:CB	2.19	0.56
14:T:130:ILE:HD11	14:T:148:ILE:HD11	1.86	0.56
4:D:84:PHE:HB3	4:D:97:LEU:CB	2.31	0.56
7:G:41:VAL:HG21	7:G:56:VAL:HB	1.86	0.56
7:G:160:VAL:HG12	7:G:161:GLU:N	2.21	0.56
2:B:112:TYR:CZ	9:I:84:ILE:HD11	2.37	0.56
2:B:210:ARG:HD3	21:q:76:ASP:HB2	1.88	0.56
6:F:412:LEU:HD21	6:F:435:VAL:HG13	1.87	0.56
7:G:253:VAL:HG13	7:G:520:ALA:CB	2.35	0.56
7:G:600:GLU:OE1	7:G:600:GLU:N	2.39	0.56
8:H:190:LEU:HD21	8:H:270:PHE:CD1	2.40	0.56
8:H:210:GLY:HA2	8:H:213:VAL:HG23	1.87	0.56
9:I:168:VAL:HG21	9:I:201:ILE:HG21	1.87	0.56
11:Q:165:SER:HB3	11:Q:168:LYS:O	2.06	0.56
19:a:1:MET:HG3	30:q:201:CDL:HB21	1.87	0.56
6:F:171:VAL:HA	6:F:174:ARG:HH12	1.70	0.56
8:H:142:TYR:HE1	8:H:285:LEU:CD2	2.19	0.56
11:Q:110:PRO:HB3	12:R:43:TYR:OH	2.06	0.56
11:Q:167:ASN:O	11:Q:168:LYS:HG2	2.04	0.56
12:R:36:GLN:HG2	21:q:127:TYR:CD2	2.40	0.56
2:B:92:PRO:HG3	2:B:119:VAL:CG1	2.36	0.56
5:E:40:HIS:HB2	7:G:209:TYR:CZ	2.41	0.56
5:E:130:HIS:NE2	5:E:171:ILE:HD12	2.21	0.56
5:E:182:ALA:HB3	5:E:183:PRO:HD3	1.88	0.56
5:E:200:ILE:O	5:E:204:ILE:HG13	2.06	0.56
7:G:546:PHE:CZ	7:G:569:GLN:HB2	2.40	0.56
5:E:151:LEU:CD2	5:E:170:LEU:HD13	2.35	0.56
7:G:572:HIS:CE1	7:G:700:ILE:HG12	2.41	0.56
8:H:19:PHE:HB3	19:a:12:MET:HG3	1.87	0.56
8:H:307:LEU:HB3	8:H:308:PRO:HD3	1.88	0.56
9:I:80:GLU:HB3	22:r:26:LEU:HD11	1.88	0.56
12:R:77:ILE:HD11	12:R:111:PHE:CG	2.41	0.56
7:G:456:ALA:O	7:G:499:LYS:HE2	2.06	0.56
7:G:639:LEU:O	7:G:643:ARG:HG2	2.06	0.56
28:H:401:3PE:HN3	20:b:18:VAL:HG23	1.70	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:35:THR:CG2	22:r:107:SER:HA	2.36	0.56
10:P:208:GLY:H	10:P:211:ASP:CB	2.18	0.56
19:a:31:ASN:HD21	19:a:36:LYS:HB2	1.71	0.56
6:F:39:ASP:HB3	6:F:265:PHE:HZ	1.69	0.55
7:G:206:VAL:O	7:G:206:VAL:HG12	2.05	0.55
10:P:251:ASN:OD1	10:P:254:LYS:HE3	2.06	0.55
18:Z:53:TRP:O	18:Z:57:ARG:HG3	2.06	0.55
18:Z:56:GLU:HA	18:Z:59:ARG:HH11	1.72	0.55
19:a:14:VAL:O	19:a:18:ILE:HG13	2.06	0.55
7:G:671:LEU:HD21	13:S:45:LYS:HG2	1.88	0.55
10:P:235:THR:OG1	10:P:273:LEU:CB	2.54	0.55
17:X:20:VAL:HG13	17:X:24:VAL:HB	1.87	0.55
17:X:53:PRO:HD3	18:Z:116:TRP:CD1	2.41	0.55
21:q:68:MET:SD	21:q:81:MET:CB	2.95	0.55
21:q:68:MET:HE1	21:q:81:MET:O	2.06	0.55
6:F:152:ARG:HD3	23:s:57:LEU:HD11	1.87	0.55
7:G:172:ILE:O	7:G:172:ILE:HG22	2.06	0.55
7:G:707:MET:O	7:G:711:VAL:HG23	2.05	0.55
18:Z:85:GLN:O	18:Z:89:GLU:HG3	2.06	0.55
2:B:69:SER:O	2:B:70:ARG:C	2.48	0.55
4:D:169:TRP:CD1	4:D:352:PRO:HD3	2.41	0.55
4:D:329:ARG:CD	4:D:453:THR:HB	2.36	0.55
6:F:270:ASN:OD1	6:F:270:ASN:C	2.48	0.55
7:G:483:ARG:HH21	7:G:489:ILE:HD11	1.70	0.55
8:H:318:MET:HE3	18:Z:57:ARG:HH21	1.71	0.55
10:P:315:THR:O	10:P:316:LYS:C	2.49	0.55
17:X:124:GLN:C	17:X:125:LEU:HD12	2.31	0.55
20:b:38:TYR:HA	20:b:41:TYR:CD2	2.42	0.55
1:A:17:LEU:HB3	8:H:222:LEU:HD11	1.88	0.55
1:A:54:LYS:HE3	1:A:111:LEU:O	2.06	0.55
1:A:96:THR:O	1:A:100:LEU:HG	2.06	0.55
1:A:103:ALA:O	1:A:107:THR:HG23	2.06	0.55
7:G:215:MET:SD	7:G:714:VAL:HG22	2.46	0.55
7:G:264:SER:HB2	7:G:272:ARG:HG2	1.88	0.55
8:H:26:LYS:O	8:H:30:TYR:HD2	1.89	0.55
10:P:188:GLU:HA	10:P:191:VAL:HG12	1.89	0.55
10:P:376:ASN:OD1	10:P:376:ASN:C	2.50	0.55
5:E:84:LEU:HD12	23:s:46:LEU:HD13	1.88	0.55
5:E:180:VAL:HG21	6:F:286:CYS:HA	1.87	0.55
7:G:94:MET:CE	7:G:100:TRP:HH2	2.20	0.55
7:G:192:VAL:HG11	7:G:214:PHE:CE1	2.42	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:617:ARG:HH12	16:W:128:GLY:C	2.14	0.55
8:H:4:ILE:H	8:H:4:ILE:HD12	1.71	0.55
8:H:183:MET:HB3	9:I:63:TRP:CH2	2.41	0.55
10:P:196:PRO:O	10:P:197:GLU:HB2	2.07	0.55
10:P:258:ALA:HA	10:P:263:PHE:HZ	1.71	0.55
17:X:39:THR:HG23	17:X:40:ASN:N	2.20	0.55
1:A:105:GLU:CG	1:A:111:LEU:HB3	2.37	0.55
3:C:124:ARG:NH1	3:C:125:PHE:HZ	1.98	0.55
6:F:336:LEU:HD11	6:F:338:ASP:CG	2.32	0.55
7:G:64:CYS:HG	7:G:75:CYS:HG	1.52	0.55
7:G:356:ASP:O	7:G:360:LYS:HG3	2.06	0.55
7:G:525:ALA:O	7:G:530:TYR:HB2	2.07	0.55
10:P:273:LEU:O	10:P:277:VAL:HG23	2.06	0.55
20:b:8:PHE:O	20:b:9:LEU:C	2.50	0.55
1:A:22:PHE:O	1:A:25:PRO:HD2	2.05	0.55
4:D:254:ARG:HH11	22:r:25:GLN:CA	2.19	0.55
4:D:322:SER:O	4:D:323:ARG:C	2.47	0.55
6:F:213:ILE:CG2	6:F:235:VAL:HA	2.36	0.55
10:P:206:ILE:HG13	29:P:401:NDP:H42N	1.88	0.55
4:D:145:MET:HB3	4:D:148:GLU:OE2	2.07	0.55
4:D:280:ALA:CB	15:V:11:LEU:CG	2.81	0.55
4:D:359:ASP:CB	7:G:150:ARG:HH22	2.15	0.55
5:E:135:THR:OG1	5:E:135:THR:O	2.21	0.55
7:G:218:LEU:HD21	7:G:413:LEU:CD2	2.37	0.55
10:P:195:PHE:HD1	10:P:198:ALA:HB2	1.71	0.55
10:P:213:PHE:CE2	10:P:239:PRO:HB3	2.42	0.55
10:P:265:PHE:CZ	10:P:338:LEU:HD12	2.41	0.55
11:Q:163:ASN:OD1	11:Q:163:ASN:C	2.49	0.55
6:F:424:ILE:HG12	7:G:76:ARG:HH11	1.72	0.55
7:G:274:LEU:C	7:G:274:LEU:HD12	2.32	0.55
10:P:61:ALA:HB3	10:P:82:ILE:HG23	1.89	0.55
10:P:64:PHE:HE1	10:P:209:ARG:O	1.90	0.55
10:P:145:PHE:O	10:P:149:PRO:HG2	2.06	0.55
14:T:87:LEU:HD22	14:T:104:PHE:CZ	2.41	0.55
1:A:68:GLU:CD	1:A:98:LEU:HG	2.33	0.54
2:B:107:MET:HE3	2:B:114:MET:HE2	1.88	0.54
2:B:141:MET:CE	4:D:115:LEU:HD23	2.37	0.54
3:C:73:GLN:NE2	15:V:107:PRO:HB3	2.22	0.54
4:D:97:LEU:HG	4:D:99:LEU:HD21	1.89	0.54
4:D:278:VAL:CG1	4:D:438:MET:HG2	2.37	0.54
6:F:386:ARG:HB3	6:F:387:GLU:OE1	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:98:ARG:O	9:I:169:GLU:HB3	2.07	0.54
10:P:199:ILE:HD13	10:P:258:ALA:HB1	1.89	0.54
14:T:128:PHE:CE2	14:T:130:ILE:HG13	2.42	0.54
16:W:53:MET:HB2	16:W:55:LEU:HG	1.90	0.54
3:C:172:MET:HE3	3:C:187:LEU:CD1	2.37	0.54
4:D:355:GLU:HG2	4:D:357:LYS:H	1.72	0.54
6:F:67:GLU:O	6:F:71:LYS:HG2	2.07	0.54
7:G:68:ARG:HE	7:G:283:GLU:HG3	1.73	0.54
7:G:666:GLN:NE2	13:S:38:VAL:HG13	2.21	0.54
8:H:212:ASN:HB3	8:H:215:TYR:HB2	1.89	0.54
17:X:64:ASN:O	17:X:68:LEU:HG	2.07	0.54
20:b:8:PHE:CG	20:b:9:LEU:N	2.74	0.54
4:D:232:VAL:HG23	4:D:356:ILE:HD13	1.88	0.54
6:F:388:GLY:CA	6:F:419:ILE:HD11	2.37	0.54
7:G:472:PRO:O	7:G:510:TRP:NE1	2.32	0.54
10:P:219:ASN:ND2	10:P:313:TRP:HE1	2.04	0.54
17:X:121:ASP:O	17:X:122:LEU:C	2.50	0.54
19:a:58:ASN:HB2	19:a:61:TYR:CD2	2.43	0.54
2:B:95:PHE:HE2	2:B:97:LEU:HD11	1.71	0.54
2:B:170:TYR:HB2	9:I:153:ILE:CG2	2.33	0.54
4:D:145:MET:O	4:D:148:GLU:N	2.40	0.54
4:D:166:ARG:O	4:D:170:ILE:HG12	2.07	0.54
5:E:192:TYR:CB	5:E:195:LEU:HD11	2.37	0.54
7:G:49:VAL:HG11	7:G:80:VAL:HG21	1.89	0.54
7:G:547:LEU:HD11	7:G:566:ILE:HD12	1.90	0.54
7:G:688:GLN:HA	7:G:693:ASP:HB3	1.89	0.54
8:H:51:ASP:CA	8:H:54:LYS:HG2	2.37	0.54
9:I:130:ILE:HG12	9:I:145:TYR:CD1	2.42	0.54
10:P:311:GLU:O	10:P:312:PRO:C	2.49	0.54
17:X:52:ASP:N	17:X:52:ASP:OD1	2.40	0.54
18:Z:24:ASN:OD1	18:Z:24:ASN:O	2.24	0.54
2:B:135:GLY:O	2:B:165:ALA:HB2	2.08	0.54
4:D:154:ALA:HB2	4:D:398:THR:CG2	2.37	0.54
6:F:382:CYS:SG	24:F:502:SF4:FE2	1.89	0.54
9:I:208:ASP:OD1	9:I:211:TYR:HB2	2.08	0.54
14:T:97:LYS:HG3	14:T:97:LYS:O	2.08	0.54
3:C:160:ILE:HB	4:D:286:TYR:CD1	2.43	0.54
6:F:275:LEU:HA	6:F:289:GLU:HA	1.90	0.54
10:P:300:TRP:O	10:P:304:LEU:HG	2.07	0.54
10:P:355:ARG:HH11	10:P:356:HIS:CE1	2.25	0.54
11:Q:52:LEU:HG	16:W:21:LYS:HG2	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Q:160:TYR:CZ	11:Q:164:PHE:HZ	2.26	0.54
3:C:124:ARG:HD2	11:Q:140:LYS:NZ	2.23	0.54
3:C:224:GLU:OE1	10:P:48:ARG:O	2.26	0.54
6:F:339:PHE:O	6:F:343:VAL:HG23	2.07	0.54
7:G:126:LEU:CD1	12:R:89:PRO:HB2	2.37	0.54
7:G:395:GLU:OE2	7:G:417:ARG:NH1	2.41	0.54
7:G:617:ARG:NH1	16:W:128:GLY:C	2.66	0.54
7:G:639:LEU:HD21	7:G:643:ARG:CZ	2.36	0.54
10:P:106:LEU:HD21	12:R:49:VAL:HG11	1.89	0.54
10:P:211:ASP:OD2	10:P:352:VAL:HG11	2.08	0.54
10:P:318:LYS:HA	10:P:321:ARG:NH1	2.22	0.54
15:V:50:GLN:HE22	22:r:94:ALA:H	1.54	0.54
18:Z:53:TRP:NE1	18:Z:57:ARG:HD2	2.23	0.54
1:A:49:LEU:HD12	1:A:50:PRO:HD2	1.90	0.54
2:B:114:MET:SD	2:B:119:VAL:HG12	2.48	0.54
7:G:50:LEU:O	7:G:54:GLU:HG2	2.07	0.54
7:G:163:LYS:HB3	7:G:211:GLU:OE1	2.07	0.54
7:G:189:ILE:HG13	7:G:285:TRP:CZ2	2.43	0.54
8:H:11:VAL:O	8:H:12:PRO:C	2.49	0.54
8:H:40:VAL:CG1	8:H:47:GLN:NE2	2.71	0.54
8:H:69:SER:O	8:H:72:ILE:HG13	2.08	0.54
10:P:209:ARG:N	10:P:352:VAL:HG22	2.23	0.54
13:S:79:LEU:HA	13:S:82:LEU:CD1	2.24	0.54
14:T:118:ILE:HG23	14:T:122:MET:CE	2.37	0.54
21:q:64:TYR:CE2	21:q:82:VAL:HG13	2.42	0.54
3:C:217:ARG:HH12	16:W:112:GLU:CB	2.13	0.54
7:G:68:ARG:NE	7:G:283:GLU:HG3	2.23	0.54
7:G:278:HIS:HB3	7:G:281:ILE:HG13	1.90	0.54
7:G:566:ILE:HD11	7:G:579:MET:O	2.07	0.54
7:G:684:LEU:HD12	7:G:684:LEU:O	2.08	0.54
8:H:142:TYR:HA	8:H:289:LEU:HD13	1.86	0.54
20:b:68:SER:O	20:b:69:HIS:C	2.51	0.54
4:D:81:THR:HG22	4:D:100:GLU:HG2	1.88	0.54
4:D:84:PHE:CZ	4:D:91:ALA:HB2	2.42	0.54
4:D:202:TRP:CH2	9:I:72:MET:HG2	2.42	0.54
5:E:179:CYS:O	5:E:180:VAL:C	2.51	0.54
6:F:109:ARG:HE	6:F:239:PRO:HD3	1.73	0.54
7:G:482:GLN:HG3	7:G:518:ARG:HH21	1.73	0.54
8:H:40:VAL:HG11	8:H:47:GLN:NE2	2.23	0.54
8:H:88:PRO:HG2	8:H:105:ILE:HD11	1.90	0.54
8:H:303:TRP:CZ3	20:b:28:LEU:HG	2.43	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:132:ALA:O	9:I:133:GLU:HG3	2.07	0.54
11:Q:117:THR:HG22	11:Q:119:ASP:H	1.73	0.54
16:W:67:ARG:HD2	16:W:71:MET:HE2	1.89	0.54
20:b:28:LEU:HA	20:b:31:ILE:HG22	1.90	0.54
21:q:95:ASP:OD1	21:q:96:ASP:N	2.41	0.54
4:D:319:PRO:HG3	4:D:336:GLU:HG3	1.89	0.53
5:E:77:ALA:C	5:E:80:PRO:HD2	2.33	0.53
6:F:159:ARG:HB3	6:F:162:PHE:CD2	2.43	0.53
6:F:171:VAL:HA	6:F:174:ARG:NH1	2.23	0.53
6:F:325:PRO:HG3	6:F:433:TRP:HB3	1.88	0.53
7:G:170:LYS:O	7:G:231:LEU:HA	2.08	0.53
7:G:355:LYS:HG3	7:G:366:LEU:CD1	2.38	0.53
7:G:534:VAL:HG21	7:G:554:CYS:HB3	1.91	0.53
8:H:51:ASP:OD1	8:H:51:ASP:C	2.52	0.53
10:P:370:LYS:HG3	10:P:370:LYS:O	2.08	0.53
14:T:140:CYS:HB2	14:T:143:GLU:HG2	1.90	0.53
21:q:88:ARG:HD2	21:q:94:THR:OG1	2.08	0.53
1:A:58:VAL:HG11	8:H:286:MET:HE1	1.89	0.53
6:F:270:ASN:ND2	6:F:338:ASP:HB2	2.22	0.53
7:G:94:MET:HE2	7:G:100:TRP:HH2	1.73	0.53
10:P:258:ALA:HA	10:P:263:PHE:CZ	2.43	0.53
13:S:16:LEU:HD13	13:S:19:ILE:CD1	2.38	0.53
4:D:202:TRP:CZ2	9:I:76:TYR:CE2	2.96	0.53
4:D:217:VAL:CG1	4:D:240:LEU:HD22	2.38	0.53
4:D:253:LEU:HB2	22:r:23:LYS:HD2	1.89	0.53
4:D:335:GLU:OE2	9:I:37:LYS:NZ	2.41	0.53
6:F:117:ALA:CB	6:F:158:ILE:HG22	2.37	0.53
6:F:422:HIS:NE2	7:G:112:ALA:CA	2.68	0.53
11:Q:58:LYS:O	11:Q:59:LEU:C	2.49	0.53
16:W:43:TYR:CE1	16:W:63:ARG:HD3	2.43	0.53
18:Z:12:PRO:HD3	18:Z:16:TYR:CE1	2.43	0.53
19:a:3:PHE:HE2	30:q:201:CDL:H112	1.73	0.53
2:B:92:PRO:CD	2:B:121:PHE:H	2.18	0.53
7:G:68:ARG:NH2	7:G:283:GLU:HB2	2.23	0.53
7:G:360:LYS:HB2	7:G:632:ILE:CD1	2.28	0.53
7:G:557:ARG:CD	7:G:579:MET:HB2	2.38	0.53
7:G:600:GLU:OE2	7:G:602:ARG:NH1	2.42	0.53
7:G:634:LEU:HD13	7:G:636:TYR:CZ	2.43	0.53
8:H:102:ILE:CD1	8:H:154:LEU:HD21	2.39	0.53
8:H:317:TYR:O	8:H:318:MET:C	2.52	0.53
10:P:94:LEU:O	10:P:97:MET:HG2	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:R:94:ASN:OD1	12:R:96:ASP:HB2	2.08	0.53
3:C:168:GLU:CA	3:C:186:ILE:HD11	2.38	0.53
4:D:86:PRO:CB	4:D:95:LEU:H	2.22	0.53
4:D:129:TYR:OH	4:D:391:VAL:HG21	2.08	0.53
6:F:152:ARG:CZ	23:s:60:PRO:HG3	2.38	0.53
7:G:161:GLU:OE1	12:R:97:LYS:HE2	2.09	0.53
8:H:23:VAL:O	8:H:23:VAL:HG12	2.07	0.53
8:H:172:MET:HE1	18:Z:46:GLY:HA3	1.91	0.53
11:Q:82:PRO:O	11:Q:94:THR:HG23	2.08	0.53
3:C:64:VAL:HG11	3:C:85:ILE:HD13	1.91	0.53
7:G:370:GLU:OE2	7:G:478:SER:CB	2.56	0.53
8:H:1:MET:HA	8:H:4:ILE:HD13	1.89	0.53
9:I:78:PHE:CG	22:r:8:ILE:HG23	2.44	0.53
10:P:315:THR:HG22	10:P:316:LYS:N	2.21	0.53
12:R:95:LEU:HD21	12:R:111:PHE:CB	2.37	0.53
12:R:98:GLU:HA	12:R:113:GLN:CD	2.33	0.53
13:S:30:SER:O	13:S:31:GLN:C	2.49	0.53
15:V:114:TRP:O	15:V:115:PRO:C	2.52	0.53
5:E:129:TYR:CZ	5:E:207:LEU:HB3	2.43	0.53
7:G:435:PRO:O	7:G:435:PRO:HG2	2.08	0.53
7:G:679:VAL:HG23	7:G:679:VAL:O	2.09	0.53
8:H:172:MET:HE2	8:H:177:PRO:CD	2.22	0.53
10:P:142:GLU:HA	10:P:146:VAL:HG12	1.90	0.53
10:P:164:PHE:HB3	10:P:198:ALA:CB	2.38	0.53
10:P:353:LEU:HA	10:P:356:HIS:HD2	1.74	0.53
13:S:82:LEU:HD13	13:S:86:GLU:OE1	2.08	0.53
17:X:120:PRO:HG3	20:b:71:GLN:HE21	1.73	0.53
19:a:42:GLN:O	19:a:43:TYR:C	2.50	0.53
21:q:3:LEU:HD13	30:q:201:CDL:OB6	2.09	0.53
21:q:132:LYS:HD3	21:q:135:HIS:ND1	2.23	0.53
2:B:113:ASP:OD1	8:H:34:ARG:HD2	2.08	0.53
4:D:210:MET:O	4:D:211:PHE:C	2.50	0.53
4:D:368:ARG:HA	4:D:371:MET:HG2	1.90	0.53
5:E:94:ILE:HD13	7:G:209:TYR:HE2	1.74	0.53
6:F:276:PHE:HD1	6:F:352:ALA:HB1	1.72	0.53
7:G:307:VAL:HG21	7:G:325:ARG:HG3	1.91	0.53
7:G:546:PHE:HD1	7:G:567:VAL:CG2	2.22	0.53
3:C:96:LEU:HD12	3:C:155:ILE:HG21	1.91	0.53
6:F:113:LEU:HD23	6:F:154:ALA:CB	2.39	0.53
7:G:260:ASN:H	7:G:281:ILE:CD1	2.21	0.53
7:G:651:PRO:HD3	13:S:56:ARG:HB3	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:146:MET:HE1	8:H:192:GLU:HB2	1.90	0.53
9:I:100:GLU:HB2	9:I:175:PHE:CE2	2.44	0.53
10:P:217:PHE:HA	10:P:220:TYR:CD2	2.42	0.53
10:P:275:HIS:HA	10:P:278:LYS:HG2	1.91	0.53
12:R:69:VAL:HG12	12:R:112:LYS:N	2.24	0.53
15:V:95:LEU:HA	15:V:100:TRP:CH2	2.35	0.53
16:W:88:LYS:O	16:W:92:GLU:HG2	2.08	0.53
17:X:25:LEU:HD11	19:a:50:ARG:CZ	2.39	0.53
21:q:29:ARG:HD3	21:q:74:PHE:CE1	2.44	0.53
2:B:125:PRO:HG3	2:B:148:VAL:HG13	1.90	0.53
2:B:173:TYR:O	3:C:203:LEU:HD22	2.09	0.53
2:B:192:PRO:HG2	9:I:175:PHE:CD1	2.43	0.53
3:C:107:PHE:CD1	3:C:133:SER:HB3	2.43	0.53
4:D:363:VAL:O	4:D:389:TYR:HE1	1.92	0.53
5:E:131:ILE:HD13	5:E:151:LEU:HD11	1.90	0.53
6:F:297:LYS:O	6:F:301:GLU:HG2	2.08	0.53
7:G:30:ASN:O	7:G:44:GLU:HA	2.09	0.53
7:G:261:ILE:HD13	7:G:273:ILE:HG23	1.91	0.53
9:I:209:TYR:HA	9:I:212:ARG:CG	2.38	0.53
11:Q:59:LEU:HD21	16:W:80:ARG:HH12	1.74	0.53
11:Q:72:ILE:HD13	11:Q:143:TRP:NE1	2.24	0.53
19:a:6:LEU:O	19:a:7:PRO:C	2.52	0.53
4:D:95:LEU:HB2	4:D:458:PHE:CZ	2.44	0.52
6:F:346:GLN:NE2	6:F:440:ARG:HD2	2.24	0.52
7:G:640:ASP:OD1	7:G:641:GLN:N	2.42	0.52
14:T:87:LEU:HD23	14:T:122:MET:HE1	1.91	0.52
17:X:77:HIS:HD2	17:X:115:LEU:HD21	1.75	0.52
21:q:6:VAL:HG11	30:q:201:CDL:HB4	1.91	0.52
3:C:114:THR:CG2	4:D:421:ARG:HH12	2.17	0.52
4:D:141:TYR:CB	4:D:223:HIS:HE1	2.22	0.52
5:E:178:ALA:HA	6:F:125:CYS:SG	2.49	0.52
6:F:235:VAL:HG12	6:F:240:THR:OG1	2.09	0.52
7:G:163:LYS:HE2	12:R:97:LYS:NZ	2.24	0.52
7:G:203:ASP:C	7:G:203:ASP:OD1	2.52	0.52
7:G:438:LEU:HD12	7:G:442:TYR:CD1	2.44	0.52
7:G:617:ARG:NH1	16:W:129:HIS:N	2.57	0.52
9:I:118:LEU:CD1	9:I:161:ALA:HB1	2.39	0.52
4:D:148:GLU:OE2	4:D:227:ILE:HG13	2.10	0.52
6:F:63:TYR:H	6:F:256:ARG:HH21	1.57	0.52
7:G:608:VAL:HG23	11:Q:103:THR:HG1	1.73	0.52
9:I:94:SER:CB	9:I:95:PRO:HD2	2.29	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:153:ILE:HD12	9:I:153:ILE:O	2.09	0.52
10:P:166:HIS:CE1	10:P:168:SER:HB2	2.45	0.52
10:P:283:MET:HE2	10:P:366:ILE:HG22	1.92	0.52
12:R:113:GLN:CD	12:R:113:GLN:N	2.66	0.52
17:X:80:GLU:HB3	17:X:81:PRO:HD3	1.91	0.52
19:a:64:LYS:HG3	19:a:66:LEU:H	1.75	0.52
2:B:116:ARG:O	8:H:39:ILE:HG22	2.09	0.52
7:G:371:ILE:HG12	7:G:533:GLY:CA	2.38	0.52
8:H:23:VAL:HG11	19:a:9:LEU:CD2	2.39	0.52
8:H:174:LEU:C	8:H:177:PRO:HD2	2.34	0.52
8:H:179:TRP:CG	8:H:180:PRO:HD3	2.43	0.52
6:F:396:MET:HE2	6:F:438:LEU:HD13	1.91	0.52
7:G:30:ASN:O	7:G:45:PRO:HD3	2.09	0.52
7:G:347:ASP:N	7:G:347:ASP:OD1	2.41	0.52
18:Z:65:LEU:HB2	20:b:50:PRO:HG2	1.91	0.52
4:D:80:MET:SD	8:H:126:LYS:HD3	2.49	0.52
6:F:326:LEU:CD2	6:F:363:ILE:HD11	2.40	0.52
6:F:383:THR:HG21	7:G:120:LEU:HD21	1.91	0.52
6:F:422:HIS:NE2	7:G:112:ALA:CB	2.72	0.52
7:G:386:LEU:HD21	7:G:523:VAL:HG13	1.91	0.52
18:Z:64:ASP:OD1	18:Z:65:LEU:N	2.42	0.52
1:A:8:PHE:O	1:A:12:LEU:HG	2.09	0.52
7:G:128:CYS:N	7:G:129:PRO:HD2	2.24	0.52
7:G:528:LEU:HD21	7:G:653:LEU:CD1	2.39	0.52
8:H:222:LEU:O	8:H:223:PHE:C	2.50	0.52
10:P:195:PHE:CD1	10:P:198:ALA:HB2	2.45	0.52
14:T:79:ILE:CG2	14:T:145:VAL:HG13	2.40	0.52
15:V:48:THR:HA	15:V:51:ILE:HD12	1.90	0.52
21:q:89:TRP:HB2	21:q:98:PRO:HD3	1.92	0.52
4:D:128:THR:N	4:D:131:GLN:HE21	2.04	0.52
5:E:118:TYR:HE2	6:F:206:CYS:SG	2.33	0.52
7:G:140:GLN:HG3	7:G:141:ASP:OD1	2.09	0.52
7:G:164:ASN:ND2	7:G:166:GLY:H	2.08	0.52
7:G:231:LEU:HD12	7:G:231:LEU:O	2.10	0.52
7:G:382:ARG:HD2	13:S:56:ARG:HD3	1.90	0.52
7:G:385:TYR:HA	7:G:515:ILE:CD1	2.39	0.52
7:G:563:ASP:O	7:G:564:CYS:C	2.51	0.52
7:G:614:GLY:O	16:W:129:HIS:NE2	2.41	0.52
8:H:85:LEU:CD2	8:H:108:THR:HB	2.37	0.52
14:T:130:ILE:CG2	14:T:131:PRO:HD2	2.40	0.52
2:B:103:GLU:O	2:B:106:HIS:HB2	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:192:TYR:CE2	5:E:213:PRO:HB2	2.45	0.52
5:E:240:PRO:HG3	6:F:60:GLY:HA2	1.91	0.52
7:G:358:LEU:HD12	7:G:366:LEU:CD2	2.40	0.52
8:H:273:ILE:HG23	8:H:277:TYR:CD2	2.45	0.52
10:P:55:VAL:HG22	10:P:79:GLN:HB3	1.91	0.52
6:F:159:ARG:HG2	6:F:161:GLU:HB2	1.91	0.52
7:G:177:ILE:HG12	7:G:228:VAL:HG21	1.92	0.52
7:G:445:LEU:HD22	7:G:460:HIS:CE1	2.44	0.52
8:H:33:LEU:HD11	9:I:76:TYR:HD1	1.74	0.52
8:H:186:PHE:CZ	8:H:270:PHE:CD1	2.98	0.52
15:V:62:GLU:HB3	15:V:68:LEU:HD13	1.92	0.52
21:q:56:PHE:HD1	21:q:59:HIS:NE2	2.06	0.52
21:q:65:THR:CG2	21:q:66:THR:N	2.72	0.52
1:A:104:TYR:O	1:A:105:GLU:C	2.51	0.51
7:G:275:PRO:HB2	11:Q:86:ASN:ND2	2.25	0.51
8:H:90:PRO:CG	8:H:240:ILE:HG21	2.39	0.51
10:P:239:PRO:HG2	10:P:345:LEU:CD1	2.40	0.51
21:q:88:ARG:HB2	21:q:93:MET:HB2	1.91	0.51
21:q:125:VAL:HG23	21:q:125:VAL:O	2.08	0.51
7:G:136:GLU:HB3	11:Q:87:MET:HB3	1.92	0.51
7:G:422:TRP:CZ2	7:G:441:ARG:HB3	2.45	0.51
7:G:639:LEU:HD23	7:G:639:LEU:C	2.35	0.51
8:H:51:ASP:O	8:H:54:LYS:HG2	2.10	0.51
8:H:223:PHE:O	8:H:224:PHE:C	2.53	0.51
14:T:130:ILE:HG23	14:T:131:PRO:CD	2.40	0.51
16:W:73:ASN:O	16:W:76:VAL:HG12	2.10	0.51
18:Z:61:LEU:O	18:Z:64:ASP:OD1	2.28	0.51
20:b:82:LYS:O	20:b:83:ASN:C	2.52	0.51
21:q:29:ARG:HD3	21:q:74:PHE:CD1	2.44	0.51
5:E:129:TYR:CE2	5:E:207:LEU:HB3	2.46	0.51
6:F:66:LYS:C	6:F:66:LYS:HD3	2.34	0.51
7:G:304:GLU:HB2	7:G:316:TYR:HD2	1.75	0.51
7:G:340:ALA:HB1	7:G:354:LEU:HD21	1.91	0.51
7:G:421:SER:HB3	7:G:427:LEU:CD1	2.41	0.51
7:G:704:SER:HB2	7:G:707:MET:HB2	1.92	0.51
8:H:2:PHE:CE2	8:H:6:ILE:HD11	2.46	0.51
8:H:172:MET:HE1	18:Z:46:GLY:HA2	1.93	0.51
2:B:125:PRO:O	2:B:152:MET:HA	2.10	0.51
2:B:202:LEU:HD12	9:I:86:TYR:CG	2.43	0.51
4:D:462:ASP:O	4:D:463:ARG:C	2.53	0.51
5:E:47:ASN:OD1	5:E:50:THR:HG23	2.09	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:25:LEU:O	17:X:29:ALA:N	2.44	0.51
17:X:129:THR:CG2	20:b:68:SER:HA	2.39	0.51
2:B:126:ARG:HG3	8:H:214:GLU:HA	1.91	0.51
6:F:409:ILE:CG2	6:F:446:LEU:HD23	2.40	0.51
7:G:75:CYS:SG	7:G:76:ARG:N	2.84	0.51
7:G:355:LYS:HA	7:G:366:LEU:CD1	2.37	0.51
7:G:367:CYS:HB3	7:G:533:GLY:O	2.10	0.51
8:H:230:ASN:O	8:H:231:ILE:C	2.53	0.51
9:I:38:TYR:HB3	9:I:41:LYS:HB2	1.93	0.51
9:I:149:MET:HE3	9:I:185:TYR:CE2	2.45	0.51
2:B:79:ASP:OD2	2:B:216:GLN:HA	2.10	0.51
3:C:115:ALA:HB2	3:C:127:ILE:HD13	1.92	0.51
4:D:106:VAL:HG21	4:D:447:VAL:CG2	2.40	0.51
4:D:253:LEU:HB2	22:r:23:LYS:HD3	1.92	0.51
4:D:299:GLN:OE1	22:r:104:TRP:HB2	2.10	0.51
4:D:382:PHE:O	4:D:386:THR:HG23	2.11	0.51
7:G:329:MET:HE3	7:G:333:PHE:CE2	2.45	0.51
7:G:379:THR:HG23	7:G:526:LEU:O	2.11	0.51
7:G:421:SER:HB3	7:G:427:LEU:HD11	1.91	0.51
7:G:488:ALA:HB2	7:G:677:GLN:CB	2.41	0.51
9:I:149:MET:CE	9:I:185:TYR:CD2	2.94	0.51
10:P:66:GLY:O	10:P:67:ARG:C	2.54	0.51
11:Q:91:VAL:HG13	11:Q:95:LYS:NZ	2.26	0.51
17:X:5:VAL:O	17:X:6:GLU:C	2.54	0.51
2:B:174:SER:HA	3:C:203:LEU:CD2	2.41	0.51
7:G:382:ARG:O	7:G:386:LEU:HD12	2.10	0.51
7:G:621:LYS:O	7:G:622:ILE:C	2.54	0.51
8:H:30:TYR:OH	19:a:4:GLU:HB2	2.11	0.51
10:P:122:HIS:CB	12:R:46:VAL:CG1	2.85	0.51
14:T:114:ASP:OD1	16:W:67:ARG:NH1	2.42	0.51
19:a:1:MET:HG3	30:q:201:CDL:CB2	2.41	0.51
21:q:6:VAL:HG12	30:q:201:CDL:OA9	2.11	0.51
21:q:13:GLN:HE22	30:q:201:CDL:CA3	2.21	0.51
4:D:218:SER:CB	4:D:224:ALA:HB1	2.40	0.51
7:G:47:THR:O	7:G:96:VAL:HG12	2.10	0.51
7:G:403:VAL:CG1	7:G:476:LEU:HA	2.41	0.51
8:H:176:LEU:HB2	8:H:177:PRO:HD3	1.93	0.51
9:I:71:GLY:HA2	25:I:301:PC1:H351	1.93	0.51
17:X:56:CYS:HA	17:X:135:ARG:NH1	2.25	0.51
21:q:88:ARG:HG3	21:q:89:TRP:N	2.26	0.51
4:D:106:VAL:HG11	4:D:109:CYS:SG	2.51	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:166:ARG:CZ	18:Z:8:GLN:HG2	2.41	0.51
5:E:55:THR:O	5:E:56:PRO:C	2.53	0.51
5:E:227:ALA:HB3	6:F:284:HIS:ND1	2.26	0.51
7:G:41:VAL:HG21	7:G:56:VAL:CB	2.41	0.51
10:P:157:LYS:O	10:P:158:GLU:C	2.54	0.51
10:P:172:ALA:H	10:P:202:ARG:NH2	2.08	0.51
10:P:348:LYS:HB3	10:P:351:GLU:OE2	2.11	0.51
1:A:19:LEU:O	1:A:20:VAL:C	2.50	0.51
1:A:87:MET:HE1	8:H:309:ILE:HD11	1.92	0.51
5:E:39:VAL:CG2	7:G:205:GLN:HE22	2.16	0.51
5:E:43:THR:HG23	5:E:46:ASN:H	1.75	0.51
5:E:135:THR:O	6:F:369:ARG:NE	2.41	0.51
5:E:136:THR:HG22	5:E:137:THR:N	2.26	0.51
7:G:253:VAL:O	7:G:253:VAL:HG12	2.11	0.51
7:G:401:LEU:HD21	7:G:466:LEU:HD21	1.92	0.51
8:H:142:TYR:CE1	8:H:285:LEU:HD21	2.46	0.51
9:I:130:ILE:HD11	9:I:145:TYR:CE1	2.46	0.51
11:Q:77:VAL:HG12	11:Q:101:PHE:CG	2.46	0.51
12:R:72:VAL:HG12	12:R:73:GLU:N	2.26	0.51
17:X:38:LYS:O	17:X:42:GLU:HG3	2.11	0.51
20:b:11:ASN:OD1	20:b:12:ALA:N	2.44	0.51
1:A:59:ALA:O	1:A:62:PHE:HB3	2.11	0.50
5:E:152:GLN:HE21	5:E:159:VAL:HB	1.76	0.50
6:F:42:PHE:CE1	6:F:130:ILE:HD12	2.46	0.50
7:G:401:LEU:HD21	7:G:462:PHE:CE2	2.46	0.50
7:G:546:PHE:HD1	7:G:567:VAL:HG23	1.73	0.50
7:G:671:LEU:CD1	13:S:42:VAL:HG12	2.41	0.50
8:H:103:LEU:HG	8:H:160:TYR:CD1	2.46	0.50
1:A:57:LEU:O	1:A:61:THR:HG23	2.12	0.50
4:D:259:GLU:C	4:D:261:MET:N	2.68	0.50
5:E:180:VAL:HG22	5:E:221:ARG:HH12	1.75	0.50
5:E:188:ASN:O	5:E:189:ASP:HB3	2.10	0.50
6:F:225:LEU:HB2	11:Q:160:TYR:CD2	2.45	0.50
6:F:295:PRO:HD2	6:F:298:GLU:OE2	2.11	0.50
7:G:517:HIS:H	7:G:599:THR:CG2	2.23	0.50
8:H:152:SER:CB	8:H:181:MET:HE1	2.41	0.50
8:H:172:MET:SD	18:Z:46:GLY:HA2	2.52	0.50
10:P:374:THR:HG23	10:P:374:THR:O	2.10	0.50
15:V:90:LEU:HD21	15:V:94:MET:HE3	1.93	0.50
20:b:66:VAL:HG22	20:b:75:GLY:CA	2.40	0.50
4:D:176:GLU:O	4:D:177:ILE:C	2.53	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:304:GLU:HB2	7:G:316:TYR:CD2	2.46	0.50
8:H:26:LYS:O	8:H:30:TYR:CD2	2.64	0.50
10:P:207:PHE:O	10:P:241:TYR:HA	2.10	0.50
11:Q:75:ARG:HH12	11:Q:104:ARG:HG2	1.76	0.50
11:Q:167:ASN:C	11:Q:168:LYS:HG2	2.36	0.50
13:S:36:PHE:CZ	13:S:44:LEU:HD11	2.36	0.50
15:V:44:TYR:O	15:V:48:THR:HG22	2.10	0.50
22:r:28:TYR:O	22:r:29:GLN:C	2.53	0.50
3:C:216:LYS:HG3	10:P:209:ARG:HH11	1.76	0.50
4:D:266:ARG:HD3	28:H:401:3PE:O12	2.11	0.50
6:F:217:GLU:CD	11:Q:166:TRP:HE1	2.18	0.50
9:I:149:MET:HE3	9:I:185:TYR:CD2	2.46	0.50
10:P:208:GLY:N	10:P:211:ASP:HB3	2.20	0.50
10:P:305:PHE:CG	10:P:314:THR:HG22	2.46	0.50
11:Q:167:ASN:HA	23:s:64:ARG:HD3	1.94	0.50
14:T:90:TYR:CE2	14:T:92:LYS:HB2	2.46	0.50
4:D:444:LEU:HD21	8:H:206:GLU:O	2.12	0.50
6:F:391:TRP:HZ3	7:G:118:GLU:HG2	1.76	0.50
6:F:392:MET:HE2	6:F:416:SER:HA	1.94	0.50
7:G:183:ILE:CD1	7:G:206:VAL:HG13	2.40	0.50
8:H:17:MET:CE	8:H:225:MET:HB3	2.41	0.50
8:H:142:TYR:CE1	8:H:285:LEU:CD2	2.94	0.50
8:H:269:THR:O	8:H:273:ILE:HG12	2.11	0.50
14:T:87:LEU:HD23	14:T:122:MET:CE	2.41	0.50
14:T:105:MET:HB2	14:T:139:MET:SD	2.52	0.50
17:X:7:LEU:CD1	18:Z:87:LEU:HB3	2.41	0.50
17:X:7:LEU:HD13	18:Z:87:LEU:HB3	1.93	0.50
17:X:119:ARG:HD2	17:X:120:PRO:HD2	1.94	0.50
20:b:36:SER:HB3	20:b:39:THR:OG1	2.10	0.50
5:E:227:ALA:H	6:F:284:HIS:HB3	1.76	0.50
5:E:233:LEU:HD13	6:F:48:ARG:HH22	1.76	0.50
7:G:36:VAL:CG1	7:G:56:VAL:HG11	2.34	0.50
7:G:283:GLU:O	7:G:285:TRP:CZ3	2.65	0.50
7:G:346:VAL:HG21	7:G:548:LEU:CD2	2.41	0.50
7:G:429:VAL:HG11	7:G:440:TYR:CE1	2.46	0.50
8:H:91:MET:O	8:H:92:PRO:C	2.54	0.50
4:D:259:GLU:C	4:D:261:MET:H	2.18	0.50
5:E:82:LEU:HD21	5:E:115:ALA:HB2	1.93	0.50
8:H:184:MET:SD	8:H:296:LEU:HD23	2.52	0.50
8:H:228:TYR:HA	8:H:231:ILE:CD1	2.40	0.50
9:I:118:LEU:C	9:I:118:LEU:HD12	2.37	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:V:12:VAL:CG1	15:V:13:GLY:N	2.72	0.50
19:a:4:GLU:O	19:a:7:PRO:HD2	2.11	0.50
1:A:97:ILE:HG13	1:A:98:LEU:HD22	1.93	0.50
3:C:112:ASP:OD1	3:C:113:LEU:N	2.45	0.50
5:E:244:VAL:HG23	6:F:256:ARG:CG	2.42	0.50
6:F:113:LEU:HB3	6:F:154:ALA:HB2	1.92	0.50
6:F:345:ALA:C	6:F:346:GLN:HG2	2.34	0.50
7:G:403:VAL:HG13	7:G:476:LEU:HD12	1.93	0.50
7:G:557:ARG:CG	7:G:579:MET:HE3	2.33	0.50
10:P:40:VAL:HB	10:P:53:GLY:HA2	1.93	0.50
12:R:67:GLN:HG2	12:R:109:LEU:HD21	1.94	0.50
14:T:140:CYS:HB2	14:T:143:GLU:CG	2.40	0.50
17:X:9:THR:HG23	17:X:12:GLU:H	1.77	0.50
22:r:6:ARG:HG2	22:r:6:ARG:O	2.11	0.50
3:C:100:ARG:HH12	15:V:86:LYS:NZ	2.10	0.50
3:C:141:ARG:NH1	4:D:410:TYR:CE1	2.77	0.50
5:E:130:HIS:O	5:E:132:GLN:HG3	2.12	0.50
5:E:244:VAL:HG23	6:F:256:ARG:HG3	1.93	0.50
6:F:174:ARG:O	6:F:178:GLU:HG3	2.11	0.50
6:F:296:LEU:HD21	6:F:317:VAL:HG11	1.94	0.50
7:G:68:ARG:HD2	7:G:285:TRP:CZ3	2.47	0.50
8:H:148:ILE:HG22	8:H:297:THR:HG22	1.94	0.50
8:H:202:GLU:OE2	8:H:211:PHE:HB3	2.12	0.50
10:P:68:TYR:CD1	10:P:242:VAL:HG21	2.46	0.50
10:P:150:ARG:O	10:P:151:ALA:C	2.55	0.50
13:S:42:VAL:O	13:S:46:LYS:HG3	2.12	0.50
14:T:140:CYS:O	14:T:144:ILE:HG13	2.12	0.50
15:V:31:THR:HA	15:V:88:LEU:HD13	1.92	0.50
17:X:52:ASP:CG	18:Z:116:TRP:HB3	2.37	0.50
18:Z:66:GLU:HA	18:Z:69:ILE:HG12	1.93	0.50
3:C:146:ALA:HB2	3:C:152:ILE:HD11	1.93	0.49
4:D:235:ASP:OD2	18:Z:8:GLN:NE2	2.41	0.49
5:E:91:TRP:CE3	5:E:125:PRO:HB3	2.47	0.49
7:G:344:GLY:O	7:G:345:LEU:HB2	2.12	0.49
7:G:382:ARG:NH1	7:G:652:ASN:HD22	2.09	0.49
8:H:33:LEU:HD23	22:r:25:GLN:HG2	1.92	0.49
8:H:186:PHE:CZ	8:H:270:PHE:HE1	2.19	0.49
10:P:346:GLU:H	10:P:346:GLU:CD	2.20	0.49
15:V:7:LYS:O	15:V:8:THR:OG1	2.29	0.49
15:V:12:VAL:CG1	15:V:13:GLY:H	2.22	0.49
2:B:191:VAL:HG21	2:B:201:LEU:HD12	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:105:MET:SD	4:D:441:GLY:HA2	2.53	0.49
4:D:289:SER:N	4:D:293:LEU:HG	2.27	0.49
6:F:35:LEU:HB2	6:F:291:GLU:HB2	1.94	0.49
7:G:43:VAL:CG1	7:G:55:LYS:HD3	2.41	0.49
7:G:405:THR:HB	7:G:477:GLY:HA3	1.94	0.49
7:G:447:ASP:OD1	7:G:447:ASP:O	2.29	0.49
8:H:74:ALA:HB3	8:H:75:PRO:HD3	1.93	0.49
14:T:138:LEU:HD13	14:T:144:ILE:CD1	2.42	0.49
2:B:115:ASP:O	2:B:116:ARG:C	2.54	0.49
3:C:172:MET:SD	3:C:196:PRO:HG2	2.52	0.49
3:C:232:PHE:CD1	7:G:243:TRP:HD1	2.30	0.49
4:D:128:THR:HG22	4:D:131:GLN:CD	2.38	0.49
4:D:198:THR:CG2	8:H:275:ALA:HB1	2.42	0.49
5:E:128:LYS:CB	5:E:167:LEU:HA	2.42	0.49
6:F:122:PRO:HG3	6:F:373:PHE:CZ	2.46	0.49
7:G:162:ASP:O	7:G:163:LYS:HD3	2.12	0.49
8:H:63:PRO:O	8:H:66:THR:HG22	2.12	0.49
8:H:102:ILE:HG13	8:H:162:LEU:CD1	2.41	0.49
13:S:24:CYS:N	13:S:58:CYS:SG	2.85	0.49
18:Z:129:THR:HG22	18:Z:131:GLU:H	1.77	0.49
20:b:28:LEU:HA	20:b:31:ILE:CG2	2.42	0.49
4:D:460:GLU:O	4:D:463:ARG:HG2	2.12	0.49
5:E:97:MET:HE2	5:E:115:ALA:CB	2.42	0.49
6:F:371:ILE:HD11	6:F:435:VAL:CG2	2.41	0.49
7:G:160:VAL:HG12	7:G:161:GLU:H	1.77	0.49
8:H:66:THR:HA	8:H:124:ASN:OD1	2.12	0.49
8:H:116:ILE:HA	8:H:211:PHE:HE1	1.75	0.49
10:P:367:GLU:HG2	10:P:368:GLU:N	2.26	0.49
12:R:70:ASN:HD22	12:R:111:PHE:HE1	1.60	0.49
15:V:39:PRO:HB2	15:V:42:ALA:HB2	1.94	0.49
4:D:152:SER:O	4:D:153:ILE:C	2.56	0.49
5:E:43:THR:OG1	5:E:44:PRO:CD	2.60	0.49
5:E:191:TYR:OH	6:F:161:GLU:HB3	2.13	0.49
7:G:79:LEU:HD22	7:G:88:VAL:HG23	1.93	0.49
7:G:262:VAL:CG2	7:G:276:ARG:HB3	2.34	0.49
7:G:298:LYS:O	21:q:134:ILE:HA	2.12	0.49
7:G:593:SER:OG	7:G:639:LEU:HD13	2.12	0.49
8:H:85:LEU:HB3	8:H:233:LEU:CD2	2.42	0.49
8:H:93:HIS:O	19:a:23:THR:HG22	2.12	0.49
12:R:32:THR:CG2	12:R:36:GLN:H	2.18	0.49
16:W:95:GLU:HB3	16:W:101:LYS:HG3	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:4:ILE:CG2	17:X:5:VAL:N	2.50	0.49
19:a:3:PHE:CE2	30:q:201:CDL:H112	2.46	0.49
2:B:194:CYS:HB2	9:I:153:ILE:O	2.12	0.49
4:D:207:ARG:O	4:D:208:GLU:C	2.53	0.49
4:D:383:LYS:HD3	7:G:140:GLN:CD	2.38	0.49
6:F:127:ASP:HB3	6:F:245:VAL:CG2	2.38	0.49
6:F:157:TYR:CD2	6:F:212:LEU:HD11	2.47	0.49
6:F:212:LEU:O	6:F:216:ILE:HG12	2.13	0.49
7:G:53:CYS:O	7:G:56:VAL:HG12	2.13	0.49
8:H:179:TRP:N	8:H:180:PRO:CD	2.76	0.49
10:P:211:ASP:O	10:P:215:ASN:HB2	2.12	0.49
10:P:221:ARG:HD2	10:P:286:ARG:HD3	1.91	0.49
10:P:265:PHE:HZ	10:P:338:LEU:HD12	1.77	0.49
2:B:173:TYR:HE2	9:I:126:GLN:HB2	1.76	0.49
3:C:53:THR:O	3:C:54:HIS:C	2.55	0.49
4:D:259:GLU:OE1	4:D:263:THR:HB	2.13	0.49
6:F:171:VAL:O	6:F:175:GLU:HG2	2.12	0.49
11:Q:99:MET:SD	11:Q:128:PHE:HE2	2.35	0.49
17:X:73:GLN:OE1	17:X:117:TRP:HZ2	1.96	0.49
18:Z:140:PHE:O	18:Z:141:THR:C	2.56	0.49
4:D:141:TYR:HB3	4:D:223:HIS:CE1	2.45	0.49
4:D:182:ASN:HD21	4:D:404:LYS:NZ	2.10	0.49
4:D:250:ASN:O	4:D:251:PHE:C	2.53	0.49
5:E:97:MET:HE2	5:E:115:ALA:HB1	1.95	0.49
5:E:235:GLU:HB2	6:F:37:ASP:CB	2.43	0.49
7:G:360:LYS:CE	7:G:632:ILE:HB	2.41	0.49
14:T:88:LYS:NZ	14:T:96:GLU:H	2.11	0.49
17:X:112:LEU:HD13	17:X:118:VAL:HG22	1.94	0.49
1:A:24:LEU:N	1:A:25:PRO:CD	2.76	0.49
2:B:113:ASP:CG	8:H:34:ARG:HD2	2.38	0.49
2:B:170:TYR:CE2	4:D:134:PRO:HB2	2.47	0.49
4:D:145:MET:O	4:D:146:CYS:C	2.54	0.49
4:D:213:PHE:O	4:D:217:VAL:HG13	2.12	0.49
4:D:266:ARG:HG2	4:D:266:ARG:O	2.13	0.49
5:E:57:GLU:CA	5:E:60:LYS:HE2	2.31	0.49
5:E:133:VAL:HG22	5:E:185:VAL:HG12	1.94	0.49
6:F:36:LYS:HB3	6:F:38:GLU:HG2	1.93	0.49
6:F:224:ARG:HD2	11:Q:164:PHE:CE1	2.48	0.49
7:G:371:ILE:N	7:G:482:GLN:OE1	2.46	0.49
7:G:565:PHE:HA	7:G:581:ASP:OD2	2.12	0.49
8:H:12:PRO:O	19:a:15:CYS:HB3	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:185:TRP:O	8:H:189:THR:HG23	2.12	0.49
28:H:401:3PE:H3I2	28:H:401:3PE:H3E1	1.95	0.49
10:P:122:HIS:HB3	12:R:46:VAL:CG1	2.43	0.49
10:P:168:SER:O	10:P:202:ARG:HA	2.13	0.49
10:P:298:TYR:HA	10:P:301:ILE:HG12	1.95	0.49
2:B:170:TYR:OH	4:D:131:GLN:O	2.30	0.49
3:C:160:ILE:HB	4:D:286:TYR:HD1	1.78	0.49
4:D:145:MET:O	4:D:148:GLU:CG	2.40	0.49
4:D:279:THR:HG22	4:D:280:ALA:N	2.28	0.49
4:D:329:ARG:O	4:D:330:TYR:C	2.53	0.49
6:F:66:LYS:HG2	6:F:189:SER:HB3	1.95	0.49
6:F:339:PHE:CE1	6:F:349:LEU:HB3	2.47	0.49
7:G:117:MET:HE3	7:G:143:SER:N	2.27	0.49
7:G:175:ARG:HB2	7:G:230:ALA:CA	2.43	0.49
8:H:239:THR:CG2	8:H:262:GLU:HB2	2.43	0.49
10:P:354:ARG:NH2	16:W:56:ASP:OD1	2.45	0.49
11:Q:72:ILE:HD13	11:Q:143:TRP:HE1	1.76	0.49
15:V:56:LEU:HA	15:V:59:VAL:HB	1.94	0.49
22:r:12:ARG:HE	22:r:20:LEU:HD21	1.78	0.49
1:A:84:THR:HG23	20:b:46:ASN:HD21	1.78	0.48
4:D:82:LEU:O	4:D:83:ASN:C	2.53	0.48
4:D:339:GLN:HE21	9:I:37:LYS:NZ	2.11	0.48
4:D:365:PRO:HA	4:D:384:LEU:HD12	1.95	0.48
7:G:32:ILE:N	7:G:43:VAL:O	2.46	0.48
7:G:357:LEU:HD13	7:G:627:SER:OG	2.12	0.48
7:G:421:SER:HB2	7:G:427:LEU:HD11	1.93	0.48
8:H:311:THR:O	8:H:312:ALA:C	2.56	0.48
9:I:180:HIS:CE1	10:P:100:LEU:HD21	2.48	0.48
10:P:246:SER:O	10:P:247:LYS:C	2.55	0.48
17:X:69:ASN:O	17:X:70:PHE:C	2.56	0.48
17:X:115:LEU:HD13	17:X:117:TRP:CZ3	2.48	0.48
1:A:18:ILE:O	1:A:21:ALA:HB3	2.13	0.48
4:D:339:GLN:NE2	9:I:37:LYS:HZ2	2.11	0.48
5:E:201:GLU:HA	5:E:204:ILE:HD12	1.95	0.48
6:F:146:GLY:O	6:F:150:GLY:N	2.46	0.48
7:G:386:LEU:HD21	7:G:523:VAL:HG11	1.95	0.48
7:G:432:ILE:CG2	7:G:451:ILE:HD11	2.39	0.48
9:I:154:TYR:N	9:I:154:TYR:CD1	2.81	0.48
1:A:89:ILE:O	1:A:93:ILE:HG12	2.13	0.48
25:B:302:PC1:H132	21:q:29:ARG:HA	1.96	0.48
3:C:89:PRO:O	3:C:92:VAL:HG23	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:151:PRO:HB2	3:C:178:PHE:CE2	2.47	0.48
6:F:116:ASN:O	6:F:245:VAL:HG13	2.13	0.48
6:F:146:GLY:HA3	6:F:193:PHE:CE2	2.48	0.48
7:G:261:ILE:HD13	7:G:273:ILE:CG2	2.43	0.48
7:G:566:ILE:CD1	7:G:579:MET:HE2	2.43	0.48
9:I:80:GLU:CB	22:r:26:LEU:HD11	2.43	0.48
15:V:11:LEU:HD23	15:V:14:LEU:HD13	1.95	0.48
15:V:35:LEU:HD13	15:V:48:THR:HG23	1.96	0.48
20:b:35:ILE:O	20:b:35:ILE:CD1	2.59	0.48
2:B:91:TRP:N	2:B:91:TRP:CD1	2.80	0.48
2:B:224:ARG:HG3	10:P:85:ARG:HH12	1.78	0.48
6:F:57:LEU:HD23	6:F:61:ASP:OD1	2.13	0.48
11:Q:82:PRO:HG2	11:Q:93:ASN:O	2.14	0.48
14:T:90:TYR:HE2	14:T:92:LYS:HB3	1.78	0.48
19:a:37:ARG:CB	19:a:48:MET:HE2	2.43	0.48
2:B:182:ASP:C	2:B:182:ASP:OD1	2.56	0.48
3:C:227:GLN:HE21	3:C:230:ARG:HH11	1.52	0.48
4:D:260:GLU:HG3	18:Z:25:LEU:CD2	2.44	0.48
6:F:289:GLU:O	6:F:289:GLU:CD	2.56	0.48
6:F:326:LEU:HD12	6:F:326:LEU:O	2.13	0.48
7:G:183:ILE:CD1	7:G:197:THR:HG23	2.43	0.48
8:H:20:LEU:HA	19:a:12:MET:SD	2.53	0.48
16:W:46:VAL:N	16:W:47:PRO:HD2	2.29	0.48
3:C:197:PHE:CE2	4:D:121:GLU:OE1	2.67	0.48
5:E:45:GLU:HB3	5:E:91:TRP:HH2	1.78	0.48
6:F:443:ARG:N	6:F:444:PRO:HD2	2.28	0.48
7:G:383:SER:HB3	7:G:663:ASN:HB2	1.95	0.48
7:G:435:PRO:O	7:G:435:PRO:CG	2.61	0.48
8:H:70:LEU:HD22	8:H:121:TRP:CZ3	2.48	0.48
8:H:88:PRO:HG3	8:H:104:PHE:CD1	2.48	0.48
10:P:79:GLN:NE2	10:P:102:GLN:O	2.47	0.48
10:P:178:SER:O	10:P:179:LYS:C	2.55	0.48
1:A:18:ILE:HG12	8:H:222:LEU:HD22	1.94	0.48
2:B:210:ARG:CD	21:q:76:ASP:HB2	2.43	0.48
3:C:134:LEU:H	3:C:134:LEU:HD12	1.79	0.48
6:F:314:LEU:HD13	6:F:356:VAL:HG13	1.95	0.48
7:G:66:HIS:HB3	7:G:69:LEU:HB2	1.96	0.48
7:G:404:GLY:CA	7:G:684:LEU:HD11	2.44	0.48
7:G:662:THR:HB	13:S:25:GLN:NE2	2.28	0.48
8:H:179:TRP:CZ3	9:I:62:MET:HE1	2.48	0.48
14:T:104:PHE:CZ	14:T:118:ILE:HG21	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:a:18:ILE:N	19:a:19:PRO:CD	2.76	0.48
21:q:60:ARG:HH12	21:q:95:ASP:HA	1.78	0.48
1:A:105:GLU:HG3	1:A:111:LEU:HD22	1.95	0.48
2:B:107:MET:HE3	2:B:114:MET:CE	2.44	0.48
4:D:142:VAL:HG13	4:D:207:ARG:HH12	1.78	0.48
4:D:184:ILE:HD11	4:D:251:PHE:CZ	2.49	0.48
6:F:288:VAL:O	6:F:289:GLU:HB3	2.13	0.48
8:H:90:PRO:CG	8:H:162:LEU:HB3	2.31	0.48
10:P:340:VAL:HG13	10:P:340:VAL:O	2.14	0.48
15:V:90:LEU:HD23	15:V:94:MET:HG2	1.94	0.48
2:B:97:LEU:CD2	4:D:94:VAL:HG11	2.44	0.48
8:H:154:LEU:HD13	8:H:160:TYR:CE1	2.49	0.48
8:H:196:ALA:HB2	8:H:274:ARG:CG	2.42	0.48
9:I:116:CYS:O	9:I:117:LYS:HB2	2.13	0.48
10:P:197:GLU:HA	10:P:260:GLY:HA2	1.96	0.48
10:P:235:THR:HB	10:P:273:LEU:HB2	1.95	0.48
10:P:328:MET:O	10:P:330:THR:HG23	2.12	0.48
12:R:79:CYS:O	12:R:88:HIS:CE1	2.67	0.48
14:T:119:ILE:HG13	14:T:135:ALA:HB1	1.95	0.48
21:q:14:VAL:HG13	21:q:23:LEU:HD22	1.96	0.48
2:B:154:GLU:HB2	8:H:59:GLU:HB2	1.95	0.48
3:C:127:ILE:HB	3:C:144:THR:CG2	2.43	0.48
4:D:303:ARG:HG3	4:D:401:GLU:HG3	1.96	0.48
4:D:379:ILE:HD13	7:G:140:GLN:HA	1.95	0.48
5:E:45:GLU:HB3	5:E:91:TRP:CH2	2.48	0.48
6:F:387:GLU:OE1	6:F:387:GLU:N	2.47	0.48
7:G:68:ARG:NE	7:G:283:GLU:CG	2.76	0.48
7:G:403:VAL:HG13	7:G:476:LEU:HA	1.96	0.48
7:G:496:MET:HG2	7:G:500:ILE:CD1	2.43	0.48
8:H:96:ILE:HG12	18:Z:143:TYR:OH	2.14	0.48
8:H:210:GLY:HA2	8:H:213:VAL:CG2	2.44	0.48
9:I:98:ARG:HA	9:I:169:GLU:HB3	1.95	0.48
20:b:46:ASN:OD1	20:b:47:LYS:N	2.47	0.48
4:D:456:ILE:HD12	4:D:461:ILE:HD11	1.96	0.47
6:F:364:VAL:HG12	6:F:400:VAL:HG22	1.96	0.47
10:P:294:PRO:HB3	10:P:296:PHE:HD1	1.79	0.47
17:X:17:GLU:HB3	17:X:19:LYS:HG3	1.96	0.47
20:b:38:TYR:HA	20:b:41:TYR:HD2	1.76	0.47
21:q:97:PRO:C	21:q:99:THR:N	2.70	0.47
22:r:113:LEU:HD12	22:r:113:LEU:HA	1.77	0.47
23:s:64:ARG:HD2	23:s:64:ARG:N	2.29	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:260:GLU:CG	18:Z:25:LEU:HD22	2.43	0.47
4:D:329:ARG:O	4:D:332:CYS:HB2	2.13	0.47
5:E:134:CYS:SG	5:E:139:CYS:SG	3.11	0.47
6:F:227:PRO:HG3	7:G:94:MET:SD	2.54	0.47
7:G:297:LEU:O	7:G:297:LEU:HD23	2.14	0.47
7:G:688:GLN:HA	7:G:693:ASP:CB	2.43	0.47
10:P:116:ILE:HG21	10:P:152:ILE:HA	1.96	0.47
17:X:52:ASP:HA	17:X:53:PRO:HD3	1.40	0.47
21:q:76:ASP:OD1	21:q:76:ASP:C	2.57	0.47
2:B:98:ALA:HB3	2:B:135:GLY:CA	2.44	0.47
25:B:302:PC1:H232	25:B:302:PC1:C32	2.37	0.47
6:F:336:LEU:HD11	6:F:338:ASP:OD2	2.14	0.47
7:G:68:ARG:CD	7:G:285:TRP:HZ3	2.25	0.47
8:H:116:ILE:CG1	8:H:117:LEU:N	2.74	0.47
8:H:235:ASN:CG	8:H:270:PHE:CE2	2.92	0.47
9:I:171:PRO:HG2	9:I:200:GLU:CD	2.39	0.47
10:P:304:LEU:O	10:P:307:LEU:HB3	2.14	0.47
10:P:360:ARG:HD3	10:P:360:ARG:O	2.14	0.47
13:S:50:ASN:O	13:S:51:LEU:C	2.57	0.47
15:V:116:ILE:O	15:V:116:ILE:CG2	2.62	0.47
17:X:8:PRO:HB3	17:X:12:GLU:CD	2.39	0.47
17:X:39:THR:CG2	17:X:40:ASN:N	2.77	0.47
17:X:120:PRO:HB2	17:X:125:LEU:CD1	2.43	0.47
20:b:78:LEU:HA	20:b:80:TRP:CD1	2.48	0.47
2:B:126:ARG:HB2	2:B:127:GLN:NE2	2.29	0.47
6:F:238:CYS:O	6:F:239:PRO:C	2.54	0.47
7:G:284:GLU:OE2	11:Q:84:ARG:NH2	2.47	0.47
7:G:496:MET:HG2	7:G:500:ILE:HD12	1.95	0.47
7:G:605:GLN:NE2	7:G:643:ARG:HH22	2.13	0.47
10:P:85:ARG:HE	29:P:401:NDP:C2A	2.27	0.47
6:F:369:ARG:O	6:F:373:PHE:N	2.47	0.47
7:G:651:PRO:CD	13:S:56:ARG:HB3	2.45	0.47
8:H:9:LEU:O	8:H:9:LEU:HD13	2.14	0.47
16:W:103:ARG:O	16:W:104:THR:C	2.55	0.47
21:q:23:LEU:HD11	21:q:33:ILE:HG12	1.96	0.47
4:D:254:ARG:NH1	22:r:25:GLN:N	2.62	0.47
5:E:221:ARG:HH22	6:F:285:PRO:HB2	1.78	0.47
7:G:136:GLU:OE1	11:Q:87:MET:HG3	2.15	0.47
7:G:217:GLU:C	7:G:219:SER:H	2.21	0.47
7:G:265:THR:HG23	7:G:265:THR:O	2.14	0.47
7:G:517:HIS:CD2	7:G:523:VAL:HG22	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:697:THR:O	7:G:702:ARG:NH1	2.48	0.47
8:H:154:LEU:HD22	8:H:160:TYR:HA	1.97	0.47
8:H:200:LEU:CD2	8:H:285:LEU:HD13	2.44	0.47
11:Q:99:MET:SD	11:Q:128:PHE:CE2	3.08	0.47
2:B:95:PHE:CE2	2:B:97:LEU:HD11	2.50	0.47
4:D:302:LEU:HB2	4:D:401:GLU:CG	2.33	0.47
6:F:46:TYR:O	6:F:48:ARG:HG3	2.15	0.47
6:F:213:ILE:HG23	6:F:235:VAL:CA	2.41	0.47
6:F:338:ASP:OD1	6:F:338:ASP:O	2.33	0.47
6:F:370:LEU:O	6:F:373:PHE:HB3	2.15	0.47
8:H:64:LEU:H	8:H:64:LEU:CD2	2.25	0.47
8:H:130:PHE:O	8:H:134:ARG:HG3	2.14	0.47
8:H:306:SER:OG	20:b:33:PRO:HG3	2.15	0.47
10:P:157:LYS:HD3	10:P:194:VAL:O	2.14	0.47
10:P:169:HIS:N	10:P:184:LYS:HE3	2.29	0.47
12:R:36:GLN:HG2	21:q:127:TYR:HD2	1.78	0.47
13:S:79:LEU:CA	13:S:82:LEU:HD12	2.26	0.47
14:T:117:GLU:HG2	16:W:43:TYR:CZ	2.49	0.47
16:W:46:VAL:O	16:W:50:VAL:HG23	2.14	0.47
17:X:40:ASN:O	17:X:41:LYS:C	2.58	0.47
18:Z:87:LEU:HD21	18:Z:119:PRO:HG3	1.97	0.47
21:q:55:PHE:CZ	21:q:58:ARG:HG3	2.50	0.47
4:D:84:PHE:HZ	4:D:91:ALA:HB2	1.79	0.47
4:D:303:ARG:HG3	4:D:401:GLU:HB2	1.96	0.47
5:E:226:PRO:HD2	5:E:230:LEU:HB3	1.97	0.47
6:F:41:ILE:CD1	6:F:262:PHE:HE1	2.25	0.47
6:F:209:GLU:OE2	6:F:230:PRO:HG2	2.15	0.47
6:F:382:CYS:HA	7:G:74:ASN:O	2.15	0.47
7:G:401:LEU:HD12	7:G:474:VAL:HG22	1.96	0.47
10:P:97:MET:O	10:P:103:LEU:HD11	2.15	0.47
5:E:92:LEU:HG	5:E:92:LEU:O	2.14	0.47
6:F:168:ASN:ND2	23:s:40:TYR:HE2	2.13	0.47
7:G:82:ILE:CD1	7:G:102:ILE:HG13	2.43	0.47
7:G:140:GLN:HG3	7:G:141:ASP:N	2.30	0.47
7:G:373:PRO:HD3	7:G:481:LEU:HB3	1.96	0.47
7:G:429:VAL:HG11	7:G:440:TYR:HE1	1.80	0.47
10:P:287:THR:HG23	10:P:289:ILE:HD11	1.97	0.47
11:Q:166:TRP:CZ3	23:s:67:PRO:HG2	2.50	0.47
14:T:87:LEU:CD2	14:T:104:PHE:HZ	2.12	0.47
16:W:32:LYS:O	16:W:36:ARG:HG3	2.15	0.47
20:b:41:TYR:HD1	20:b:80:TRP:CZ3	2.33	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:q:68:MET:SD	21:q:81:MET:HG2	2.55	0.47
22:r:109:ASP:O	22:r:110:GLN:OE1	2.32	0.47
4:D:266:ARG:NH2	9:I:63:TRP:HA	2.30	0.47
8:H:75:PRO:HA	8:H:223:PHE:CE1	2.49	0.47
10:P:276:LEU:O	10:P:280:ILE:HG13	2.15	0.47
13:S:58:CYS:HB2	13:S:61:VAL:CG1	2.43	0.47
16:W:50:VAL:HA	16:W:55:LEU:HD12	1.97	0.47
17:X:129:THR:HG23	20:b:68:SER:CA	2.44	0.47
18:Z:72:MET:N	18:Z:73:PRO:CD	2.78	0.47
20:b:55:VAL:HG13	20:b:56:PRO:HD2	1.97	0.47
1:A:73:LEU:N	1:A:74:PRO:CD	2.76	0.46
1:A:106:TRP:CZ2	8:H:291:LYS:HA	2.49	0.46
2:B:104:MET:HE3	2:B:132:ILE:HD12	1.97	0.46
4:D:339:GLN:HE21	9:I:37:LYS:HZ2	1.61	0.46
5:E:154:LYS:HE3	5:E:201:GLU:HB2	1.97	0.46
6:F:230:PRO:HA	6:F:233:VAL:O	2.15	0.46
6:F:420:GLU:O	6:F:429:ASP:OD1	2.32	0.46
7:G:382:ARG:NH1	7:G:386:LEU:HD11	2.30	0.46
8:H:127:TYR:HD2	8:H:207:LEU:HG	1.78	0.46
10:P:209:ARG:O	10:P:210:GLU:HB3	2.15	0.46
16:W:120:ASP:OD1	16:W:121:PHE:N	2.46	0.46
17:X:35:GLN:HG3	17:X:70:PHE:HE1	1.80	0.46
2:B:107:MET:O	2:B:112:TYR:O	2.32	0.46
4:D:84:PHE:H	4:D:97:LEU:C	2.23	0.46
4:D:142:VAL:HG21	4:D:185:MET:HG2	1.98	0.46
4:D:320:ILE:HG12	9:I:36:TYR:HB2	1.97	0.46
5:E:83:ASP:O	5:E:87:ARG:HG2	2.14	0.46
5:E:109:MET:HE3	5:E:113:GLU:HG2	1.98	0.46
5:E:173:VAL:HG22	5:E:174:GLU:N	2.31	0.46
8:H:249:ILE:HG13	19:a:35:GLU:OE2	2.15	0.46
19:a:22:SER:O	19:a:23:THR:C	2.57	0.46
1:A:6:VAL:HG11	8:H:87:VAL:HG21	1.96	0.46
4:D:151:TYR:CZ	4:D:155:VAL:HG21	2.50	0.46
4:D:211:PHE:O	4:D:214:TYR:HB2	2.16	0.46
5:E:141:LEU:HD22	6:F:281:HIS:NE2	2.30	0.46
6:F:159:ARG:HB3	6:F:162:PHE:CE2	2.49	0.46
8:H:1:MET:HE3	19:a:29:PHE:CE1	2.50	0.46
8:H:291:LYS:HE2	8:H:291:LYS:HB2	1.80	0.46
10:P:44:GLY:HA2	11:Q:107:TRP:CE3	2.49	0.46
10:P:163:ARG:HH11	10:P:199:ILE:HD11	1.81	0.46
19:a:58:ASN:HB2	19:a:61:TYR:CE2	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:s:49:ASN:HA	23:s:52:LEU:HD12	1.97	0.46
1:A:60:ILE:O	1:A:64:LEU:HG	2.16	0.46
3:C:49:ARG:NH2	3:C:54:HIS:CD2	2.84	0.46
4:D:117:HIS:HD2	4:D:462:ASP:O	1.97	0.46
4:D:381:HIS:HE1	9:I:161:ALA:O	1.99	0.46
6:F:446:LEU:O	6:F:450:MET:HG2	2.15	0.46
8:H:30:TYR:HE1	19:a:1:MET:O	1.96	0.46
8:H:116:ILE:HG13	8:H:117:LEU:H	1.76	0.46
12:R:72:VAL:HG21	12:R:77:ILE:HG21	1.97	0.46
15:V:22:GLU:O	15:V:26:ILE:HG12	2.15	0.46
15:V:56:LEU:HD12	15:V:57:ASP:CA	2.44	0.46
17:X:80:GLU:O	17:X:81:PRO:C	2.56	0.46
22:r:12:ARG:HB3	22:r:20:LEU:CD2	2.44	0.46
1:A:52:SER:HB3	1:A:55:PHE:CD2	2.51	0.46
2:B:107:MET:HE1	2:B:201:LEU:HD23	1.96	0.46
3:C:62:GLU:O	3:C:63:TYR:C	2.58	0.46
4:D:216:ARG:HG3	4:D:240:LEU:HD13	1.97	0.46
4:D:432:LEU:O	4:D:433:ALA:C	2.58	0.46
5:E:47:ASN:H	5:E:50:THR:HG23	1.79	0.46
5:E:134:CYS:SG	5:E:175:CYS:HA	2.56	0.46
6:F:292:MET:HG2	6:F:293:SER:H	1.80	0.46
6:F:318:ILE:HB	6:F:355:ILE:HB	1.98	0.46
6:F:395:VAL:HG22	7:G:155:GLU:OE2	2.15	0.46
7:G:544:MET:HA	7:G:565:PHE:O	2.16	0.46
11:Q:166:TRP:CE3	23:s:67:PRO:HG2	2.51	0.46
12:R:39:ASP:CG	12:R:40:GLU:N	2.73	0.46
17:X:115:LEU:HD13	17:X:117:TRP:CZ2	2.51	0.46
30:q:201:CDL:OB7	30:q:201:CDL:HB62	2.16	0.46
1:A:22:PHE:HA	8:H:60:PRO:HG2	1.98	0.46
4:D:88:HIS:HB2	4:D:89:PRO:HD2	1.97	0.46
8:H:1:MET:O	8:H:2:PHE:C	2.58	0.46
9:I:48:VAL:O	20:b:10:LYS:NZ	2.49	0.46
10:P:227:PRO:HA	10:P:291:TYR:O	2.16	0.46
17:X:53:PRO:CD	17:X:54:ARG:H	2.24	0.46
19:a:49:GLU:CD	19:a:52:ARG:HH11	2.22	0.46
21:q:14:VAL:HA	21:q:23:LEU:HD22	1.98	0.46
1:A:75:LEU:O	1:A:79:ILE:HG12	2.16	0.46
2:B:164:CYS:SG	24:B:301:SF4:S4	3.14	0.46
6:F:358:ASP:C	6:F:360:SER:H	2.23	0.46
6:F:391:TRP:CZ3	7:G:118:GLU:HG2	2.51	0.46
10:P:95:ARG:HG2	10:P:105:PHE:CE2	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:328:MET:HB2	10:P:329:PRO:HD2	1.98	0.46
11:Q:77:VAL:HG21	11:Q:99:MET:HE3	1.97	0.46
17:X:20:VAL:CG2	17:X:24:VAL:HG21	2.40	0.46
21:q:71:LYS:HB2	21:q:73:THR:HG23	1.98	0.46
1:A:7:ILE:HA	1:A:10:ASN:ND2	2.31	0.46
4:D:198:THR:HG23	8:H:275:ALA:O	2.15	0.46
4:D:375:MET:HE2	4:D:375:MET:HB2	1.66	0.46
5:E:141:LEU:O	5:E:142:ARG:HB2	2.15	0.46
7:G:217:GLU:HG3	7:G:412:PRO:HB3	1.97	0.46
8:H:150:LEU:HD21	8:H:241:ILE:HD13	1.97	0.46
10:P:207:PHE:CZ	10:P:345:LEU:HA	2.51	0.46
13:S:19:ILE:HD12	13:S:94:VAL:CG1	2.44	0.46
13:S:42:VAL:HB	13:S:46:LYS:HE3	1.98	0.46
14:T:87:LEU:CD2	14:T:122:MET:HE1	2.46	0.46
18:Z:28:ARG:O	18:Z:28:ARG:CG	2.64	0.46
20:b:28:LEU:O	20:b:32:MET:HG2	2.15	0.46
21:q:86:TRP:HA	21:q:98:PRO:HG2	1.98	0.46
1:A:63:LEU:O	1:A:67:LEU:HG	2.15	0.46
2:B:154:GLU:O	10:P:89:TYR:OH	2.33	0.46
7:G:168:LEU:HD21	7:G:710:CYS:SG	2.56	0.46
7:G:251:ILE:HG13	7:G:604:GLN:HB3	1.98	0.46
7:G:260:ASN:N	7:G:281:ILE:HD11	2.30	0.46
7:G:406:ASN:ND2	7:G:436:VAL:CG2	2.76	0.46
8:H:248:TYR:CD1	8:H:254:LEU:HD23	2.51	0.46
8:H:316:PRO:HA	18:Z:58:ARG:HH11	1.80	0.46
10:P:206:ILE:HB	29:P:401:NDP:N7N	2.30	0.46
12:R:38:TYR:CD1	12:R:44:ARG:HB2	2.50	0.46
15:V:32:LEU:O	15:V:36:LYS:HG2	2.16	0.46
21:q:74:PHE:HD2	21:q:75:TRP:CD1	2.33	0.46
30:q:201:CDL:OB7	22:r:8:ILE:HD11	2.16	0.46
4:D:243:ASP:C	4:D:245:TYR:N	2.72	0.46
5:E:204:ILE:O	5:E:208:LYS:HG3	2.16	0.46
6:F:69:LEU:HD22	6:F:147:ARG:HB2	1.98	0.46
6:F:81:LYS:HE3	6:F:96:GLY:C	2.41	0.46
7:G:269:GLU:HG2	7:G:271:MET:HE3	1.98	0.46
7:G:545:LEU:O	7:G:566:ILE:HA	2.16	0.46
8:H:28:LEU:HD11	8:H:274:ARG:HH11	1.81	0.46
8:H:250:ASN:OD1	8:H:250:ASN:N	2.49	0.46
10:P:68:TYR:CZ	10:P:242:VAL:HG11	2.51	0.46
10:P:170:LEU:HD13	10:P:264:ALA:HB1	1.97	0.46
10:P:210:GLU:HG3	10:P:210:GLU:O	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:S:65:LEU:HD23	13:S:65:LEU:O	2.16	0.46
2:B:123:ALA:HB3	8:H:204:GLU:OE2	2.16	0.45
4:D:214:TYR:O	4:D:217:VAL:HG22	2.16	0.45
4:D:241:LEU:HD22	4:D:348:LEU:HD23	1.98	0.45
4:D:289:SER:HA	4:D:293:LEU:CD1	2.46	0.45
6:F:295:PRO:O	6:F:296:LEU:C	2.60	0.45
7:G:33:GLU:HB2	7:G:42:MET:HE3	1.99	0.45
7:G:83:GLU:HB2	7:G:101:ASN:HB3	1.98	0.45
7:G:401:LEU:HD11	7:G:466:LEU:HD21	1.98	0.45
7:G:592:LYS:HA	7:G:608:VAL:HG12	1.98	0.45
10:P:55:VAL:HA	10:P:79:GLN:O	2.17	0.45
10:P:169:HIS:ND1	29:P:401:NDP:H5N	2.32	0.45
14:T:117:GLU:HA	14:T:120:MET:CE	2.41	0.45
15:V:84:ALA:HA	15:V:87:GLU:CD	2.41	0.45
17:X:94:MET:O	17:X:95:GLN:C	2.59	0.45
17:X:134:ASP:O	17:X:135:ARG:C	2.58	0.45
5:E:45:GLU:CD	5:E:45:GLU:H	2.23	0.45
6:F:47:GLY:C	6:F:49:HIS:H	2.24	0.45
6:F:111:LYS:HG2	6:F:239:PRO:HB2	1.97	0.45
6:F:146:GLY:HA3	6:F:193:PHE:HE2	1.81	0.45
6:F:342:LEU:HD12	6:F:349:LEU:HA	1.97	0.45
7:G:373:PRO:CG	7:G:481:LEU:HD22	2.47	0.45
9:I:56:ASN:O	9:I:60:ILE:HG13	2.16	0.45
10:P:285:HIS:CE1	10:P:364:SER:HB3	2.51	0.45
14:T:103:HIS:HD1	14:T:140:CYS:HG	1.56	0.45
16:W:83:ASP:O	16:W:87:ILE:HG12	2.17	0.45
2:B:72:GLU:HA	2:B:72:GLU:OE2	2.16	0.45
3:C:102:HIS:CE1	15:V:44:TYR:HE1	2.35	0.45
4:D:124:ILE:HG21	4:D:422:CYS:SG	2.56	0.45
5:E:246:ALA:O	5:E:247:GLY:C	2.60	0.45
6:F:50:ASP:HB3	6:F:55:GLY:HA3	1.98	0.45
6:F:270:ASN:C	6:F:292:MET:HE3	2.40	0.45
7:G:36:VAL:O	7:G:39:GLN:HG2	2.16	0.45
28:H:401:3PE:H331	9:I:63:TRP:CZ2	2.51	0.45
9:I:80:GLU:N	19:a:1:MET:HE1	2.31	0.45
10:P:192:ARG:HH11	10:P:197:GLU:HA	1.81	0.45
10:P:208:GLY:N	10:P:211:ASP:OD2	2.49	0.45
15:V:8:THR:CG2	15:V:9:THR:N	2.79	0.45
15:V:56:LEU:HD13	15:V:60:LYS:HE2	1.98	0.45
21:q:6:VAL:HG13	30:q:201:CDL:CA2	2.47	0.45
23:s:48:LEU:O	23:s:52:LEU:HG	2.15	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:LEU:HB2	8:H:155:LEU:HD21	1.99	0.45
1:A:109:LYS:HG2	1:A:112:GLU:HB2	1.98	0.45
2:B:94:THR:HG21	4:D:89:PRO:N	2.31	0.45
4:D:238:LEU:HA	18:Z:9:ASP:HB2	1.97	0.45
4:D:251:PHE:O	4:D:252:SER:C	2.56	0.45
5:E:135:THR:OG1	5:E:172:GLU:OE2	2.31	0.45
5:E:184:MET:HG3	5:E:192:TYR:O	2.16	0.45
7:G:169:VAL:HG22	7:G:223:ILE:CD1	2.40	0.45
7:G:301:ARG:NE	7:G:613:PRO:HG3	2.30	0.45
7:G:347:ASP:HB2	7:G:594:ALA:HB1	1.99	0.45
7:G:447:ASP:O	7:G:447:ASP:CG	2.59	0.45
8:H:148:ILE:CG2	8:H:297:THR:HG22	2.45	0.45
8:H:239:THR:O	8:H:239:THR:CG2	2.63	0.45
10:P:157:LYS:O	10:P:160:GLY:N	2.49	0.45
10:P:264:ALA:O	10:P:266:THR:HG23	2.17	0.45
14:T:119:ILE:CD1	14:T:138:LEU:HD11	2.43	0.45
17:X:53:PRO:O	17:X:57:LEU:HG	2.16	0.45
1:A:55:PHE:CZ	8:H:282:TYR:CE2	2.85	0.45
1:A:109:LYS:HG2	1:A:109:LYS:O	2.17	0.45
4:D:342:ARG:O	4:D:346:GLN:HG3	2.17	0.45
5:E:137:THR:HA	5:E:140:MET:HE2	1.98	0.45
6:F:86:ARG:HB2	6:F:88:ARG:HH12	1.81	0.45
7:G:128:CYS:N	7:G:129:PRO:CD	2.80	0.45
7:G:259:SER:HA	7:G:281:ILE:HD13	1.99	0.45
7:G:652:ASN:OD1	7:G:653:LEU:HG	2.16	0.45
8:H:16:ALA:HB2	19:a:15:CYS:HB2	1.99	0.45
8:H:181:MET:O	8:H:185:TRP:N	2.49	0.45
9:I:89:GLU:HG3	21:q:61:TRP:HB3	1.97	0.45
21:q:10:GLY:HA2	30:q:201:CDL:CA5	2.45	0.45
4:D:134:PRO:O	4:D:138:ARG:NH1	2.48	0.45
4:D:300:TRP:CE3	4:D:305:THR:HG21	2.52	0.45
5:E:128:LYS:HB3	5:E:167:LEU:CA	2.46	0.45
5:E:173:VAL:HG11	5:E:176:LEU:HD11	1.99	0.45
5:E:180:VAL:CG2	6:F:286:CYS:HA	2.46	0.45
6:F:119:GLU:HG3	6:F:127:ASP:HB2	1.99	0.45
6:F:179:ALA:HB3	6:F:181:LEU:HG	1.98	0.45
6:F:234:GLY:HA3	6:F:240:THR:HB	1.98	0.45
7:G:127:ASP:HB2	7:G:130:ILE:HD12	1.98	0.45
8:H:4:ILE:HD12	8:H:4:ILE:N	2.30	0.45
8:H:27:ILE:O	8:H:31:MET:HG3	2.16	0.45
8:H:240:ILE:HD11	8:H:259:PHE:CD1	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Q:99:MET:HG2	11:Q:128:PHE:HE2	1.82	0.45
14:T:87:LEU:CD2	14:T:104:PHE:CE1	2.94	0.45
14:T:118:ILE:CG2	14:T:122:MET:HE3	2.47	0.45
15:V:56:LEU:HD11	15:V:57:ASP:OD1	2.17	0.45
1:A:62:PHE:O	1:A:63:LEU:C	2.60	0.45
2:B:107:MET:CE	2:B:201:LEU:HD23	2.46	0.45
2:B:131:MET:HE3	2:B:152:MET:HE2	1.96	0.45
3:C:243:ALA:C	7:G:105:ASN:ND2	2.75	0.45
4:D:198:THR:HA	8:H:32:GLN:HG2	1.98	0.45
6:F:154:ALA:HB2	6:F:193:PHE:HZ	1.82	0.45
7:G:381:LEU:HD23	13:S:55:ILE:HG13	1.98	0.45
7:G:454:ASP:OD1	7:G:459:ARG:NH2	2.50	0.45
8:H:10:LEU:O	8:H:11:VAL:C	2.59	0.45
13:S:37:ILE:HD12	13:S:55:ILE:HD12	1.98	0.45
2:B:138:THR:HG21	4:D:116:LEU:HA	1.97	0.45
3:C:207:VAL:N	3:C:223:VAL:HG23	2.32	0.45
4:D:154:ALA:HB2	4:D:398:THR:HG22	1.97	0.45
4:D:245:TYR:O	4:D:246:GLU:C	2.60	0.45
5:E:81:VAL:O	5:E:82:LEU:C	2.60	0.45
5:E:87:ARG:HD2	23:s:42:THR:HB	1.98	0.45
5:E:238:LYS:HE2	5:E:242:PHE:CZ	2.51	0.45
7:G:263:VAL:HG22	7:G:273:ILE:HG12	1.99	0.45
7:G:282:ASN:HB2	7:G:285:TRP:O	2.17	0.45
7:G:624:ARG:HA	7:G:634:LEU:HD12	1.99	0.45
8:H:2:PHE:O	8:H:6:ILE:HG13	2.17	0.45
8:H:200:LEU:HD22	8:H:282:TYR:HD1	1.82	0.45
8:H:293:PHE:CE1	28:H:401:3PE:H32	2.51	0.45
9:I:76:TYR:O	9:I:77:LEU:C	2.59	0.45
10:P:55:VAL:HA	10:P:79:GLN:HB3	1.99	0.45
10:P:172:ALA:N	10:P:202:ARG:HH21	2.13	0.45
14:T:83:VAL:HG21	14:T:145:VAL:HG22	1.99	0.45
17:X:122:LEU:HD21	20:b:81:LEU:HD23	1.98	0.45
18:Z:66:GLU:HA	18:Z:69:ILE:CG1	2.47	0.45
3:C:204:THR:CB	3:C:225:LEU:HD11	2.47	0.45
4:D:294:ARG:HD2	4:D:318:VAL:CG1	2.47	0.45
4:D:446:ASP:O	4:D:450:ILE:HG13	2.16	0.45
5:E:40:HIS:HB2	7:G:209:TYR:CE2	2.52	0.45
5:E:180:VAL:HG11	5:E:224:CYS:CB	2.47	0.45
6:F:117:ALA:HB3	6:F:158:ILE:HG22	1.98	0.45
6:F:383:THR:CG2	7:G:120:LEU:HD23	2.47	0.45
7:G:296:GLY:HA2	7:G:703:ALA:O	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:308:ARG:HH11	7:G:580:ALA:H	1.64	0.45
7:G:462:PHE:CD2	7:G:466:LEU:HG	2.52	0.45
7:G:509:GLU:HG2	7:G:510:TRP:N	2.32	0.45
8:H:305:ILE:O	8:H:308:PRO:HD2	2.17	0.45
10:P:334:GLY:O	10:P:337:ASP:HB3	2.16	0.45
14:T:133:ILE:HG23	14:T:134:ASP:N	2.32	0.45
16:W:42:TRP:O	16:W:46:VAL:HG23	2.17	0.45
19:a:2:TRP:HZ2	30:q:201:CDL:OB7	2.00	0.45
2:B:192:PRO:HD3	9:I:176:SER:HA	1.98	0.45
5:E:54:PHE:HE2	5:E:103:VAL:HG21	1.82	0.45
5:E:55:THR:O	5:E:58:ASN:N	2.50	0.45
5:E:94:ILE:O	5:E:98:ASN:ND2	2.50	0.45
6:F:168:ASN:HD21	23:s:40:TYR:HE2	1.64	0.45
6:F:251:SER:N	6:F:252:PRO:HD2	2.32	0.45
7:G:306:MET:HA	7:G:316:TYR:HA	1.99	0.45
7:G:404:GLY:HA2	7:G:684:LEU:HD13	1.83	0.45
8:H:91:MET:HB3	8:H:92:PRO:HD2	1.99	0.45
8:H:146:MET:HE1	8:H:192:GLU:CB	2.47	0.45
11:Q:77:VAL:CG1	11:Q:101:PHE:CD2	3.00	0.45
13:S:62:GLN:HB2	13:S:80:ASN:CG	2.42	0.45
14:T:82:ARG:NH2	14:T:126:PHE:HD1	2.15	0.45
14:T:90:TYR:O	14:T:91:ASP:HB2	2.17	0.45
14:T:130:ILE:CG2	14:T:131:PRO:CD	2.95	0.45
3:C:149:LEU:CD1	16:W:80:ARG:HH21	2.23	0.44
4:D:174:PHE:HZ	4:D:240:LEU:HD21	1.82	0.44
4:D:258:VAL:O	4:D:261:MET:HB2	2.17	0.44
4:D:361:ALA:O	4:D:384:LEU:HD11	2.18	0.44
5:E:179:CYS:SG	6:F:123:GLY:HA2	2.57	0.44
6:F:42:PHE:CD1	6:F:130:ILE:HD12	2.53	0.44
6:F:116:ASN:HB3	6:F:212:LEU:HD22	1.99	0.44
6:F:274:LYS:HZ2	6:F:352:ALA:HB3	1.82	0.44
6:F:296:LEU:HD13	6:F:337:MET:HE3	1.98	0.44
6:F:409:ILE:CG1	6:F:446:LEU:HD23	2.47	0.44
7:G:185:PHE:CE2	7:G:285:TRP:NE1	2.85	0.44
7:G:473:MET:HE3	7:G:514:ASN:HD21	1.83	0.44
8:H:223:PHE:O	8:H:226:ALA:N	2.50	0.44
10:P:182:ARG:O	10:P:186:VAL:HG23	2.17	0.44
10:P:298:TYR:C	10:P:300:TRP:N	2.71	0.44
10:P:315:THR:CG2	10:P:316:LYS:N	2.80	0.44
17:X:9:THR:O	17:X:12:GLU:HB3	2.17	0.44
17:X:115:LEU:HB3	17:X:117:TRP:CE2	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Z:53:TRP:CE2	18:Z:57:ARG:HD2	2.52	0.44
4:D:82:LEU:HD22	8:H:126:LYS:HD2	1.99	0.44
4:D:128:THR:HG22	4:D:131:GLN:HG2	1.99	0.44
7:G:259:SER:HA	7:G:281:ILE:HD12	1.98	0.44
11:Q:65:THR:HG23	11:Q:67:VAL:HG23	1.99	0.44
13:S:48:HIS:HE1	13:S:95:LEU:CD2	2.25	0.44
16:W:45:GLU:O	16:W:46:VAL:C	2.58	0.44
17:X:120:PRO:HB3	17:X:125:LEU:HD11	1.94	0.44
1:A:21:ALA:CB	8:H:218:GLY:HA3	2.47	0.44
5:E:104:LEU:O	5:E:106:VAL:HG13	2.17	0.44
5:E:128:LYS:HD3	5:E:167:LEU:HG	2.00	0.44
6:F:158:ILE:HD13	6:F:166:ALA:HB2	1.98	0.44
7:G:114:GLU:HG3	7:G:148:SER:HB3	2.00	0.44
7:G:127:ASP:C	7:G:127:ASP:OD1	2.59	0.44
8:H:288:LEU:O	8:H:293:PHE:N	2.50	0.44
10:P:55:VAL:HG11	10:P:122:HIS:O	2.18	0.44
10:P:178:SER:O	10:P:182:ARG:HG3	2.17	0.44
11:Q:85:ASN:N	11:Q:85:ASN:OD1	2.48	0.44
20:b:38:TYR:O	20:b:39:THR:C	2.58	0.44
1:A:106:TRP:N	1:A:106:TRP:CD1	2.85	0.44
4:D:256:ASP:OD1	4:D:338:ARG:NH2	2.42	0.44
5:E:49:ASP:O	5:E:50:THR:C	2.60	0.44
5:E:55:THR:N	5:E:58:ASN:HB2	2.32	0.44
6:F:110:PRO:CB	6:F:152:ARG:HH22	2.30	0.44
7:G:69:LEU:HD23	7:G:69:LEU:HA	1.83	0.44
7:G:169:VAL:HG11	7:G:231:LEU:HD13	1.99	0.44
7:G:319:TRP:CZ3	7:G:584:LEU:HD22	2.52	0.44
7:G:346:VAL:O	7:G:521:SER:HB3	2.17	0.44
7:G:671:LEU:HA	7:G:674:LEU:HD12	1.99	0.44
10:P:165:ILE:HG12	10:P:199:ILE:HB	1.99	0.44
10:P:323:HIS:O	10:P:323:HIS:CG	2.71	0.44
10:P:345:LEU:C	10:P:345:LEU:HD23	2.43	0.44
11:Q:91:VAL:HG22	11:Q:91:VAL:O	2.18	0.44
12:R:47:ARG:HG3	12:R:48:PHE:N	2.32	0.44
12:R:97:LYS:CE	12:R:100:LYS:HD3	2.45	0.44
2:B:163:SER:HB2	9:I:150:THR:O	2.18	0.44
4:D:90:ALA:HB2	8:H:205:SER:CA	2.45	0.44
4:D:217:VAL:HG23	4:D:218:SER:N	2.31	0.44
4:D:252:SER:O	4:D:253:LEU:C	2.59	0.44
4:D:330:TYR:O	4:D:331:LEU:C	2.60	0.44
7:G:278:HIS:CG	7:G:281:ILE:HG13	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:355:LYS:HG3	7:G:366:LEU:HD12	2.00	0.44
8:H:39:ILE:HG13	21:q:31:ASN:ND2	2.33	0.44
8:H:42:PRO:HB3	21:q:27:PHE:HE2	1.76	0.44
8:H:174:LEU:O	8:H:177:PRO:O	2.35	0.44
12:R:32:THR:HG21	21:q:129:THR:HG23	2.00	0.44
12:R:39:ASP:H	12:R:42:ASP:CG	2.21	0.44
13:S:74:GLU:OE1	13:S:74:GLU:N	2.50	0.44
17:X:55:ARG:O	17:X:135:ARG:NH1	2.48	0.44
17:X:139:GLU:CD	17:X:139:GLU:H	2.26	0.44
1:A:24:LEU:HD23	1:A:24:LEU:C	2.43	0.44
1:A:75:LEU:CB	8:H:155:LEU:HD21	2.48	0.44
4:D:284:LEU:HD21	4:D:298:ILE:HG21	1.99	0.44
5:E:54:PHE:CE2	5:E:103:VAL:HG21	2.53	0.44
5:E:78:VAL:HA	5:E:104:LEU:CD1	2.44	0.44
6:F:41:ILE:O	6:F:137:LYS:NZ	2.47	0.44
6:F:346:GLN:NE2	6:F:440:ARG:HD3	2.30	0.44
7:G:131:CYS:HA	7:G:175:ARG:HH12	1.83	0.44
7:G:401:LEU:HD11	7:G:466:LEU:CD2	2.47	0.44
7:G:666:GLN:HE22	13:S:38:VAL:HG13	1.83	0.44
8:H:11:VAL:O	8:H:14:LEU:N	2.51	0.44
8:H:54:LYS:CG	8:H:55:LEU:N	2.78	0.44
8:H:289:LEU:O	8:H:294:LEU:HB2	2.18	0.44
9:I:59:ARG:HA	9:I:64:THR:HG23	1.99	0.44
10:P:298:TYR:O	10:P:299:SER:C	2.60	0.44
11:Q:62:THR:HG22	11:Q:141:ASN:O	2.18	0.44
18:Z:66:GLU:HG3	20:b:50:PRO:HG3	1.98	0.44
19:a:2:TRP:NE1	30:q:201:CDL:OB4	2.51	0.44
22:r:109:ASP:O	22:r:110:GLN:CG	2.64	0.44
2:B:114:MET:SD	2:B:119:VAL:CG1	3.06	0.44
3:C:85:ILE:HD12	3:C:140:ILE:CD1	2.48	0.44
4:D:141:TYR:CB	4:D:223:HIS:CE1	3.01	0.44
6:F:431:ALA:O	6:F:434:PRO:HD2	2.18	0.44
7:G:68:ARG:CB	7:G:285:TRP:HH2	2.31	0.44
7:G:259:SER:HB2	7:G:282:ASN:HB3	1.99	0.44
7:G:607:LYS:HG2	11:Q:78:ARG:HH11	1.82	0.44
10:P:72:HIS:HB2	10:P:250:VAL:HG21	2.00	0.44
10:P:96:LEU:C	10:P:96:LEU:HD12	2.43	0.44
11:Q:77:VAL:HG21	11:Q:99:MET:CE	2.48	0.44
13:S:20:ARG:HG3	13:S:54:LEU:CB	2.43	0.44
14:T:79:ILE:O	14:T:83:VAL:HG23	2.17	0.44
14:T:113:LEU:O	14:T:116:VAL:HB	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:W:86:VAL:O	16:W:90:LYS:HG3	2.18	0.44
18:Z:98:MET:HB2	18:Z:104:TRP:CE2	2.52	0.44
18:Z:129:THR:HG22	18:Z:131:GLU:N	2.33	0.44
1:A:6:VAL:HG11	8:H:87:VAL:CG2	2.48	0.44
2:B:98:ALA:N	2:B:135:GLY:HA3	2.33	0.44
3:C:155:ILE:O	3:C:156:VAL:C	2.61	0.44
4:D:83:ASN:N	4:D:83:ASN:OD1	2.50	0.44
4:D:243:ASP:C	4:D:245:TYR:H	2.24	0.44
4:D:244:ILE:HG22	4:D:244:ILE:O	2.18	0.44
5:E:176:LEU:HB2	5:E:184:MET:HE1	2.00	0.44
6:F:147:ARG:HD2	6:F:191:TYR:CD1	2.53	0.44
6:F:168:ASN:ND2	23:s:40:TYR:CE2	2.85	0.44
7:G:281:ILE:HD12	7:G:282:ASN:H	1.83	0.44
7:G:281:ILE:HG23	7:G:602:ARG:NH1	2.32	0.44
8:H:135:ALA:HB2	8:H:201:THR:HG22	1.98	0.44
10:P:156:SER:HB2	10:P:161:VAL:CG2	2.46	0.44
18:Z:68:ARG:O	18:Z:69:ILE:C	2.60	0.44
22:r:109:ASP:OD1	22:r:110:GLN:N	2.51	0.44
4:D:88:HIS:C	4:D:90:ALA:N	2.74	0.44
4:D:133:LEU:HB3	4:D:134:PRO:HD3	2.00	0.44
4:D:201:PHE:CB	8:H:32:GLN:HB3	2.48	0.44
4:D:201:PHE:HB2	8:H:32:GLN:HB3	2.00	0.44
4:D:202:TRP:HZ2	9:I:73:THR:HG22	1.82	0.44
4:D:299:GLN:HB3	22:r:104:TRP:CE3	2.53	0.44
6:F:109:ARG:NE	6:F:239:PRO:HD3	2.33	0.44
6:F:120:GLY:O	6:F:121:GLU:C	2.61	0.44
6:F:412:LEU:CD2	6:F:435:VAL:HG13	2.48	0.44
7:G:303:THR:HB	7:G:614:GLY:HA3	1.98	0.44
7:G:338:VAL:HA	7:G:544:MET:O	2.17	0.44
8:H:89:LEU:HG	8:H:90:PRO:HD2	2.00	0.44
10:P:169:HIS:H	10:P:184:LYS:CE	2.30	0.44
13:S:30:SER:O	13:S:33:VAL:N	2.51	0.44
16:W:20:VAL:HG21	16:W:80:ARG:CZ	2.48	0.44
3:C:55:LYS:HE2	3:C:55:LYS:HB3	1.83	0.43
3:C:114:THR:HG22	3:C:115:ALA:N	2.33	0.43
3:C:124:ARG:HD2	11:Q:140:LYS:HZ1	1.83	0.43
4:D:106:VAL:N	4:D:442:HIS:O	2.41	0.43
5:E:233:LEU:CD2	6:F:40:ARG:HD3	2.48	0.43
6:F:226:LYS:O	6:F:227:PRO:C	2.60	0.43
6:F:375:LYS:HD3	6:F:390:ASP:OD1	2.17	0.43
7:G:651:PRO:HB3	13:S:57:GLU:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:S:83:SER:O	13:S:87:VAL:HG23	2.17	0.43
16:W:87:ILE:O	16:W:91:MET:HG3	2.18	0.43
19:a:37:ARG:HB2	19:a:48:MET:HE2	1.99	0.43
2:B:131:MET:HE1	2:B:149:TYR:HB2	2.00	0.43
4:D:378:LEU:HD23	7:G:126:LEU:HB2	2.00	0.43
6:F:98:LYS:HA	6:F:101:PHE:CE2	2.53	0.43
6:F:268:GLU:CG	6:F:269:ARG:H	2.30	0.43
7:G:283:GLU:OE1	7:G:283:GLU:N	2.48	0.43
10:P:321:ARG:CZ	10:P:321:ARG:HB2	2.48	0.43
11:Q:51:GLN:HB3	16:W:26:ARG:HH22	1.82	0.43
11:Q:101:PHE:CE1	11:Q:124:MET:HE3	2.53	0.43
13:S:51:LEU:CD1	13:S:95:LEU:HD12	2.46	0.43
14:T:109:GLY:O	14:T:110:LEU:C	2.61	0.43
15:V:56:LEU:C	15:V:56:LEU:CD1	2.85	0.43
1:A:105:GLU:HG2	1:A:111:LEU:HB3	1.99	0.43
1:A:105:GLU:O	1:A:110:GLY:N	2.52	0.43
2:B:95:PHE:CE2	2:B:97:LEU:HD21	2.53	0.43
4:D:86:PRO:HG3	4:D:95:LEU:N	2.32	0.43
4:D:232:VAL:CG2	4:D:356:ILE:HB	2.48	0.43
5:E:60:LYS:O	5:E:61:ARG:C	2.62	0.43
5:E:87:ARG:NH2	6:F:163:TYR:CD1	2.87	0.43
5:E:235:GLU:HB2	6:F:37:ASP:HB2	2.00	0.43
6:F:62:TRP:CH2	6:F:140:GLU:HA	2.53	0.43
7:G:185:PHE:HE2	7:G:285:TRP:CD1	2.36	0.43
7:G:388:ASN:O	7:G:511:LYS:HE2	2.19	0.43
8:H:116:ILE:HD12	8:H:135:ALA:HB3	2.00	0.43
8:H:200:LEU:HD21	8:H:285:LEU:HD13	1.99	0.43
10:P:163:ARG:NE	10:P:253:THR:HA	2.33	0.43
10:P:246:SER:O	10:P:249:ILE:N	2.51	0.43
10:P:269:ASN:ND2	10:P:271:TYR:OH	2.51	0.43
11:Q:99:MET:O	11:Q:99:MET:HG3	2.18	0.43
15:V:19:THR:N	15:V:20:PRO:CD	2.81	0.43
1:A:49:LEU:HD12	1:A:50:PRO:CD	2.47	0.43
1:A:81:THR:O	20:b:46:ASN:ND2	2.51	0.43
4:D:151:TYR:O	4:D:152:SER:C	2.59	0.43
5:E:196:THR:O	5:E:197:PRO:C	2.61	0.43
6:F:88:ARG:HH21	6:F:262:PHE:HZ	1.66	0.43
6:F:209:GLU:CD	6:F:230:PRO:HG2	2.42	0.43
6:F:226:LYS:N	6:F:227:PRO:CD	2.82	0.43
6:F:320:GLY:HA3	6:F:324:THR:HG21	1.99	0.43
6:F:409:ILE:CG1	6:F:446:LEU:CD2	2.94	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:279:GLU:HG3	11:Q:154:LYS:HG3	2.00	0.43
7:G:283:GLU:CG	7:G:285:TRP:HZ3	2.26	0.43
7:G:301:ARG:HE	7:G:613:PRO:CG	2.26	0.43
8:H:212:ASN:O	8:H:213:VAL:C	2.60	0.43
8:H:277:TYR:OH	9:I:66:LEU:HB3	2.17	0.43
9:I:76:TYR:HA	9:I:79:ARG:HD2	2.01	0.43
9:I:191:LEU:HD23	9:I:191:LEU:HA	1.91	0.43
11:Q:59:LEU:HD23	11:Q:59:LEU:HA	1.84	0.43
13:S:24:CYS:SG	13:S:61:VAL:HG12	2.58	0.43
22:r:5:THR:HG22	22:r:5:THR:O	2.18	0.43
1:A:78:ALA:HA	1:A:81:THR:HG23	2.01	0.43
2:B:71:ALA:O	2:B:75:VAL:N	2.47	0.43
2:B:126:ARG:HG3	8:H:213:VAL:O	2.18	0.43
5:E:180:VAL:HG22	5:E:221:ARG:NH1	2.33	0.43
7:G:381:LEU:HD23	13:S:55:ILE:CG1	2.49	0.43
7:G:432:ILE:HG12	7:G:451:ILE:HD11	1.99	0.43
8:H:140:ILE:HG13	8:H:141:SER:N	2.32	0.43
10:P:283:MET:HE3	10:P:357:ARG:HH11	1.83	0.43
13:S:16:LEU:CB	13:S:69:TYR:CD1	2.97	0.43
17:X:23:ALA:HB2	17:X:95:GLN:HE22	1.82	0.43
4:D:83:ASN:HA	4:D:98:VAL:CA	2.24	0.43
5:E:126:VAL:HG21	5:E:130:HIS:CG	2.53	0.43
5:E:157:ILE:HG13	5:E:161:GLU:HB3	2.01	0.43
7:G:306:MET:HG2	7:G:316:TYR:CA	2.46	0.43
7:G:358:LEU:HD12	7:G:366:LEU:HD21	1.99	0.43
7:G:467:LYS:HA	7:G:467:LYS:HD3	1.83	0.43
9:I:67:ILE:CG2	25:I:301:PC1:H381	2.38	0.43
13:S:23:LEU:HB3	13:S:33:VAL:HG12	2.01	0.43
14:T:133:ILE:O	14:T:136:GLU:N	2.46	0.43
2:B:70:ARG:HG3	2:B:70:ARG:O	2.18	0.43
2:B:111:ARG:CZ	4:D:208:GLU:HG2	2.49	0.43
3:C:93:ILE:HD11	3:C:153:ASP:HB3	1.99	0.43
4:D:156:GLU:OE1	4:D:163:PRO:HD3	2.19	0.43
4:D:184:ILE:HD12	4:D:210:MET:HE1	1.99	0.43
4:D:197:MET:HG3	8:H:32:GLN:NE2	2.34	0.43
5:E:63:GLU:O	5:E:64:ALA:C	2.61	0.43
5:E:238:LYS:HE2	5:E:242:PHE:CE1	2.54	0.43
6:F:50:ASP:OD2	6:F:52:ARG:HB2	2.17	0.43
6:F:272:GLY:O	6:F:292:MET:HB2	2.19	0.43
6:F:283:ASN:ND2	6:F:306:GLY:H	2.16	0.43
6:F:338:ASP:OD1	6:F:338:ASP:C	2.61	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:185:PHE:HE2	7:G:285:TRP:NE1	2.16	0.43
7:G:336:ASN:HB3	7:G:540:ASN:ND2	2.33	0.43
7:G:597:VAL:HG12	7:G:603:ALA:CB	2.48	0.43
10:P:126:VAL:HG23	10:P:161:VAL:HG11	1.99	0.43
10:P:203:PRO:HG2	29:P:401:NDP:C5N	2.48	0.43
10:P:362:LEU:HD23	10:P:362:LEU:HA	1.88	0.43
11:Q:59:LEU:O	11:Q:140:LYS:HA	2.18	0.43
14:T:92:LYS:O	14:T:92:LYS:HG2	2.16	0.43
20:b:31:ILE:HG23	20:b:32:MET:N	2.34	0.43
20:b:32:MET:N	20:b:33:PRO:CD	2.82	0.43
1:A:23:TRP:O	1:A:26:GLN:HG3	2.19	0.43
2:B:147:LYS:HE3	2:B:151:GLN:NE2	2.26	0.43
3:C:128:VAL:HG13	3:C:141:ARG:CG	2.49	0.43
3:C:240:ALA:O	3:C:241:PHE:C	2.62	0.43
4:D:326:CYS:CB	4:D:453:THR:HG21	2.49	0.43
5:E:147:ILE:CG2	5:E:200:ILE:HG12	2.37	0.43
6:F:410:ASP:OD1	6:F:410:ASP:C	2.62	0.43
8:H:154:LEU:CD2	8:H:160:TYR:HA	2.49	0.43
8:H:200:LEU:CD2	8:H:282:TYR:HA	2.49	0.43
8:H:220:PHE:O	8:H:224:PHE:HB2	2.19	0.43
8:H:253:GLU:O	8:H:254:LEU:C	2.62	0.43
9:I:101:HIS:CE1	9:I:169:GLU:CD	2.97	0.43
10:P:211:ASP:CG	10:P:214:LEU:HB3	2.43	0.43
10:P:216:HIS:CD2	10:P:318:LYS:HE3	2.54	0.43
11:Q:111:LEU:HD11	21:q:126:PRO:HG2	2.01	0.43
12:R:72:VAL:HG11	12:R:77:ILE:HG22	2.01	0.43
13:S:75:LYS:HE2	13:S:75:LYS:HA	2.01	0.43
15:V:56:LEU:CD1	15:V:57:ASP:OD1	2.67	0.43
17:X:10:LEU:H	17:X:10:LEU:HD12	1.84	0.43
18:Z:10:MET:HB3	18:Z:10:MET:HE2	1.71	0.43
20:b:15:LYS:O	20:b:15:LYS:HG3	2.18	0.43
5:E:62:ILE:HD12	5:E:81:VAL:HG13	2.00	0.43
6:F:64:LYS:O	6:F:68:ILE:HG13	2.19	0.43
6:F:278:ILE:CG2	6:F:282:VAL:HG21	2.46	0.43
7:G:126:LEU:HD13	12:R:89:PRO:HB3	2.01	0.43
7:G:281:ILE:HD12	7:G:282:ASN:N	2.33	0.43
10:P:170:LEU:O	10:P:171:ASN:C	2.62	0.43
10:P:212:ARG:O	10:P:213:PHE:C	2.61	0.43
12:R:45:ARG:HA	12:R:48:PHE:HE1	1.83	0.43
14:T:87:LEU:HD11	14:T:141:PRO:HB3	2.01	0.43
16:W:61:GLN:O	16:W:64:ASP:HB2	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:W:120:ASP:HB3	16:W:123:SER:OG	2.19	0.43
17:X:20:VAL:O	19:a:54:ILE:CD1	2.67	0.43
17:X:46:CYS:SG	17:X:135:ARG:NH1	2.91	0.43
19:a:55:SER:O	19:a:56:GLY:C	2.61	0.43
4:D:86:PRO:HG3	4:D:95:LEU:H	1.84	0.43
4:D:141:TYR:O	4:D:222:MET:HE3	2.18	0.43
4:D:264:ASN:O	4:D:265:ASN:C	2.57	0.43
4:D:318:VAL:HG21	22:r:104:TRP:CZ3	2.54	0.43
5:E:109:MET:O	5:E:110:ARG:C	2.62	0.43
5:E:183:PRO:HB2	5:E:195:LEU:N	2.34	0.43
5:E:230:LEU:HD13	5:E:232:SER:O	2.19	0.43
7:G:102:ILE:HD12	7:G:102:ILE:N	2.34	0.43
10:P:198:ALA:O	10:P:199:ILE:C	2.61	0.43
10:P:280:ILE:HG23	10:P:353:LEU:HD22	2.00	0.43
17:X:26:LYS:HD3	17:X:95:GLN:OE1	2.19	0.43
18:Z:102:PRO:O	18:Z:103:ASN:C	2.62	0.43
19:a:17:VAL:O	19:a:18:ILE:C	2.62	0.43
1:A:81:THR:O	1:A:82:ILE:C	2.62	0.42
3:C:213:ASP:O	3:C:214:GLU:C	2.61	0.42
4:D:194:ILE:HG23	4:D:271:ARG:NE	2.29	0.42
4:D:320:ILE:HG22	4:D:321:GLY:N	2.33	0.42
5:E:88:GLN:HG3	5:E:89:ASN:CG	2.44	0.42
6:F:113:LEU:HB3	6:F:154:ALA:CB	2.49	0.42
6:F:153:ALA:HB1	6:F:194:ASP:O	2.19	0.42
6:F:281:HIS:HB3	6:F:358:ASP:OD1	2.19	0.42
7:G:651:PRO:O	7:G:652:ASN:C	2.62	0.42
8:H:8:THR:O	8:H:9:LEU:CB	2.67	0.42
8:H:24:GLU:CA	8:H:271:LEU:CD2	2.88	0.42
8:H:77:LEU:O	8:H:81:LEU:HG	2.19	0.42
8:H:140:ILE:O	8:H:143:GLU:HB3	2.19	0.42
8:H:196:ALA:C	8:H:198:PHE:N	2.77	0.42
8:H:293:PHE:O	8:H:296:LEU:N	2.52	0.42
10:P:223:PHE:O	10:P:224:LEU:C	2.62	0.42
10:P:310:PHE:O	10:P:311:GLU:C	2.60	0.42
12:R:72:VAL:HG11	12:R:77:ILE:CG2	2.49	0.42
15:V:36:LYS:HA	15:V:36:LYS:HD3	1.89	0.42
16:W:120:ASP:OD1	16:W:120:ASP:C	2.61	0.42
1:A:7:ILE:O	1:A:10:ASN:HB2	2.19	0.42
1:A:13:LEU:HD12	1:A:13:LEU:HA	1.84	0.42
5:E:185:VAL:HG23	5:E:185:VAL:O	2.19	0.42
8:H:1:MET:O	8:H:4:ILE:N	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:17:MET:HE1	8:H:225:MET:HE3	2.00	0.42
8:H:110:SER:O	8:H:113:VAL:HG12	2.19	0.42
9:I:76:TYR:CD1	9:I:79:ARG:HD2	2.55	0.42
10:P:134:TRP:CD1	10:P:134:TRP:O	2.72	0.42
12:R:44:ARG:C	12:R:46:VAL:N	2.73	0.42
19:a:4:GLU:C	19:a:7:PRO:HD2	2.44	0.42
19:a:28:LYS:HE3	19:a:35:GLU:HG2	2.01	0.42
1:A:68:GLU:O	1:A:71:LEU:N	2.50	0.42
2:B:81:LEU:HD23	25:B:302:PC1:H251	2.00	0.42
2:B:154:GLU:CB	8:H:59:GLU:HB2	2.49	0.42
2:B:170:TYR:HE2	4:D:134:PRO:HB2	1.83	0.42
4:D:133:LEU:CD2	4:D:228:ARG:HG2	2.49	0.42
5:E:47:ASN:CG	5:E:49:ASP:HB3	2.45	0.42
6:F:383:THR:CG2	7:G:120:LEU:CD2	2.94	0.42
7:G:292:PHE:HB3	7:G:706:THR:HG21	2.01	0.42
7:G:302:LEU:HB3	7:G:585:PRO:HB3	2.01	0.42
8:H:182:ALA:O	8:H:183:MET:C	2.60	0.42
8:H:294:LEU:HB3	8:H:295:PRO:HD3	2.01	0.42
9:I:104:ARG:HD2	9:I:201:ILE:HG21	2.01	0.42
10:P:235:THR:O	10:P:273:LEU:N	2.52	0.42
10:P:238:GLN:HA	10:P:239:PRO:HD3	1.84	0.42
10:P:313:TRP:CE3	10:P:314:THR:HB	2.54	0.42
16:W:101:LYS:HB3	16:W:101:LYS:NZ	2.34	0.42
20:b:41:TYR:CD1	20:b:80:TRP:CZ3	3.07	0.42
2:B:124:SER:HB2	2:B:127:GLN:OE1	2.20	0.42
4:D:162:GLN:HB2	4:D:163:PRO:HD2	2.01	0.42
5:E:104:LEU:O	5:E:105:GLN:C	2.62	0.42
6:F:128:ARG:HD2	6:F:162:PHE:CE1	2.54	0.42
6:F:314:LEU:HD11	6:F:317:VAL:HG23	2.01	0.42
7:G:68:ARG:CD	7:G:285:TRP:CH2	3.02	0.42
7:G:329:MET:HG3	7:G:565:PHE:CZ	2.54	0.42
7:G:347:ASP:O	7:G:351:LEU:HG	2.18	0.42
7:G:414:PHE:CE2	7:G:516:LEU:CD2	3.03	0.42
7:G:567:VAL:HG23	7:G:567:VAL:O	2.20	0.42
10:P:241:TYR:HD2	10:P:243:ALA:HB3	1.84	0.42
10:P:247:LYS:NZ	10:P:340:VAL:HG23	2.35	0.42
13:S:64:LYS:HE2	13:S:66:TRP:CZ2	2.55	0.42
15:V:8:THR:HG22	15:V:9:THR:N	2.34	0.42
15:V:32:LEU:HD23	15:V:32:LEU:HA	1.91	0.42
15:V:37:HIS:O	15:V:38:PHE:C	2.63	0.42
5:E:62:ILE:HG21	5:E:103:VAL:HG11	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:81:VAL:HB	5:E:104:LEU:HD11	2.00	0.42
5:E:131:ILE:HD11	5:E:168:PHE:CD2	2.49	0.42
7:G:355:LYS:HG2	7:G:359:ASN:ND2	2.33	0.42
7:G:527:ASP:OD2	7:G:650:SER:CB	2.67	0.42
8:H:286:MET:HE2	8:H:286:MET:HB3	1.87	0.42
9:I:50:MET:O	9:I:54:THR:HG23	2.20	0.42
10:P:207:PHE:HB3	10:P:213:PHE:HD2	1.85	0.42
14:T:93:ILE:HD11	14:T:118:ILE:HD11	2.00	0.42
18:Z:74:LEU:O	18:Z:78:GLU:HG3	2.20	0.42
20:b:42:ALA:HA	20:b:45:ILE:HG22	2.01	0.42
22:r:18:GLN:OE1	22:r:18:GLN:N	2.52	0.42
1:A:94:LEU:O	1:A:97:ILE:HG12	2.19	0.42
2:B:194:CYS:O	2:B:196:PRO:HD3	2.20	0.42
2:B:202:LEU:HD13	2:B:202:LEU:O	2.19	0.42
3:C:236:SER:OG	7:G:145:MET:HE1	2.19	0.42
3:C:241:PHE:O	3:C:242:PRO:C	2.62	0.42
4:D:104:GLU:CG	8:H:130:PHE:HZ	2.32	0.42
5:E:84:LEU:HD12	23:s:46:LEU:CD1	2.49	0.42
6:F:364:VAL:HA	6:F:438:LEU:HD11	2.01	0.42
7:G:83:GLU:C	7:G:84:LYS:HG2	2.44	0.42
7:G:592:LYS:N	7:G:608:VAL:HG12	2.34	0.42
7:G:639:LEU:HD23	7:G:643:ARG:HG2	2.01	0.42
8:H:193:THR:O	8:H:194:ASN:C	2.61	0.42
13:S:19:ILE:O	13:S:53:ILE:HD12	2.20	0.42
15:V:35:LEU:HA	15:V:38:PHE:CE1	2.55	0.42
16:W:86:VAL:O	16:W:87:ILE:C	2.62	0.42
18:Z:44:ILE:HD13	18:Z:44:ILE:HA	1.85	0.42
2:B:77:LYS:HA	2:B:77:LYS:HD3	1.64	0.42
2:B:194:CYS:O	24:B:301:SF4:S2	2.78	0.42
4:D:379:ILE:HG23	7:G:140:GLN:HB2	2.01	0.42
5:E:203:ILE:HA	5:E:206:GLU:OE1	2.20	0.42
7:G:362:ASP:CB	13:S:71:PHE:CE1	2.92	0.42
7:G:643:ARG:HA	7:G:646:LEU:HD12	2.02	0.42
7:G:662:THR:HB	13:S:25:GLN:HE21	1.83	0.42
9:I:122:ILE:HG13	9:I:122:ILE:O	2.19	0.42
10:P:354:ARG:HG3	10:P:362:LEU:CD2	2.48	0.42
14:T:80:LYS:O	14:T:84:LEU:HG	2.20	0.42
14:T:90:TYR:CD2	14:T:92:LYS:HB3	2.54	0.42
17:X:120:PRO:CB	17:X:125:LEU:CD1	2.91	0.42
21:q:5:GLU:HG2	21:q:9:ARG:HE	1.85	0.42
21:q:74:PHE:HE2	21:q:75:TRP:HE1	1.68	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:r:110:GLN:HA	22:r:111:PRO:HD2	1.85	0.42
1:A:55:PHE:HZ	8:H:282:TYR:HE2	1.56	0.42
3:C:186:ILE:CD1	4:D:429:PHE:HZ	2.32	0.42
4:D:154:ALA:HB2	4:D:398:THR:HG21	2.01	0.42
5:E:179:CYS:C	5:E:181:ASN:N	2.77	0.42
6:F:65:THR:HA	6:F:68:ILE:HD12	2.01	0.42
7:G:43:VAL:HG12	7:G:55:LYS:CD	2.46	0.42
7:G:189:ILE:HG21	7:G:285:TRP:CE2	2.55	0.42
8:H:19:PHE:CB	19:a:12:MET:HG3	2.49	0.42
8:H:27:ILE:CG2	8:H:31:MET:HE3	2.42	0.42
8:H:96:ILE:HG23	18:Z:143:TYR:CE1	2.54	0.42
9:I:78:PHE:HD1	19:a:2:TRP:CD1	2.37	0.42
9:I:93:LEU:O	21:q:93:MET:CG	2.65	0.42
10:P:300:TRP:NE1	10:P:304:LEU:HD21	2.35	0.42
11:Q:58:LYS:O	11:Q:58:LYS:HG3	2.20	0.42
11:Q:75:ARG:NH1	11:Q:104:ARG:HG2	2.34	0.42
13:S:16:LEU:HD13	13:S:19:ILE:HD11	2.02	0.42
16:W:65:LYS:O	16:W:69:MET:HG2	2.19	0.42
17:X:75:LYS:O	17:X:79:ALA:HB2	2.19	0.42
19:a:12:MET:HE2	19:a:12:MET:HB3	1.90	0.42
3:C:73:GLN:HE22	3:C:145:TYR:HE1	1.66	0.42
4:D:181:LEU:HD21	4:D:210:MET:HB2	2.02	0.42
5:E:109:MET:HE1	7:G:198:THR:CG2	2.50	0.42
5:E:179:CYS:SG	6:F:123:GLY:CA	3.08	0.42
6:F:81:LYS:HE2	6:F:97:LEU:CD2	2.47	0.42
6:F:110:PRO:O	6:F:238:CYS:HB3	2.20	0.42
6:F:226:LYS:HD3	6:F:226:LYS:HA	1.86	0.42
6:F:280:GLY:O	6:F:281:HIS:C	2.63	0.42
7:G:163:LYS:HE2	12:R:97:LYS:HZ3	1.85	0.42
7:G:224:ASP:OD2	7:G:291:ARG:NH2	2.50	0.42
7:G:404:GLY:HA2	7:G:684:LEU:HD11	2.00	0.42
8:H:172:MET:HE3	8:H:176:LEU:CB	2.47	0.42
8:H:179:TRP:CE3	8:H:183:MET:HE3	2.55	0.42
8:H:287:HIS:O	8:H:291:LYS:N	2.51	0.42
16:W:53:MET:SD	16:W:106:VAL:HG21	2.60	0.42
16:W:58:THR:O	16:W:61:GLN:HB3	2.20	0.42
17:X:38:LYS:NZ	20:b:68:SER:OG	2.52	0.42
17:X:41:LYS:O	17:X:42:GLU:C	2.59	0.42
21:q:39:VAL:HG21	21:q:89:TRP:CZ2	2.55	0.42
2:B:82:ILE:CG1	8:H:57:MET:HE1	2.43	0.42
3:C:75:VAL:HG13	3:C:83:LEU:HD11	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:259:GLU:O	4:D:261:MET:N	2.53	0.42
6:F:38:GLU:HG3	6:F:39:ASP:OD1	2.20	0.42
6:F:329:LYS:HE3	6:F:359:ARG:NH1	2.35	0.42
27:F:501:FMN:H9	27:F:501:FMN:H1'1	1.88	0.42
7:G:155:GLU:CD	7:G:155:GLU:N	2.78	0.42
7:G:253:VAL:O	7:G:253:VAL:CG1	2.68	0.42
7:G:347:ASP:CB	7:G:594:ALA:HB1	2.49	0.42
7:G:408:ARG:HD3	7:G:409:PHE:CZ	2.54	0.42
7:G:524:ALA:HB2	7:G:597:VAL:HG22	2.01	0.42
8:H:186:PHE:CE2	28:H:401:3PE:H2B1	2.54	0.42
8:H:260:MET:HE2	8:H:260:MET:HB3	1.93	0.42
14:T:100:VAL:O	14:T:141:PRO:HD2	2.20	0.42
17:X:117:TRP:CD1	17:X:117:TRP:N	2.87	0.42
19:a:49:GLU:O	19:a:50:ARG:C	2.62	0.42
20:b:16:GLU:N	20:b:17:PRO:HD3	2.35	0.42
20:b:67:PRO:O	20:b:68:SER:C	2.61	0.42
23:s:66:SER:O	23:s:67:PRO:C	2.63	0.42
2:B:202:LEU:HD12	9:I:86:TYR:CE2	2.49	0.41
4:D:144:MET:HG2	4:D:223:HIS:H	1.85	0.41
4:D:208:GLU:OE1	4:D:221:ARG:NH2	2.52	0.41
4:D:261:MET:HE3	4:D:261:MET:HB3	1.90	0.41
4:D:301:ASP:N	22:r:104:TRP:HH2	2.18	0.41
4:D:384:LEU:HD23	4:D:384:LEU:HA	1.89	0.41
5:E:180:VAL:HG11	5:E:224:CYS:HB2	2.02	0.41
6:F:391:TRP:O	6:F:395:VAL:HG23	2.20	0.41
7:G:83:GLU:O	7:G:84:LYS:C	2.63	0.41
7:G:537:ILE:HG23	7:G:542:PRO:HD3	2.02	0.41
7:G:613:PRO:O	7:G:616:ALA:HB3	2.20	0.41
8:H:14:LEU:HD23	8:H:14:LEU:HA	1.86	0.41
9:I:153:ILE:CD1	9:I:155:CYS:HB3	2.38	0.41
10:P:284:THR:HG22	10:P:286:ARG:HG3	2.02	0.41
10:P:376:ASN:O	10:P:377:TYR:C	2.61	0.41
11:Q:104:ARG:HA	11:Q:104:ARG:HD3	1.88	0.41
12:R:72:VAL:HG12	12:R:73:GLU:H	1.85	0.41
17:X:130:LYS:NZ	20:b:63:MET:O	2.53	0.41
20:b:35:ILE:O	20:b:35:ILE:CG1	2.67	0.41
22:r:12:ARG:HH21	22:r:20:LEU:CD1	2.33	0.41
1:A:104:TYR:HA	1:A:107:THR:OG1	2.20	0.41
2:B:191:VAL:HG12	2:B:196:PRO:HB3	2.01	0.41
2:B:223:ARG:HG2	2:B:223:ARG:O	2.20	0.41
3:C:121:ARG:NH2	15:V:114:TRP:HA	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:140:ASP:O	4:D:147:ASN:ND2	2.53	0.41
7:G:249:GLU:HG2	7:G:262:VAL:HG22	2.01	0.41
7:G:354:LEU:HB2	7:G:623:ILE:HD13	2.02	0.41
8:H:123:SER:O	8:H:124:ASN:HB2	2.20	0.41
8:H:136:VAL:HG13	8:H:137:ALA:N	2.35	0.41
8:H:221:ALA:O	8:H:224:PHE:HB3	2.20	0.41
8:H:306:SER:O	8:H:307:LEU:C	2.63	0.41
10:P:279:TYR:O	10:P:280:ILE:C	2.62	0.41
10:P:324:ILE:HD13	10:P:324:ILE:HA	1.91	0.41
12:R:79:CYS:HG	12:R:104:CYS:HG	1.60	0.41
13:S:20:ARG:HD2	13:S:22:HIS:NE2	2.35	0.41
14:T:123:GLU:HG2	14:T:130:ILE:HD12	2.02	0.41
17:X:70:PHE:CE1	17:X:117:TRP:CZ3	3.08	0.41
21:q:21:ARG:HD2	21:q:21:ARG:HA	1.80	0.41
21:q:50:GLU:HA	21:q:59:HIS:O	2.20	0.41
4:D:198:THR:N	4:D:199:PRO:CD	2.84	0.41
4:D:240:LEU:O	4:D:241:LEU:C	2.62	0.41
4:D:375:MET:HG2	7:G:121:LEU:HD22	2.02	0.41
5:E:58:ASN:HB3	5:E:84:LEU:HD21	2.02	0.41
5:E:213:PRO:O	5:E:215:PRO:HD3	2.20	0.41
6:F:170:GLN:HG2	23:s:52:LEU:HD11	2.02	0.41
7:G:127:ASP:O	7:G:131:CYS:N	2.52	0.41
7:G:160:VAL:CG1	7:G:161:GLU:N	2.83	0.41
7:G:213:MET:HE2	7:G:215:MET:CG	2.50	0.41
10:P:201:ILE:HD13	10:P:265:PHE:CZ	2.55	0.41
10:P:355:ARG:HH11	10:P:356:HIS:HE1	1.66	0.41
11:Q:85:ASN:C	11:Q:87:MET:N	2.76	0.41
13:S:30:SER:HB3	13:S:63:PRO:HG3	2.00	0.41
14:T:115:GLN:O	14:T:116:VAL:C	2.63	0.41
15:V:98:LYS:HG2	15:V:100:TRP:CZ2	2.55	0.41
18:Z:108:GLU:O	18:Z:109:SER:C	2.61	0.41
4:D:88:HIS:C	4:D:90:ALA:H	2.28	0.41
4:D:121:GLU:HG2	4:D:424:ILE:HD12	2.02	0.41
5:E:173:VAL:HG22	5:E:174:GLU:H	1.84	0.41
5:E:180:VAL:HG13	5:E:181:ASN:N	2.34	0.41
6:F:294:VAL:HA	6:F:295:PRO:HD3	1.84	0.41
6:F:315:LEU:O	6:F:315:LEU:HD23	2.20	0.41
6:F:391:TRP:HH2	7:G:118:GLU:OE2	2.02	0.41
7:G:517:HIS:CD2	7:G:523:VAL:CG2	3.03	0.41
7:G:639:LEU:O	7:G:639:LEU:HD23	2.21	0.41
7:G:651:PRO:HG3	13:S:57:GLU:N	2.29	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:37:ASP:OD1	17:X:37:ASP:C	2.62	0.41
19:a:49:GLU:OE2	19:a:49:GLU:HA	2.20	0.41
19:a:64:LYS:CE	19:a:66:LEU:HD12	2.31	0.41
20:b:15:LYS:O	20:b:16:GLU:HB2	2.20	0.41
20:b:45:ILE:HG23	20:b:46:ASN:N	2.34	0.41
21:q:85:GLU:CG	21:q:98:PRO:HB3	2.39	0.41
30:q:201:CDL:H112	30:q:201:CDL:H312	2.02	0.41
3:C:72:VAL:HG23	3:C:72:VAL:O	2.20	0.41
4:D:151:TYR:O	4:D:155:VAL:HG23	2.20	0.41
4:D:360:ASP:C	4:D:362:LYS:N	2.71	0.41
6:F:53:LEU:O	6:F:57:LEU:HG	2.20	0.41
6:F:93:PHE:O	6:F:94:PRO:C	2.59	0.41
7:G:50:LEU:HD11	7:G:62:ARG:HD3	2.03	0.41
7:G:319:TRP:HZ3	7:G:584:LEU:HD22	1.86	0.41
7:G:365:ASN:HB3	7:G:537:ILE:HD11	2.02	0.41
8:H:289:LEU:C	8:H:289:LEU:CD2	2.93	0.41
8:H:293:PHE:O	8:H:294:LEU:C	2.63	0.41
9:I:130:ILE:HD11	9:I:145:TYR:HE1	1.85	0.41
10:P:208:GLY:O	10:P:211:ASP:N	2.53	0.41
20:b:78:LEU:O	20:b:81:LEU:N	2.53	0.41
1:A:111:LEU:HD23	1:A:112:GLU:H	1.86	0.41
2:B:76:THR:O	2:B:77:LYS:C	2.62	0.41
3:C:70:LYS:HD3	3:C:71:TYR:CZ	2.56	0.41
4:D:141:TYR:CZ	4:D:457:VAL:HG13	2.56	0.41
5:E:108:PRO:O	5:E:109:MET:C	2.63	0.41
6:F:166:ALA:O	6:F:167:SER:C	2.63	0.41
6:F:313:ASN:O	6:F:358:ASP:HA	2.20	0.41
6:F:391:TRP:CE2	7:G:153:PHE:HD1	2.39	0.41
7:G:47:THR:HG23	7:G:51:GLN:HB2	2.03	0.41
7:G:339:ALA:CB	7:G:537:ILE:HD12	2.51	0.41
8:H:283:ASP:OD1	8:H:284:GLN:N	2.53	0.41
8:H:288:LEU:C	8:H:288:LEU:HD23	2.45	0.41
9:I:54:THR:HA	20:b:13:TRP:NE1	2.35	0.41
9:I:94:SER:HB2	9:I:95:PRO:CD	2.34	0.41
9:I:149:MET:HE2	9:I:185:TYR:CD2	2.55	0.41
25:I:301:PC1:H112	18:Z:29:GLY:HA3	2.02	0.41
10:P:143:ASP:OD1	10:P:147:ASN:ND2	2.54	0.41
10:P:317:ASP:CB	10:P:321:ARG:HH22	2.31	0.41
18:Z:19:ILE:HG22	18:Z:20:ASP:N	2.36	0.41
23:s:44:THR:O	23:s:48:LEU:HG	2.21	0.41
1:A:65:PHE:O	1:A:69:ILE:HG13	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:141:ARG:HE	3:C:141:ARG:HB2	1.41	0.41
3:C:152:ILE:HG22	3:C:153:ASP:N	2.35	0.41
3:C:243:ALA:C	7:G:105:ASN:HD21	2.28	0.41
4:D:323:ARG:HG2	4:D:323:ARG:O	2.20	0.41
4:D:423:LYS:HD3	4:D:424:ILE:N	2.35	0.41
5:E:233:LEU:HB2	6:F:48:ARG:HH12	1.84	0.41
6:F:62:TRP:CE2	6:F:181:LEU:HD13	2.56	0.41
6:F:76:ILE:O	6:F:80:MET:HG2	2.21	0.41
6:F:210:THR:HG23	6:F:226:LYS:HE3	2.01	0.41
8:H:130:PHE:CZ	8:H:134:ARG:HD3	2.56	0.41
8:H:239:THR:HG23	8:H:262:GLU:HB2	2.02	0.41
10:P:214:LEU:HD23	10:P:352:VAL:HG12	2.01	0.41
10:P:293:LEU:HD12	10:P:294:PRO:HD2	2.01	0.41
13:S:41:TYR:HE1	13:S:53:ILE:HG23	1.85	0.41
14:T:87:LEU:CD2	14:T:122:MET:CE	2.98	0.41
14:T:140:CYS:HB2	14:T:143:GLU:HB2	2.02	0.41
17:X:70:PHE:O	17:X:74:ILE:HG13	2.21	0.41
21:q:87:HIS:O	21:q:91:HIS:HD2	2.04	0.41
21:q:132:LYS:HE2	21:q:135:HIS:HA	2.01	0.41
2:B:114:MET:HG3	2:B:115:ASP:N	2.36	0.41
3:C:195:HIS:HE1	16:W:88:LYS:NZ	2.19	0.41
4:D:242:ASP:O	4:D:245:TYR:HB3	2.20	0.41
6:F:42:PHE:CD2	6:F:275:LEU:HD11	2.56	0.41
6:F:102:MET:O	6:F:102:MET:HG3	2.20	0.41
6:F:115:VAL:HG22	6:F:248:VAL:HG21	2.02	0.41
6:F:274:LYS:HB3	6:F:276:PHE:CZ	2.56	0.41
7:G:41:VAL:HG21	7:G:56:VAL:CA	2.51	0.41
7:G:319:TRP:O	7:G:320:GLU:C	2.63	0.41
8:H:210:GLY:CA	8:H:213:VAL:HG23	2.50	0.41
9:I:54:THR:CG2	20:b:13:TRP:NE1	2.60	0.41
10:P:61:ALA:HA	10:P:66:GLY:HA3	2.02	0.41
14:T:120:MET:O	14:T:121:ALA:C	2.63	0.41
14:T:134:ASP:HA	14:T:137:LYS:NZ	2.36	0.41
15:V:96:LYS:HE2	15:V:96:LYS:HB2	1.95	0.41
17:X:16:GLU:CD	17:X:68:LEU:HD13	2.46	0.41
1:A:69:ILE:O	1:A:73:LEU:HG	2.21	0.41
2:B:111:ARG:NH1	4:D:212:GLU:OE2	2.54	0.41
2:B:224:ARG:HG3	10:P:85:ARG:HH22	1.85	0.41
4:D:188:THR:HG21	4:D:203:MET:HB2	2.03	0.41
4:D:265:ASN:C	4:D:267:ILE:H	2.29	0.41
4:D:310:VAL:C	4:D:312:ASP:H	2.29	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:86:GLN:NE2	5:E:121:TYR:HA	2.36	0.41
6:F:47:GLY:O	6:F:48:ARG:HB2	2.21	0.41
6:F:76:ILE:O	6:F:79:GLU:HB2	2.20	0.41
6:F:225:LEU:HD13	11:Q:160:TYR:CZ	2.56	0.41
6:F:329:LYS:HE3	6:F:359:ARG:HH11	1.86	0.41
7:G:217:GLU:C	7:G:219:SER:N	2.79	0.41
7:G:282:ASN:O	7:G:282:ASN:CG	2.63	0.41
7:G:339:ALA:HB3	7:G:542:PRO:HG3	2.03	0.41
7:G:517:HIS:CD2	7:G:599:THR:HG22	2.56	0.41
8:H:28:LEU:CD1	8:H:274:ARG:HH11	2.34	0.41
8:H:302:MET:HE2	8:H:302:MET:HB3	1.97	0.41
10:P:351:GLU:HB3	16:W:56:ASP:OD2	2.21	0.41
15:V:72:LEU:C	15:V:72:LEU:CD1	2.89	0.41
16:W:78:ASP:HB3	16:W:81:VAL:HG23	2.03	0.41
18:Z:90:ASN:O	18:Z:94:GLU:HB2	2.21	0.41
20:b:11:ASN:O	20:b:15:LYS:HG2	2.20	0.41
20:b:11:ASN:CG	20:b:15:LYS:HE3	2.46	0.41
20:b:78:LEU:C	20:b:80:TRP:N	2.77	0.41
21:q:66:THR:HG22	21:q:74:PHE:CB	2.28	0.41
1:A:18:ILE:HD13	1:A:18:ILE:HA	1.94	0.41
2:B:84:TRP:HA	2:B:87:ARG:HG2	2.02	0.41
3:C:185:ARG:O	3:C:185:ARG:HG3	2.20	0.41
4:D:106:VAL:HG21	4:D:447:VAL:HG21	2.03	0.41
5:E:190:ASN:HD22	5:E:192:TYR:HE1	1.69	0.41
7:G:48:THR:O	7:G:49:VAL:C	2.63	0.41
7:G:74:ASN:ND2	7:G:180:THR:OG1	2.54	0.41
7:G:649:VAL:HA	13:S:20:ARG:NH1	2.36	0.41
8:H:187:ILE:HG23	8:H:198:PHE:CE2	2.56	0.41
9:I:76:TYR:C	9:I:78:PHE:N	2.74	0.41
10:P:163:ARG:NH1	10:P:199:ILE:HD11	2.36	0.41
10:P:195:PHE:O	10:P:196:PRO:C	2.63	0.41
14:T:87:LEU:HD11	14:T:141:PRO:HG3	2.03	0.41
17:X:25:LEU:HB3	18:Z:71:LEU:HD22	2.03	0.41
20:b:53:TYR:CE2	20:b:55:VAL:HA	2.55	0.41
21:q:129:THR:O	21:q:129:THR:CG2	2.67	0.41
2:B:116:ARG:HG3	8:H:38:ASN:H	1.85	0.40
4:D:190:HIS:O	4:D:194:ILE:HG12	2.20	0.40
5:E:71:GLU:HB3	23:s:60:PRO:O	2.21	0.40
6:F:51:TRP:HE3	6:F:135:PRO:HG3	1.86	0.40
6:F:81:LYS:HD3	6:F:96:GLY:HA3	2.03	0.40
8:H:95:LEU:HG	8:H:96:ILE:HG13	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:149:MET:HB3	9:I:154:TYR:OH	2.20	0.40
16:W:93:LEU:O	16:W:94:GLN:C	2.64	0.40
17:X:132:LYS:HB3	17:X:132:LYS:HE2	1.84	0.40
1:A:16:THR:O	1:A:20:VAL:HG23	2.21	0.40
2:B:181:CYS:C	2:B:183:ARG:H	2.27	0.40
3:C:49:ARG:NH2	3:C:79:CYS:HA	2.36	0.40
3:C:70:LYS:O	15:V:103:LEU:HA	2.21	0.40
3:C:92:VAL:HG21	3:C:152:ILE:CG2	2.51	0.40
4:D:104:GLU:HG3	8:H:130:PHE:CZ	2.56	0.40
4:D:128:THR:HG22	4:D:131:GLN:CG	2.52	0.40
4:D:235:ASP:OD2	18:Z:8:GLN:HG3	2.21	0.40
6:F:270:ASN:CG	6:F:338:ASP:HB2	2.46	0.40
7:G:94:MET:HE3	7:G:94:MET:HB3	1.97	0.40
7:G:185:PHE:CD2	7:G:189:ILE:HB	2.56	0.40
7:G:277:MET:HE1	11:Q:153:PRO:HD3	2.03	0.40
28:H:401:3PE:O21	9:I:63:TRP:NE1	2.54	0.40
12:R:48:PHE:CD2	12:R:53:LYS:HB2	2.56	0.40
13:S:21:VAL:HG22	13:S:91:MET:HE1	2.03	0.40
14:T:107:ASP:OD1	14:T:108:LEU:N	2.54	0.40
17:X:90:ASP:OD2	19:a:62:VAL:CG1	2.50	0.40
19:a:9:LEU:O	19:a:10:ALA:C	2.64	0.40
1:A:20:VAL:O	1:A:21:ALA:C	2.62	0.40
3:C:136:PHE:CE1	22:r:96:THR:HB	2.56	0.40
4:D:116:LEU:HA	4:D:116:LEU:HD12	1.96	0.40
5:E:71:GLU:H	23:s:59:GLN:HB3	1.86	0.40
5:E:170:LEU:HD12	5:E:171:ILE:H	1.83	0.40
6:F:74:ASP:OD1	6:F:74:ASP:N	2.54	0.40
6:F:171:VAL:HG13	6:F:174:ARG:HH22	1.86	0.40
6:F:176:ALA:HB3	6:F:182:ILE:HD11	2.03	0.40
6:F:297:LYS:HG3	6:F:301:GLU:CG	2.51	0.40
7:G:64:CYS:SG	7:G:75:CYS:SG	3.14	0.40
7:G:309:ASN:CG	7:G:310:GLU:H	2.29	0.40
8:H:42:PRO:HG3	21:q:28:PHE:HE1	1.85	0.40
8:H:137:ALA:HB3	8:H:282:TYR:OH	2.22	0.40
8:H:204:GLU:OE1	8:H:204:GLU:HA	2.21	0.40
10:P:54:VAL:O	10:P:78:SER:HB3	2.21	0.40
13:S:22:HIS:CD2	13:S:66:TRP:HD1	2.39	0.40
13:S:59:SER:O	13:S:60:GLU:C	2.63	0.40
17:X:36:CYS:O	17:X:40:ASN:CG	2.65	0.40
19:a:48:MET:HE3	19:a:48:MET:HB2	1.77	0.40
20:b:67:PRO:HD2	20:b:72:ASP:CB	2.49	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:106:HIS:O	2:B:109:ALA:HB3	2.22	0.40
4:D:176:GLU:OE2	4:D:179:ARG:NH1	2.55	0.40
6:F:265:PHE:HB3	6:F:291:GLU:CG	2.51	0.40
6:F:322:SER:HB2	6:F:370:LEU:HD22	2.02	0.40
7:G:396:GLU:HG2	7:G:396:GLU:O	2.21	0.40
8:H:7:LEU:HA	8:H:7:LEU:HD13	1.75	0.40
8:H:23:VAL:O	8:H:23:VAL:CG1	2.69	0.40
8:H:153:VAL:HG11	8:H:241:ILE:HG23	2.03	0.40
9:I:36:TYR:CZ	22:r:106:LEU:HD23	2.56	0.40
9:I:162:CYS:HB3	9:I:165:ASP:HA	2.03	0.40
10:P:93:HIS:O	10:P:96:LEU:HG	2.21	0.40
13:S:23:LEU:HB3	13:S:33:VAL:CG1	2.52	0.40
14:T:113:LEU:HD22	16:W:71:MET:HE2	2.04	0.40
14:T:123:GLU:OE1	16:W:44:ARG:NH1	2.55	0.40
21:q:3:LEU:HD13	30:q:201:CDL:C51	2.51	0.40
2:B:192:PRO:HG2	9:I:175:PHE:CE1	2.56	0.40
4:D:144:MET:HE2	4:D:144:MET:HB2	1.92	0.40
6:F:176:ALA:HA	6:F:181:LEU:HD12	2.03	0.40
6:F:402:GLY:HA2	6:F:450:MET:HE2	2.04	0.40
7:G:302:LEU:N	7:G:571:HIS:O	2.45	0.40
7:G:339:ALA:HB1	7:G:537:ILE:HD12	2.03	0.40
7:G:462:PHE:HD2	7:G:466:LEU:HG	1.86	0.40
8:H:40:VAL:HG12	8:H:47:GLN:NE2	2.37	0.40
9:I:89:GLU:OE2	21:q:61:TRP:HB3	2.22	0.40
9:I:109:GLY:O	12:R:63:LEU:HD12	2.22	0.40
9:I:149:MET:HE2	9:I:185:TYR:HD2	1.86	0.40
9:I:201:ILE:O	9:I:205:ILE:HG12	2.21	0.40
10:P:236:VAL:HA	10:P:271:TYR:O	2.22	0.40
14:T:118:ILE:HD13	14:T:118:ILE:HA	1.83	0.40
20:b:69:HIS:CD2	20:b:71:GLN:H	2.39	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	A	87/115 (76%)	83 (95%)	4 (5%)	0	100	100
2	B	154/224 (69%)	142 (92%)	11 (7%)	1 (1%)	21	58
3	C	196/263 (74%)	187 (95%)	9 (5%)	0	100	100
4	D	383/463 (83%)	356 (93%)	27 (7%)	0	100	100
5	E	208/248 (84%)	193 (93%)	15 (7%)	0	100	100
6	F	422/464 (91%)	402 (95%)	20 (5%)	0	100	100
7	G	685/727 (94%)	632 (92%)	53 (8%)	0	100	100
8	H	313/318 (98%)	295 (94%)	18 (6%)	0	100	100
9	I	169/212 (80%)	169 (100%)	0	0	100	100
10	P	337/377 (89%)	314 (93%)	23 (7%)	0	100	100
11	Q	116/175 (66%)	114 (98%)	2 (2%)	0	100	100
12	R	70/116 (60%)	64 (91%)	6 (9%)	0	100	100
13	S	81/99 (82%)	77 (95%)	4 (5%)	0	100	100
14	T	73/156 (47%)	72 (99%)	1 (1%)	0	100	100
15	V	110/116 (95%)	107 (97%)	3 (3%)	0	100	100
16	W	112/131 (86%)	111 (99%)	1 (1%)	0	100	100
17	X	140/172 (81%)	131 (94%)	9 (6%)	0	100	100
18	Z	137/144 (95%)	132 (96%)	5 (4%)	0	100	100
19	a	65/70 (93%)	61 (94%)	4 (6%)	0	100	100
20	b	77/84 (92%)	69 (90%)	8 (10%)	0	100	100
21	q	118/145 (81%)	115 (98%)	3 (2%)	0	100	100
22	r	47/113 (42%)	43 (92%)	4 (8%)	0	100	100
23	s	27/104 (26%)	27 (100%)	0	0	100	100
All	All	4127/5036 (82%)	3896 (94%)	230 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	195	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	A	83/104 (80%)	83 (100%)	0	100	100
2	B	132/185 (71%)	131 (99%)	1 (1%)	73	77
3	C	180/227 (79%)	180 (100%)	0	100	100
4	D	332/395 (84%)	331 (100%)	1 (0%)	86	84
5	E	182/206 (88%)	182 (100%)	0	100	100
6	F	340/370 (92%)	340 (100%)	0	100	100
7	G	579/610 (95%)	578 (100%)	1 (0%)	87	85
8	H	279/280 (100%)	278 (100%)	1 (0%)	84	82
9	I	147/178 (83%)	147 (100%)	0	100	100
10	P	296/325 (91%)	296 (100%)	0	100	100
11	Q	105/153 (69%)	104 (99%)	1 (1%)	68	75
12	R	62/96 (65%)	61 (98%)	1 (2%)	55	69
13	S	74/80 (92%)	73 (99%)	1 (1%)	59	70
14	T	69/135 (51%)	68 (99%)	1 (1%)	59	70
15	V	100/102 (98%)	100 (100%)	0	100	100
16	W	108/114 (95%)	108 (100%)	0	100	100
17	X	129/154 (84%)	128 (99%)	1 (1%)	73	77
18	Z	120/123 (98%)	119 (99%)	1 (1%)	73	77
19	a	57/60 (95%)	57 (100%)	0	100	100
20	b	70/73 (96%)	70 (100%)	0	100	100
21	q	110/131 (84%)	110 (100%)	0	100	100
22	r	44/96 (46%)	44 (100%)	0	100	100
23	s	28/95 (30%)	28 (100%)	0	100	100
All	All	3626/4292 (84%)	3616 (100%)	10 (0%)	84	84

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	120	VAL
4	D	88	HIS
7	G	271	MET
8	H	250	ASN
11	Q	96	LYS
12	R	64	ILE
13	S	68	ARG
14	T	103	HIS
17	X	52	ASP
18	Z	7	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (87) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
2	B	106	HIS
2	B	151	GLN
2	B	209	GLN
3	C	54	HIS
3	C	73	GLN
3	C	88	HIS
3	C	123	ASN
3	C	179	ASN
3	C	195	HIS
3	C	227	GLN
3	C	235	ASN
4	D	87	GLN
4	D	117	HIS
4	D	131	GLN
4	D	147	ASN
4	D	182	ASN
4	D	234	GLN
4	D	339	GLN
4	D	346	GLN
4	D	381	HIS
4	D	454	GLN
5	E	190	ASN
5	E	245	GLN
6	F	168	ASN
6	F	270	ASN
6	F	283	ASN
6	F	303	HIS
6	F	346	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	G	59	GLN
7	G	74	ASN
7	G	105	ASN
7	G	164	ASN
7	G	205	GLN
7	G	359	ASN
7	G	388	ASN
7	G	444	HIS
7	G	495	ASN
7	G	498	GLN
7	G	540	ASN
7	G	569	GLN
7	G	571	HIS
7	G	605	GLN
7	G	666	GLN
7	G	677	GLN
7	G	705	GLN
8	H	5	ASN
8	H	32	GLN
8	H	47	GLN
8	H	93	HIS
8	H	124	ASN
8	H	138	GLN
8	H	163	GLN
8	H	169	GLN
8	H	258	ASN
8	H	292	ASN
10	P	71	ASN
10	P	79	GLN
10	P	166	HIS
10	P	219	ASN
10	P	238	GLN
10	P	269	ASN
10	P	275	HIS
10	P	341	GLN
10	P	356	HIS
11	Q	51	GLN
11	Q	88	GLN
12	R	52	GLN
13	S	48	HIS
13	S	81	ASN
15	V	41	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	V	50	GLN
16	W	54	GLN
17	X	30	HIS
17	X	77	HIS
17	X	140	ASN
19	a	31	ASN
20	b	71	GLN
20	b	83	ASN
21	q	31	ASN
21	q	52	ASN
21	q	54	GLN
21	q	87	HIS
21	q	91	HIS
21	q	123	GLN
22	r	21	GLN
22	r	110	GLN

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](#)

14 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
24	SF4	B	301	2	0,12,12	-	-	-		
30	CDL	q	201	-	56,56,99	1.21	4 (7%)	62,68,111	1.22	6 (9%)
29	NDP	P	401	-	51,52,52	1.19	5 (9%)	71,80,80	1.56	10 (14%)
24	SF4	G	801	7	0,12,12	-	-	-		
28	3PE	H	401	-	50,50,50	0.92	2 (4%)	53,55,55	1.02	2 (3%)
24	SF4	G	802	7	0,12,12	-	-	-		
26	FES	E	301	5	0,4,4	-	-	-		
24	SF4	I	303	9	0,12,12	-	-	-		
26	FES	G	803	7	0,4,4	-	-	-		
25	PC1	B	302	-	34,34,53	1.15	2 (5%)	40,42,61	1.17	4 (10%)
24	SF4	F	502	6	0,12,12	-	-	-		
27	FMN	F	501	-	33,33,33	1.41	4 (12%)	48,50,50	1.22	7 (14%)
24	SF4	I	302	9	0,12,12	-	-	-		
25	PC1	I	301	-	42,42,53	1.04	2 (4%)	48,50,61	1.05	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
30	CDL	q	201	-	-	19/67/67/110	-
24	SF4	B	301	2	-	-	0/6/5/5
29	NDP	P	401	-	-	6/34/77/77	0/5/5/5
24	SF4	G	801	7	-	-	0/6/5/5
28	3PE	H	401	-	-	12/54/54/54	-
24	SF4	G	802	7	-	-	0/6/5/5
26	FES	E	301	5	-	-	0/1/1/1
24	SF4	I	303	9	-	-	0/6/5/5
26	FES	G	803	7	-	-	0/1/1/1
25	PC1	B	302	-	-	11/38/38/57	-
24	SF4	F	502	6	-	-	0/6/5/5
27	FMN	F	501	-	-	1/18/18/18	0/3/3/3
24	SF4	I	302	9	-	-	0/6/5/5
25	PC1	I	301	-	-	8/46/46/57	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	F	501	FMN	C9A-C5A	5.09	1.49	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	P	401	NDP	C5A-C4A	4.50	1.47	1.39
30	q	201	CDL	OB8-CB7	4.26	1.45	1.33
30	q	201	CDL	OA8-CA7	4.25	1.45	1.33
25	B	302	PC1	O31-C31	4.22	1.45	1.33
25	I	301	PC1	O31-C31	4.22	1.45	1.33
28	H	401	3PE	O31-C31	4.21	1.45	1.33
28	H	401	3PE	O21-C21	4.09	1.45	1.34
25	I	301	PC1	O21-C21	4.08	1.45	1.34
30	q	201	CDL	OB6-CB5	4.08	1.45	1.34
25	B	302	PC1	O21-C21	4.02	1.45	1.34
30	q	201	CDL	OA6-CA5	4.01	1.45	1.34
27	F	501	FMN	C8-C7	3.22	1.48	1.40
29	P	401	NDP	C5A-C6A	2.72	1.48	1.41
27	F	501	FMN	C4-N3	-2.53	1.34	1.38
29	P	401	NDP	C5A-N7A	-2.39	1.34	1.39
29	P	401	NDP	C8A-N7A	2.33	1.36	1.31
27	F	501	FMN	C5A-N5	-2.24	1.35	1.39
29	P	401	NDP	C4A-N9A	-2.07	1.33	1.37

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	P	401	NDP	C5A-C4A-N3A	-5.75	118.79	126.72
29	P	401	NDP	N3A-C4A-N9A	4.53	134.87	127.17
25	B	302	PC1	O21-C21-C22	4.23	120.64	111.48
25	I	301	PC1	O21-C21-C22	3.88	119.88	111.48
30	q	201	CDL	OA6-CA5-C11	3.85	119.80	111.48
30	q	201	CDL	OB6-CB5-C51	3.80	119.70	111.48
29	P	401	NDP	C2A-N3A-C4A	3.71	120.88	111.83
29	P	401	NDP	C4A-C5A-N7A	-3.55	106.53	110.58
28	H	401	3PE	O21-C21-C22	3.35	118.73	111.48
29	P	401	NDP	N3A-C2A-N1A	-3.23	123.69	128.58
29	P	401	NDP	C4A-N9A-C8A	2.90	108.78	105.74
30	q	201	CDL	OB8-CB7-C71	2.81	120.40	111.83
28	H	401	3PE	O31-C31-C32	2.78	120.30	111.83
25	I	301	PC1	C2-O21-C21	-2.76	111.20	117.80
29	P	401	NDP	C5A-N7A-C8A	2.65	107.61	103.45
27	F	501	FMN	O4-C4-C4A	-2.63	119.58	126.53
25	I	301	PC1	O31-C31-C32	2.59	119.73	111.83
30	q	201	CDL	OA8-CA7-C31	2.58	119.71	111.83
25	B	302	PC1	O31-C31-C32	2.48	119.39	111.83
27	F	501	FMN	C4A-C10-N1	-2.42	118.66	124.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	302	PC1	C2-O21-C21	-2.35	112.16	117.80
30	q	201	CDL	CA4-OA6-CA5	-2.35	112.18	117.80
27	F	501	FMN	C4-C4A-N5	2.28	121.36	118.21
29	P	401	NDP	N9A-C8A-N7A	-2.25	110.74	113.94
29	P	401	NDP	C6A-C5A-N7A	2.19	136.30	132.09
29	P	401	NDP	C3D-C2D-C1D	2.12	105.47	101.46
27	F	501	FMN	C4A-C4-N3	2.08	118.54	113.25
27	F	501	FMN	C10-N1-C2	2.08	121.34	116.85
25	B	302	PC1	O21-C21-O22	-2.07	118.87	123.70
30	q	201	CDL	OA6-CA5-OA7	-2.07	118.87	123.70
27	F	501	FMN	C4-N3-C2	-2.06	121.98	125.64
27	F	501	FMN	O2-C2-N1	-2.02	118.44	121.80

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	B	302	PC1	C1-O11-P-O12
25	B	302	PC1	C1-O11-P-O14
25	B	302	PC1	C1-O11-P-O13
25	B	302	PC1	O22-C21-O21-C2
28	H	401	3PE	C1-O11-P-O12
28	H	401	3PE	C1-O11-P-O13
28	H	401	3PE	C1-O11-P-O14
28	H	401	3PE	C11-O13-P-O11
28	H	401	3PE	C11-O13-P-O14
29	P	401	NDP	C2N-C3N-C7N-N7N
30	q	201	CDL	CA2-OA2-PA1-OA3
30	q	201	CDL	CA3-OA5-PA1-OA2
30	q	201	CDL	OA7-CA5-OA6-CA4
30	q	201	CDL	C11-CA5-OA6-CA4
30	q	201	CDL	CB2-OB2-PB2-OB3
30	q	201	CDL	CB2-OB2-PB2-OB4
30	q	201	CDL	CB2-OB2-PB2-OB5
30	q	201	CDL	CB3-OB5-PB2-OB2
30	q	201	CDL	CB3-OB5-PB2-OB4
25	I	301	PC1	O22-C21-O21-C2
25	B	302	PC1	C22-C21-O21-C2
25	I	301	PC1	C22-C21-O21-C2
28	H	401	3PE	C32-C31-O31-C3
30	q	201	CDL	C31-CA7-OA8-CA6
28	H	401	3PE	O32-C31-O31-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	q	201	CDL	C51-CB5-OB6-CB4
30	q	201	CDL	OA9-CA7-OA8-CA6
30	q	201	CDL	OB7-CB5-OB6-CB4
25	I	301	PC1	C32-C31-O31-C3
30	q	201	CDL	CB6-CB4-OB6-CB5
25	I	301	PC1	O32-C31-O31-C3
25	B	302	PC1	C23-C24-C25-C26
25	B	302	PC1	C32-C33-C34-C35
28	H	401	3PE	C3E-C3F-C3G-C3H
28	H	401	3PE	C37-C38-C39-C3A
25	I	301	PC1	C11-C12-N-C13
29	P	401	NDP	PN-O3-PA-O2A
25	I	301	PC1	C11-C12-N-C15
29	P	401	NDP	O4D-C1D-N1N-C6N
28	H	401	3PE	C11-O13-P-O12
30	q	201	CDL	CA3-OA5-PA1-OA3
30	q	201	CDL	CB3-OB5-PB2-OB3
30	q	201	CDL	C1-CA2-OA2-PA1
27	F	501	FMN	C5'-O5'-P-O1P
29	P	401	NDP	C2B-O2B-P2B-O2X
28	H	401	3PE	C24-C25-C26-C27
25	I	301	PC1	C11-C12-N-C14
25	B	302	PC1	C1-C2-C3-O31
25	I	301	PC1	C32-C33-C34-C35
30	q	201	CDL	CA4-CA3-OA5-PA1
25	B	302	PC1	O32-C31-O31-C3
25	B	302	PC1	C3-C2-O21-C21
25	B	302	PC1	C32-C31-O31-C3
30	q	201	CDL	CB4-CB3-OB5-PB2
29	P	401	NDP	C2N-C3N-C7N-O7N
28	H	401	3PE	C33-C34-C35-C36
29	P	401	NDP	PN-O3-PA-O1A

There are no ring outliers.

12 monomers are involved in 76 short contacts:

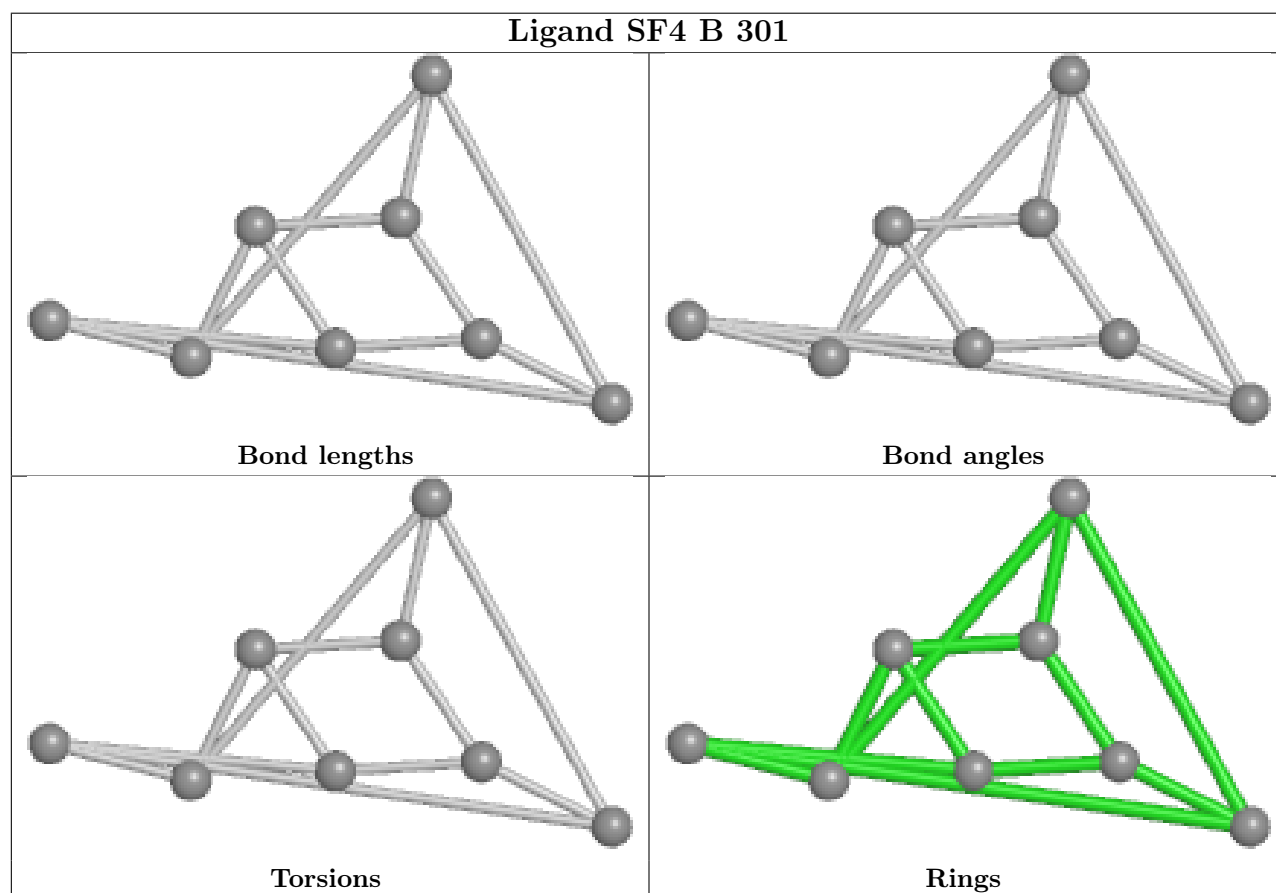
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	301	SF4	3	0
30	q	201	CDL	22	0
29	P	401	NDP	5	0
28	H	401	3PE	8	0
24	G	802	SF4	2	0

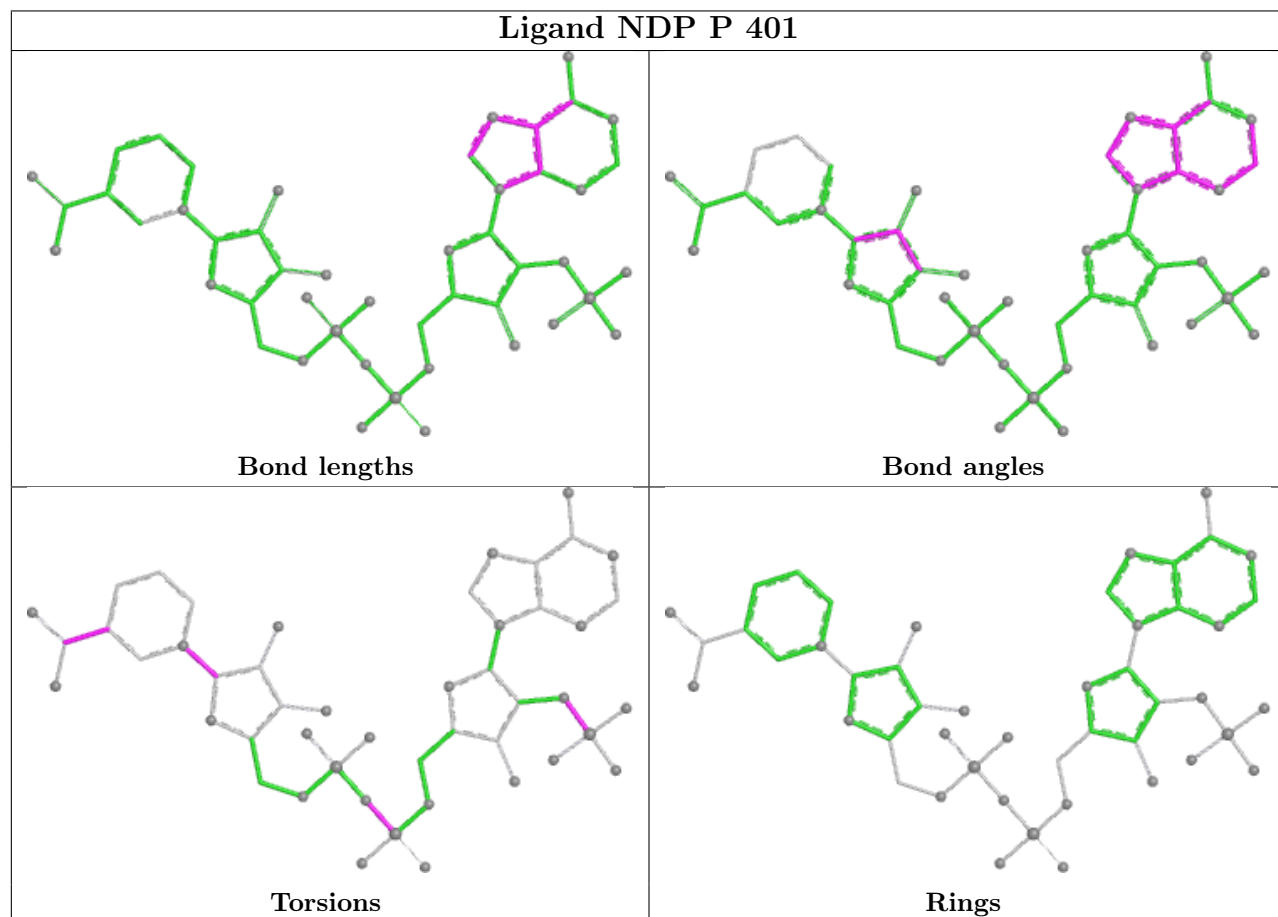
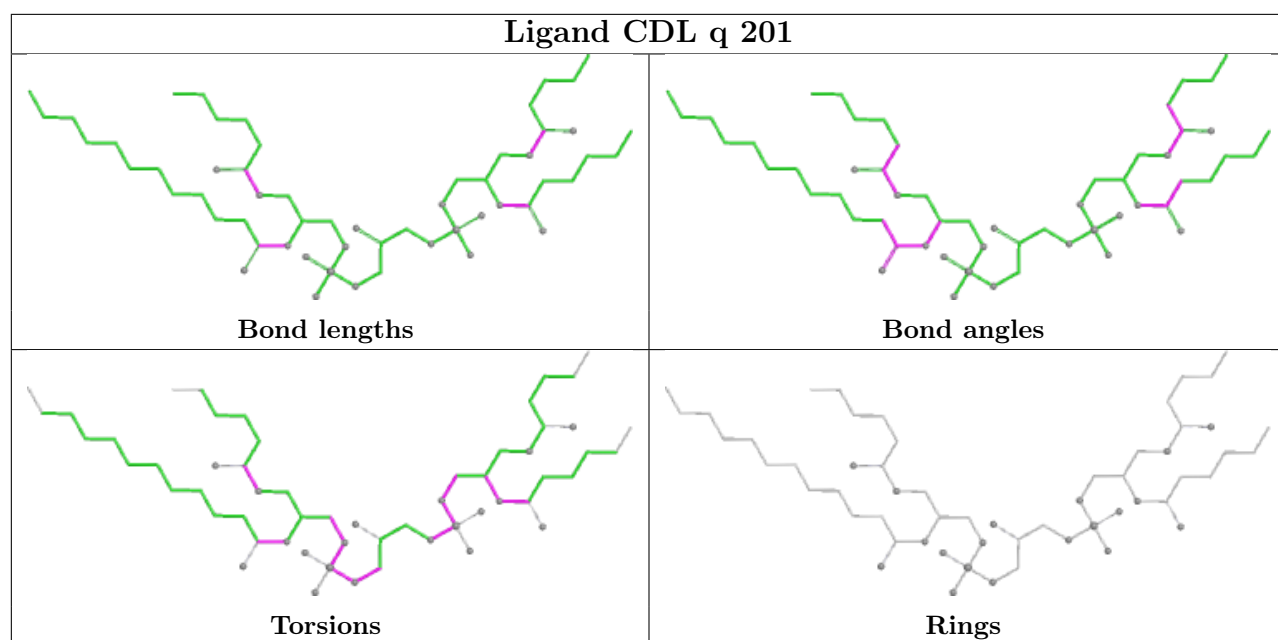
Continued on next page...

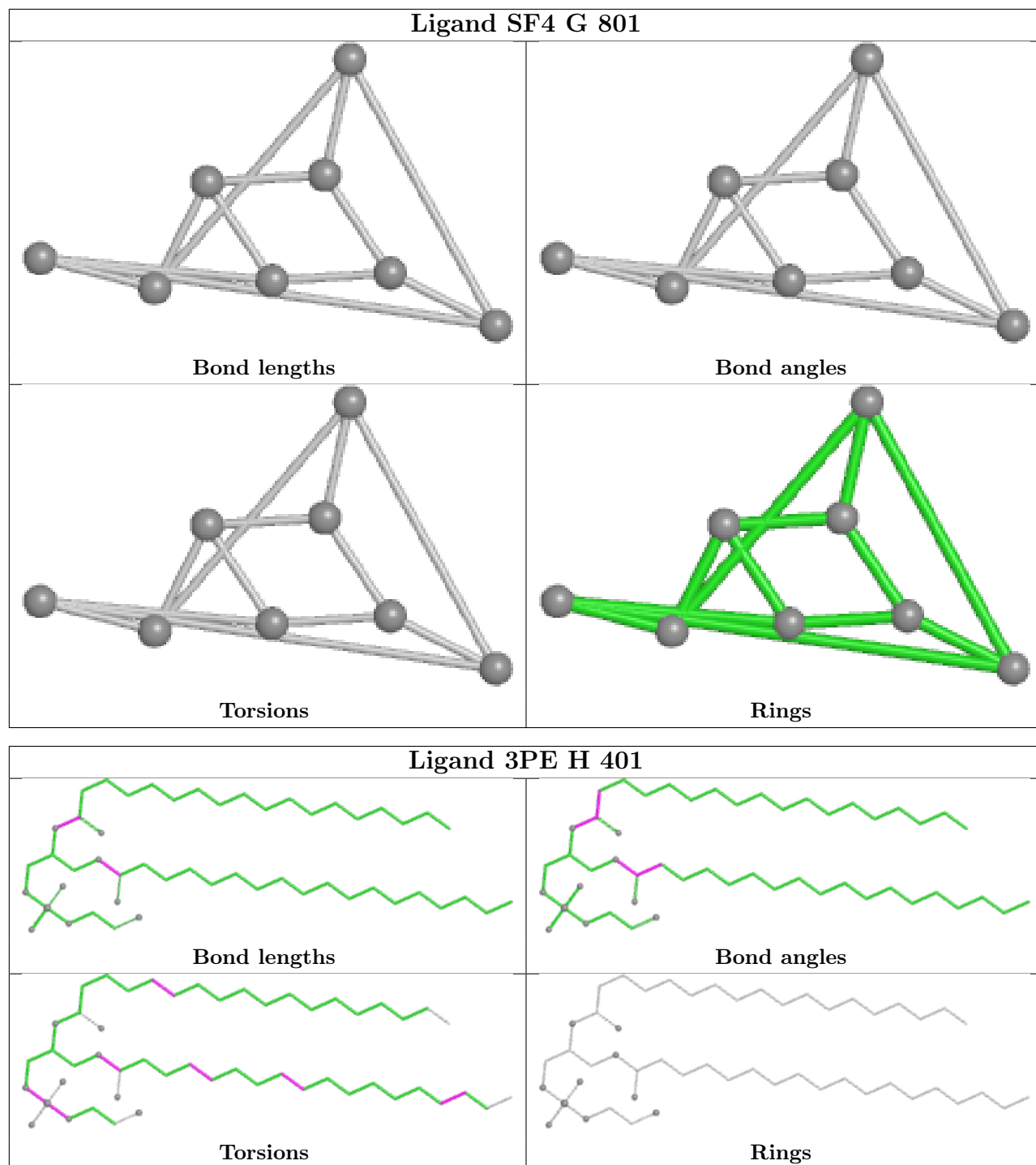
Continued from previous page...

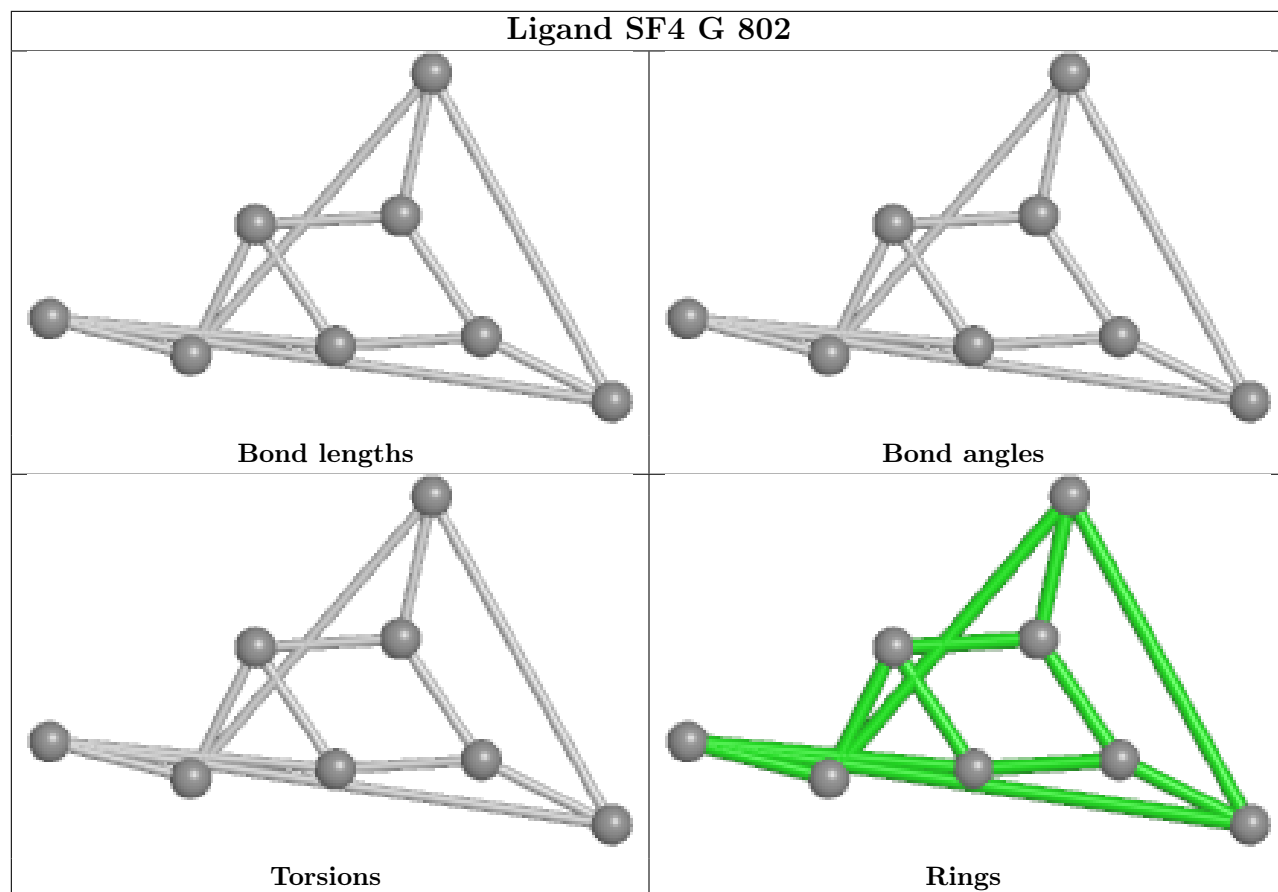
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	E	301	FES	4	0
24	I	303	SF4	5	0
26	G	803	FES	5	0
25	B	302	PC1	6	0
24	F	502	SF4	6	0
27	F	501	FMN	1	0
25	I	301	PC1	9	0

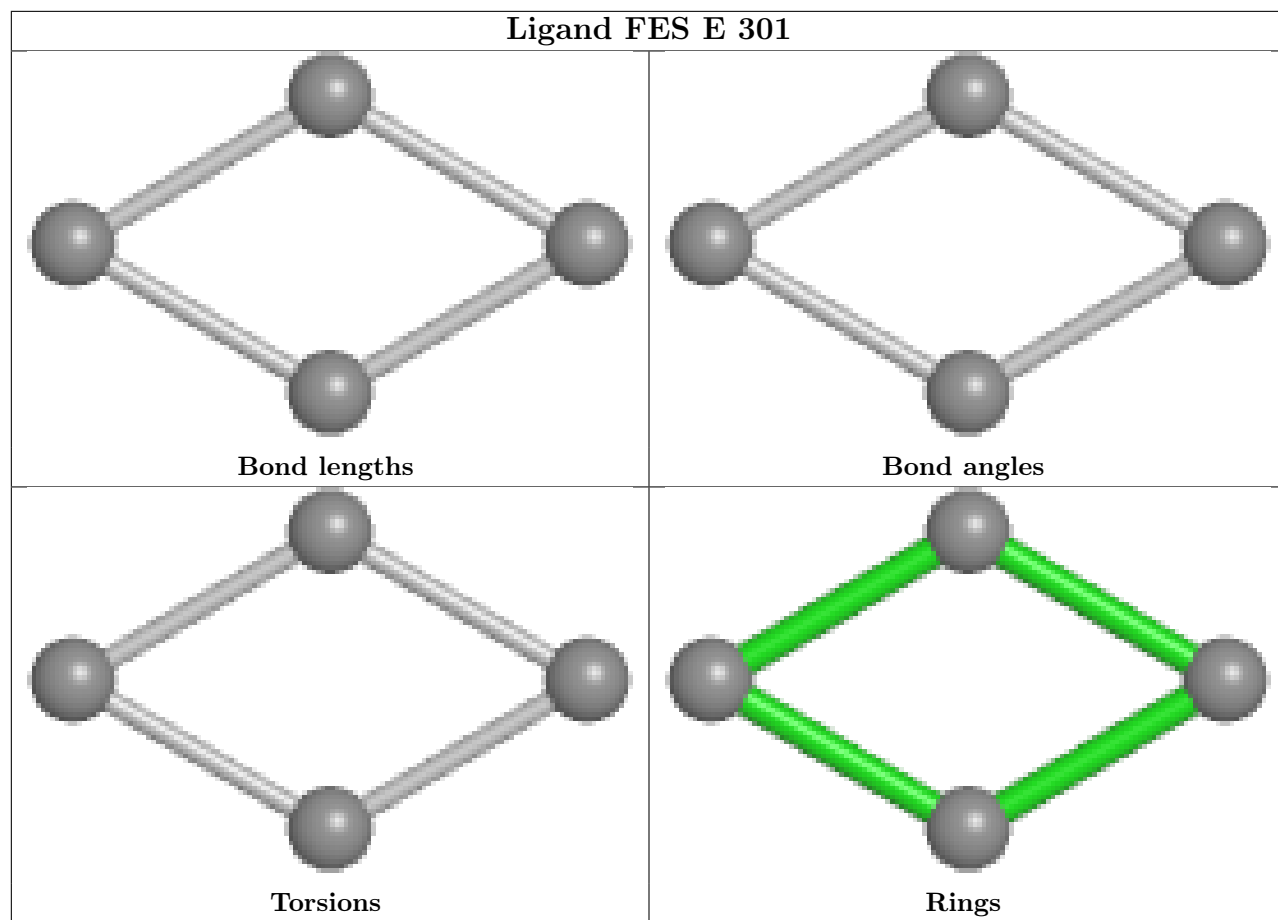
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

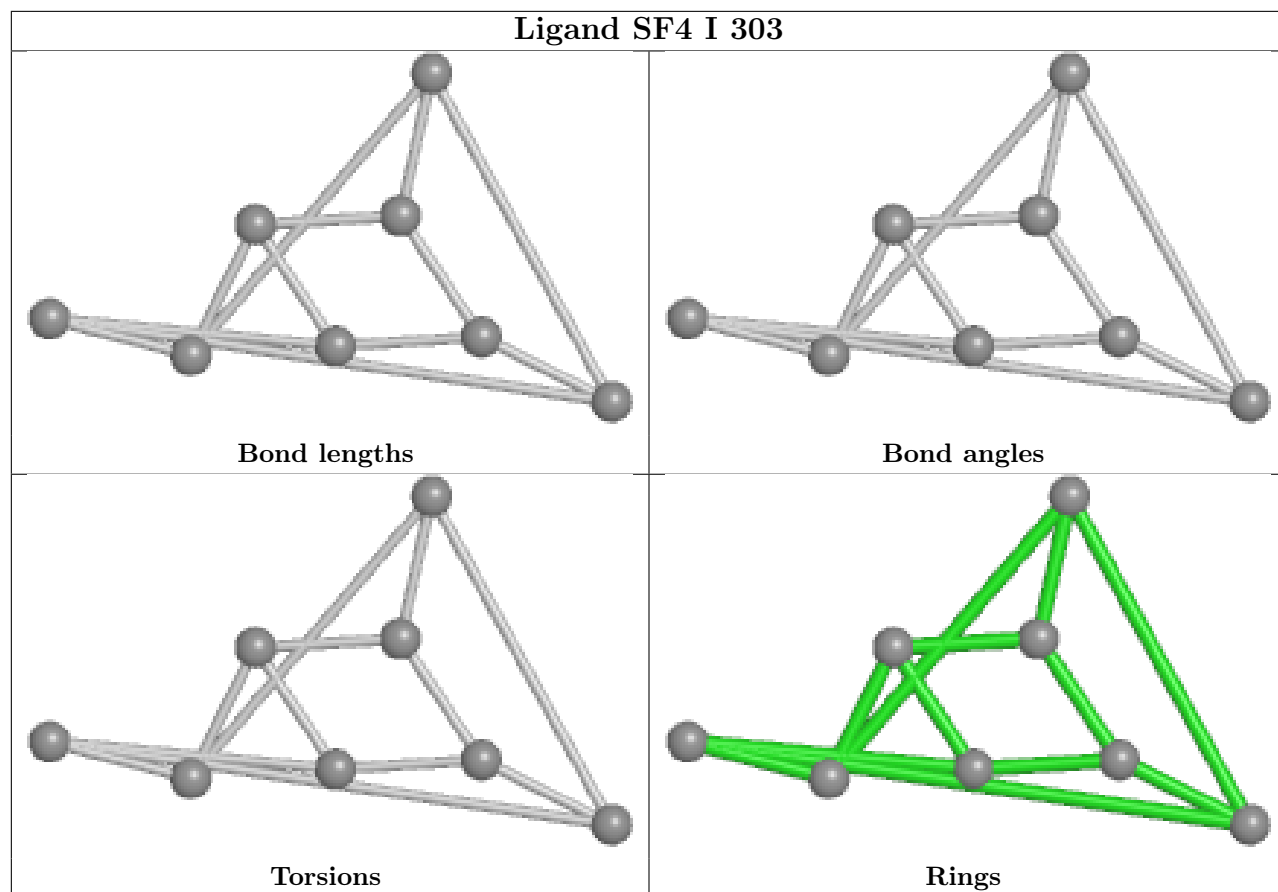


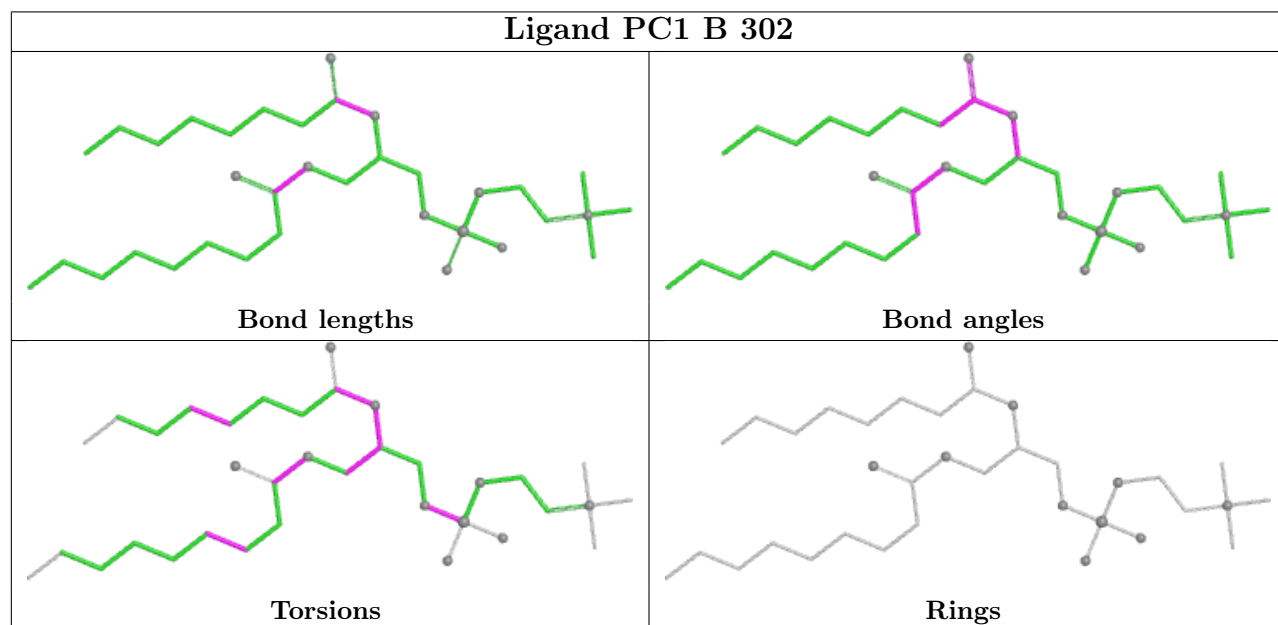
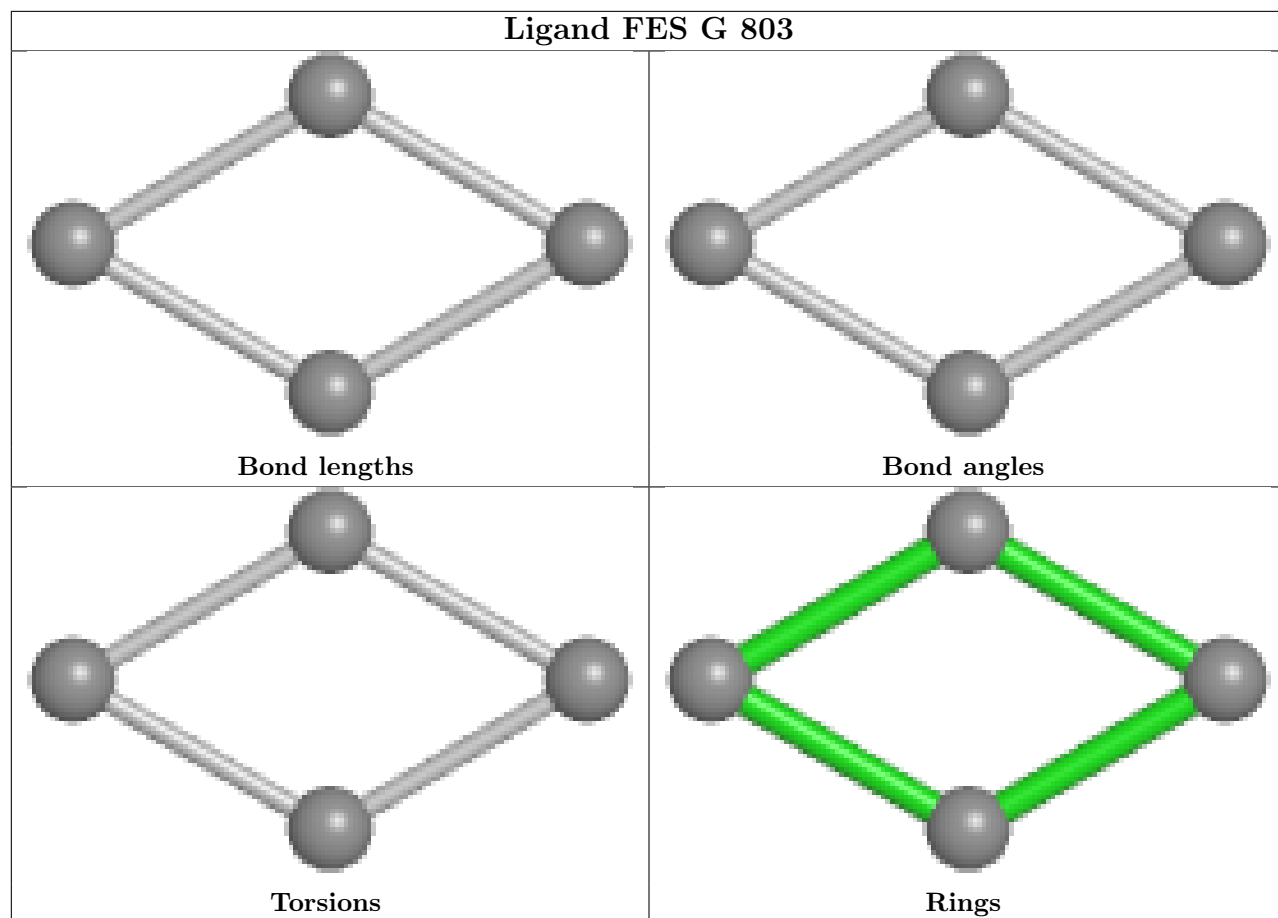


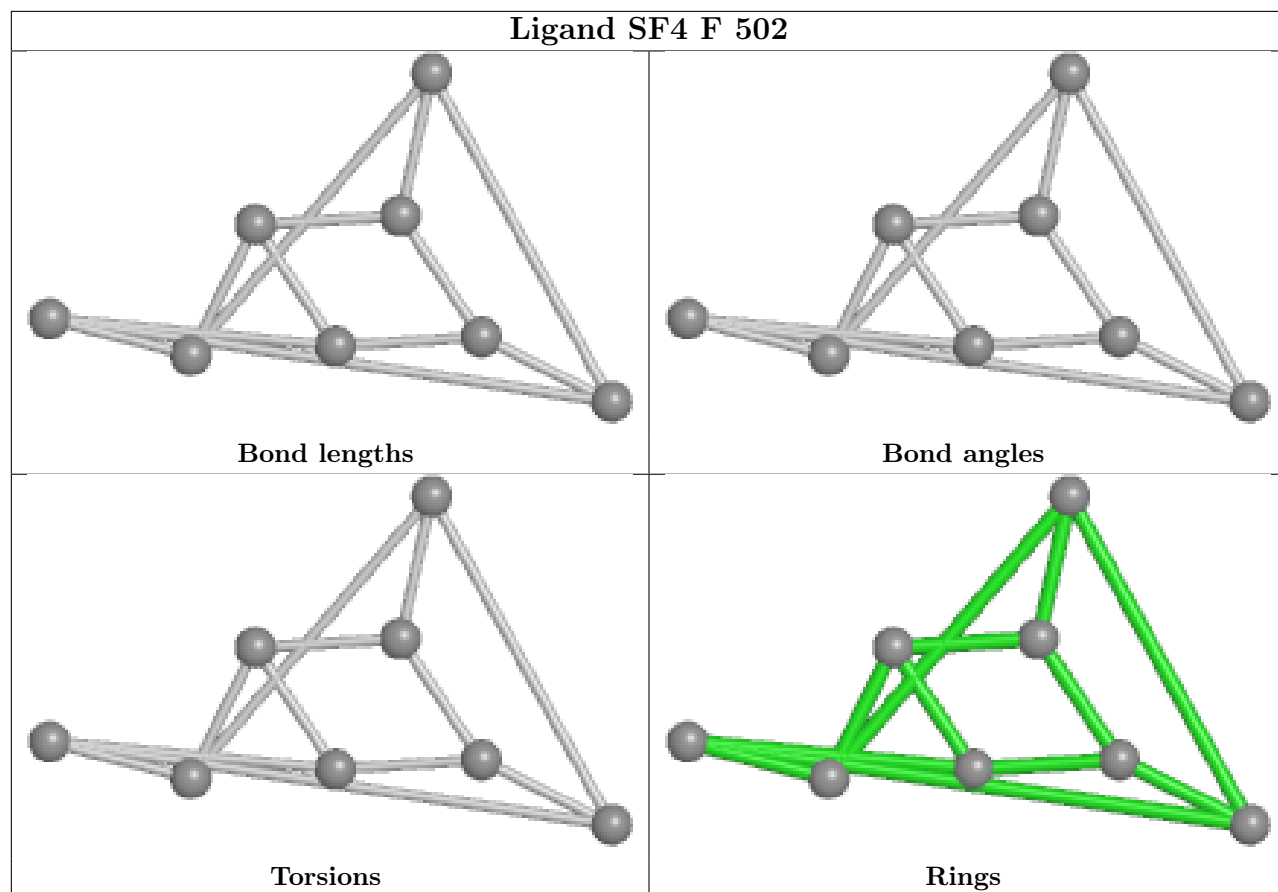


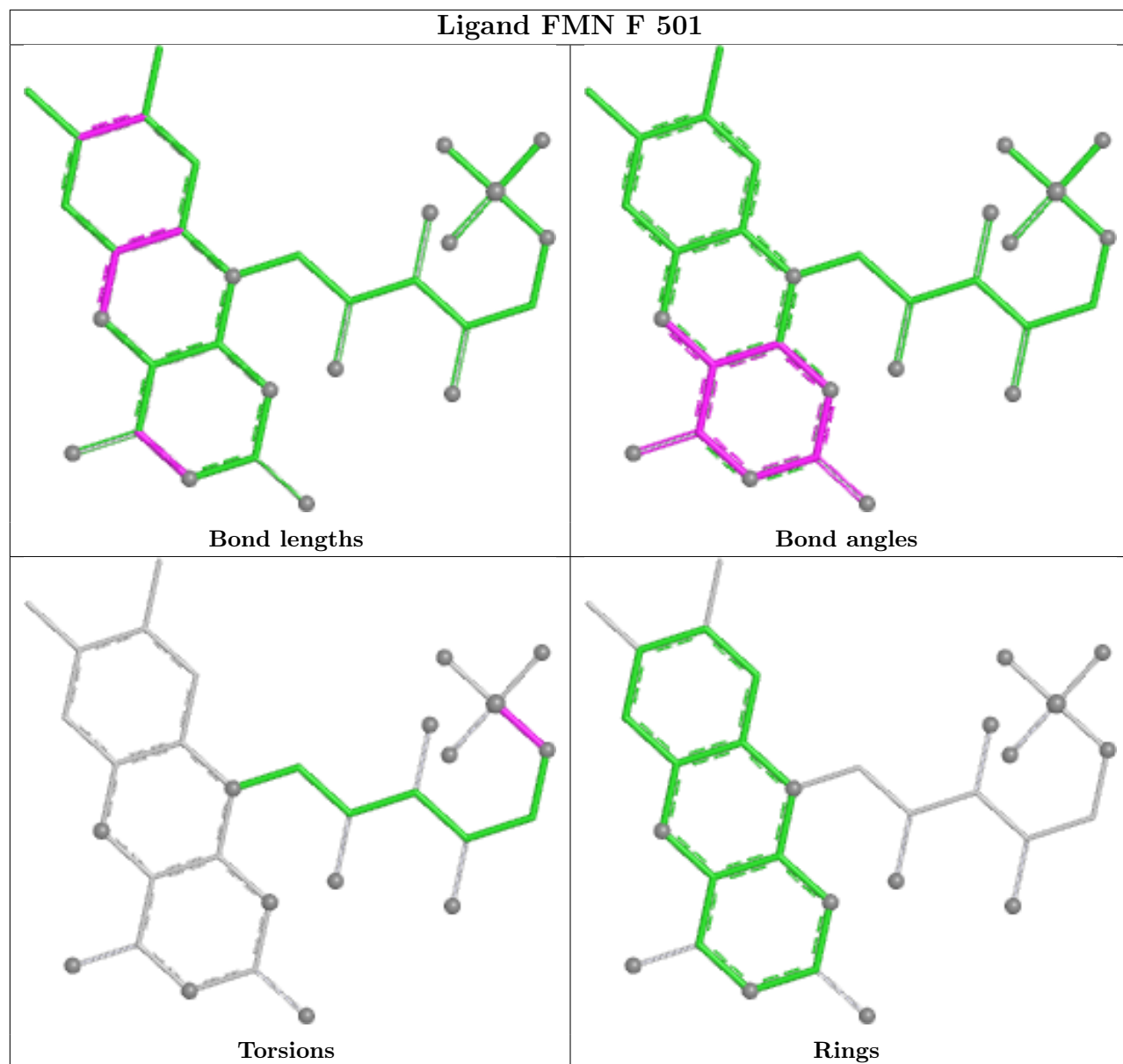


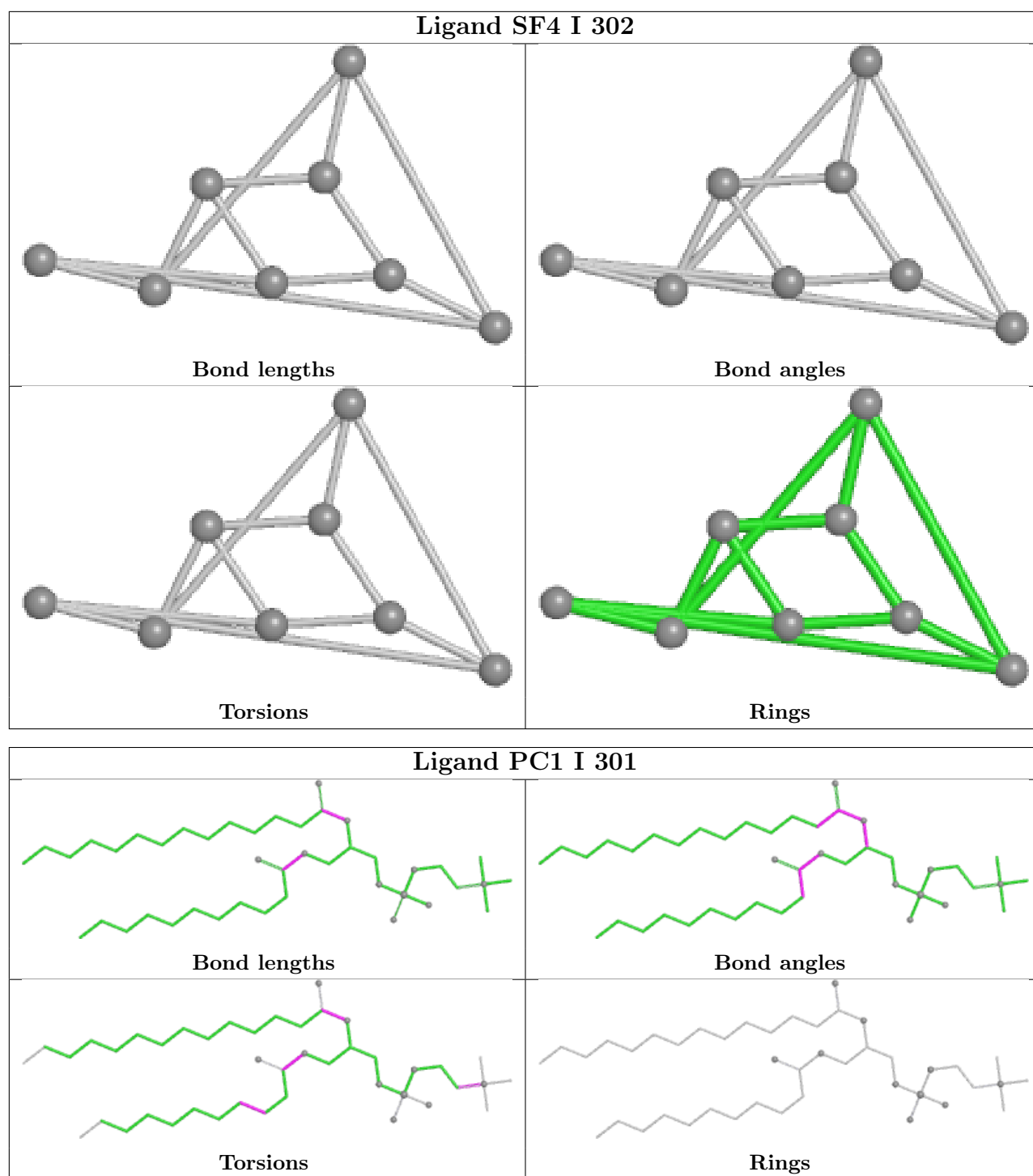












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

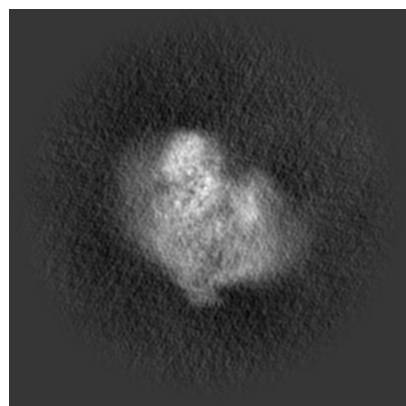
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38521. These allow visual inspection of the internal detail of the map and identification of artifacts.

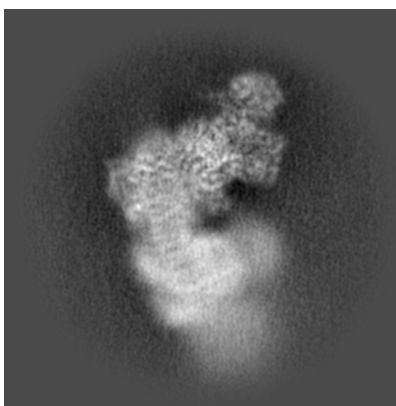
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

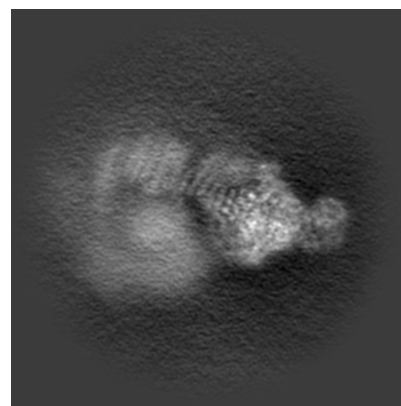
6.1.1 Primary map



X

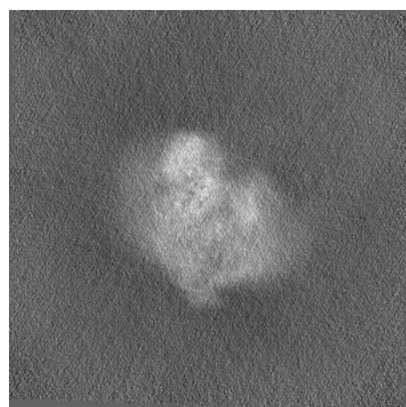


Y

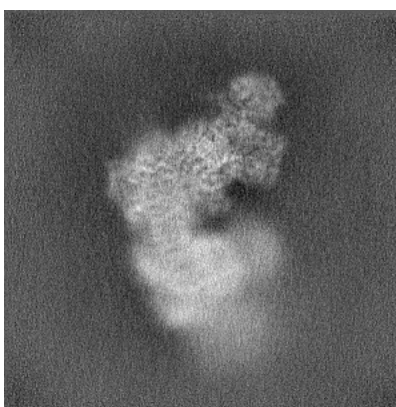


Z

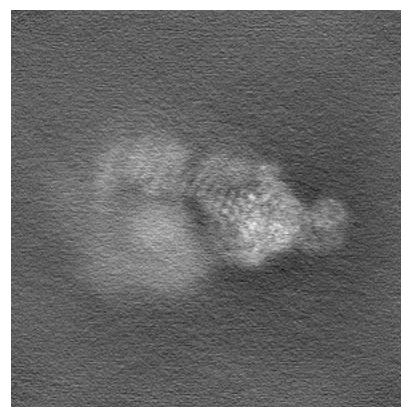
6.1.2 Raw map



X



Y

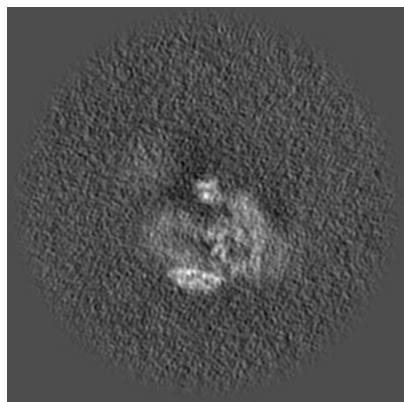


Z

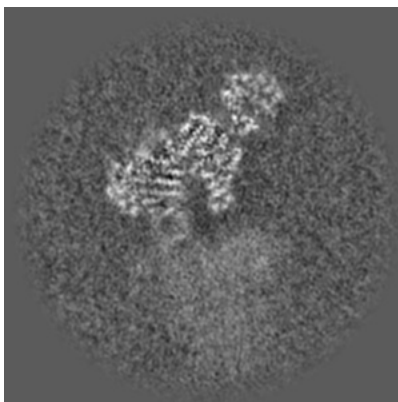
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

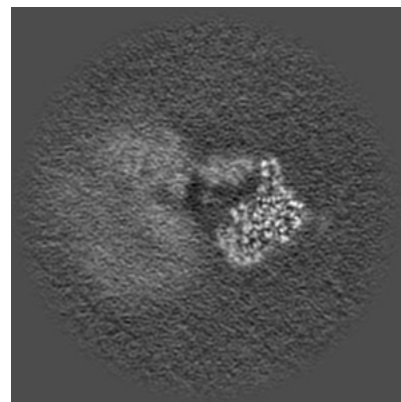
6.2.1 Primary map



X Index: 256

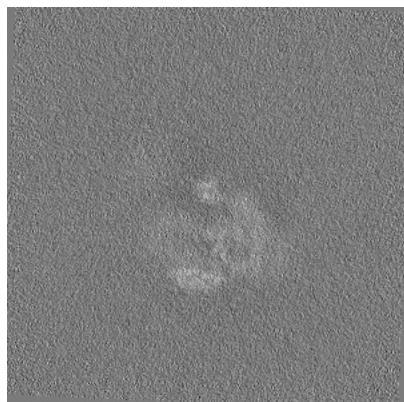


Y Index: 256

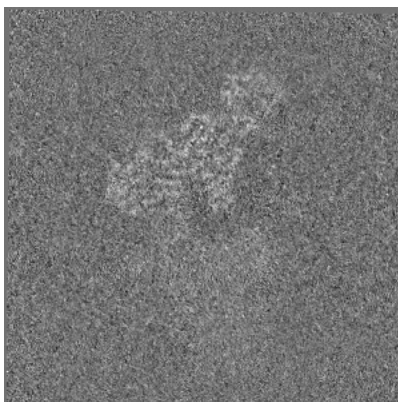


Z Index: 256

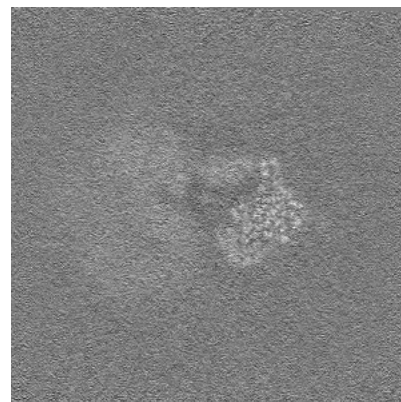
6.2.2 Raw map



X Index: 256



Y Index: 256

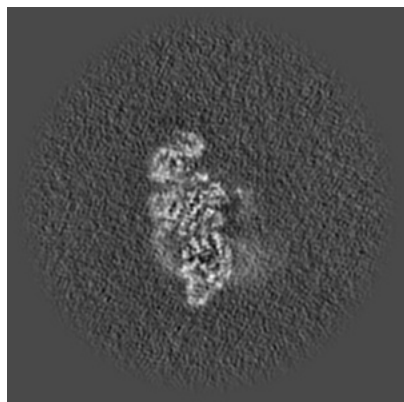


Z Index: 256

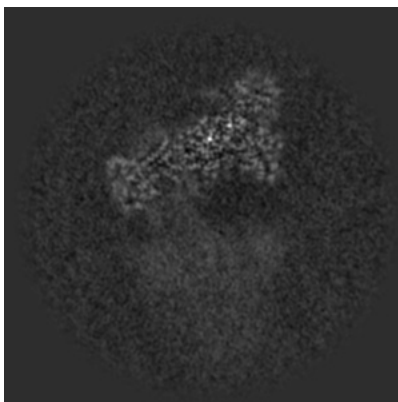
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

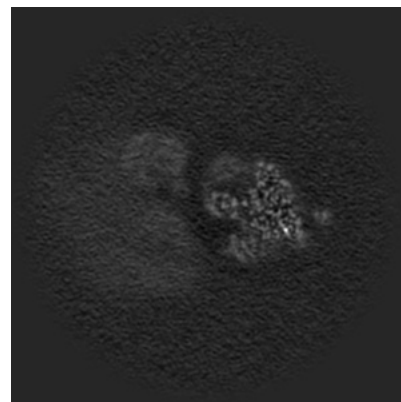
6.3.1 Primary map



X Index: 311

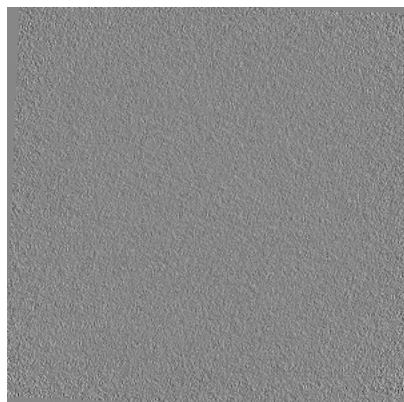


Y Index: 234

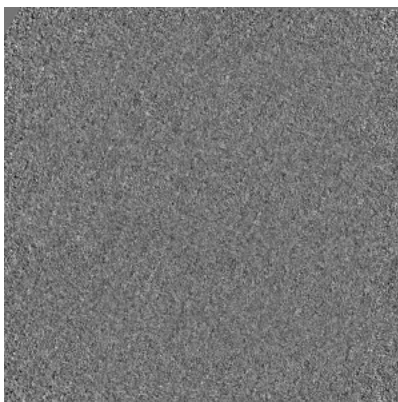


Z Index: 272

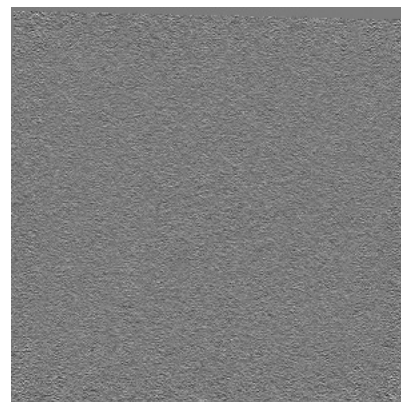
6.3.2 Raw map



X Index: 3



Y Index: 495

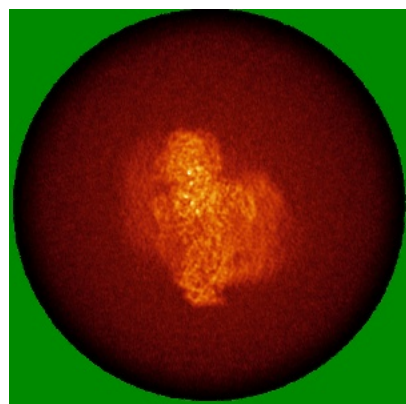


Z Index: 18

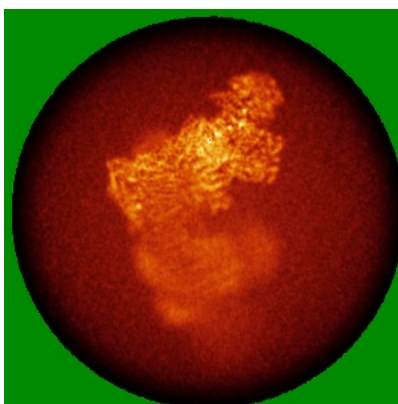
The images above show the largest variance slices of the map in three orthogonal directions.

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

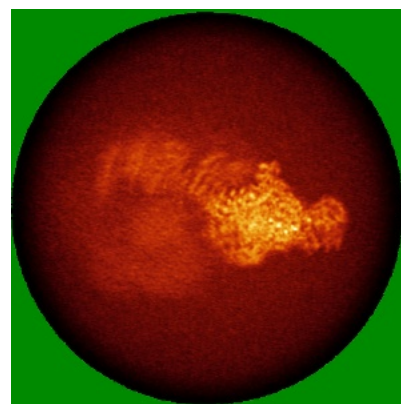
6.4.1 Primary map



X

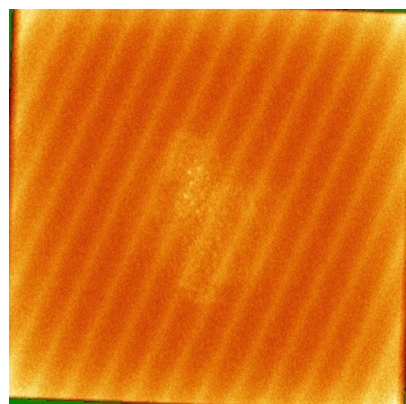


Y

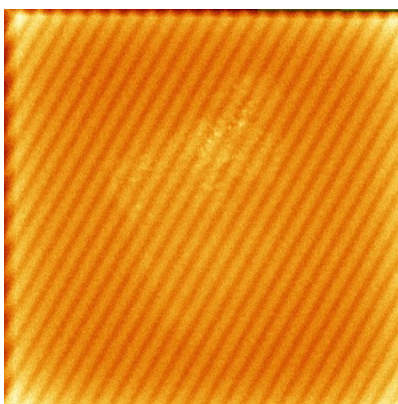


Z

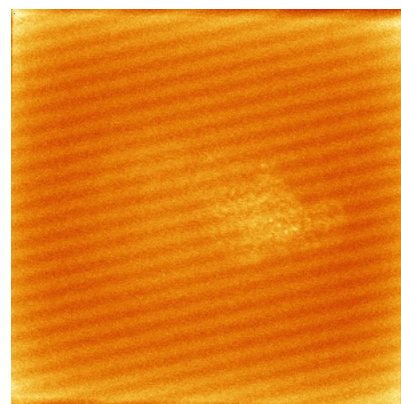
6.4.2 Raw map



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 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

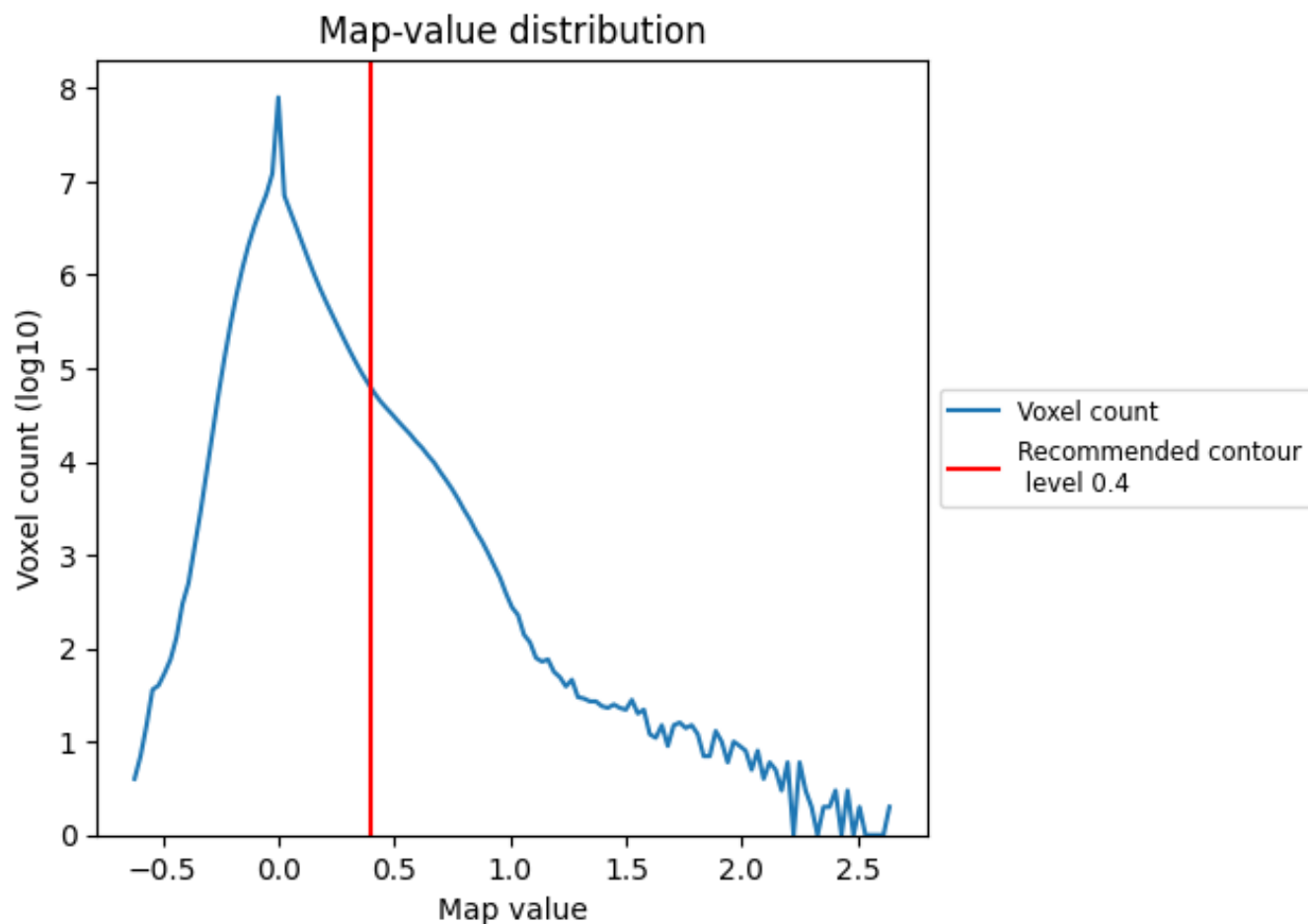
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

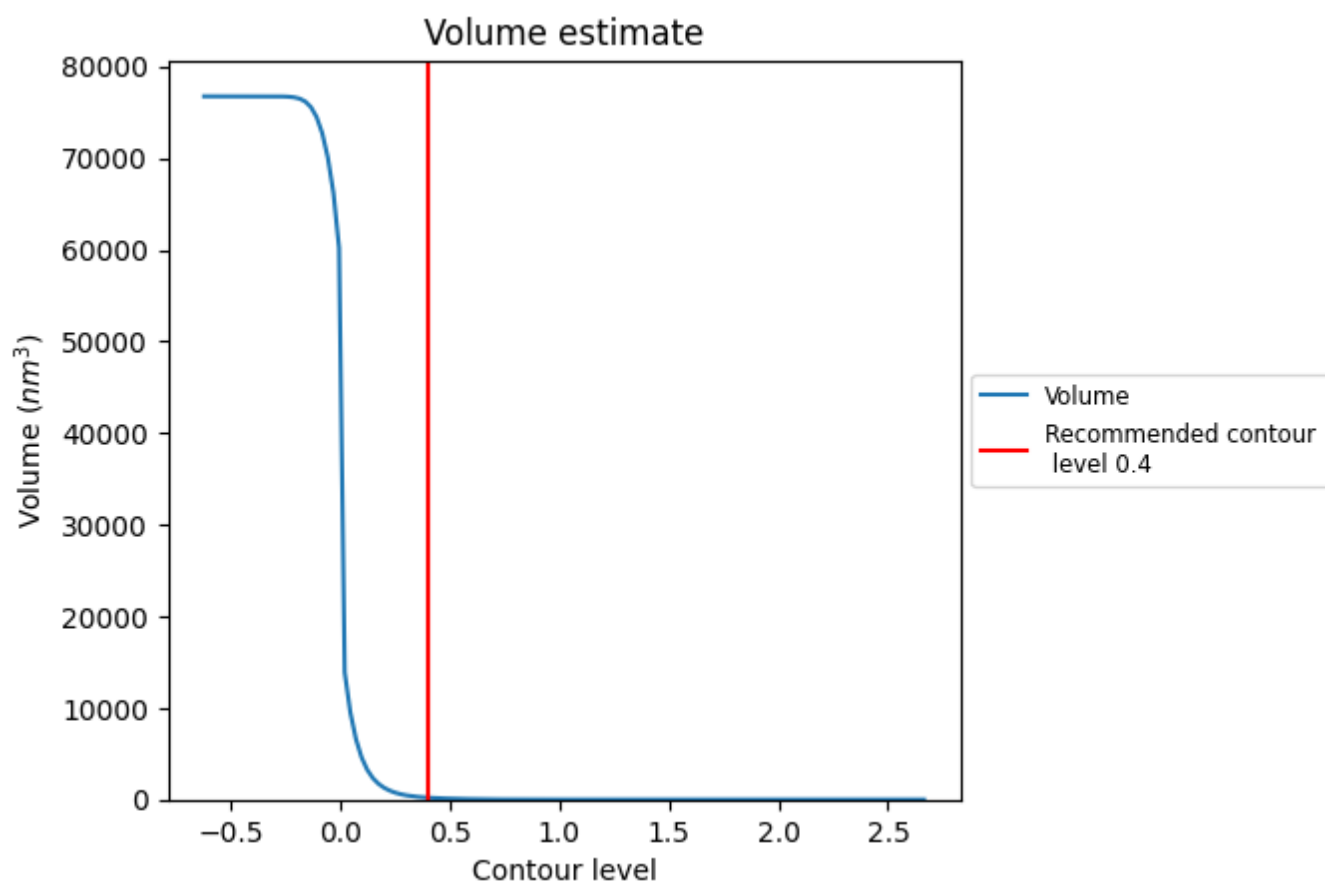
This section contains the results of statistical analysis of the map.

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.

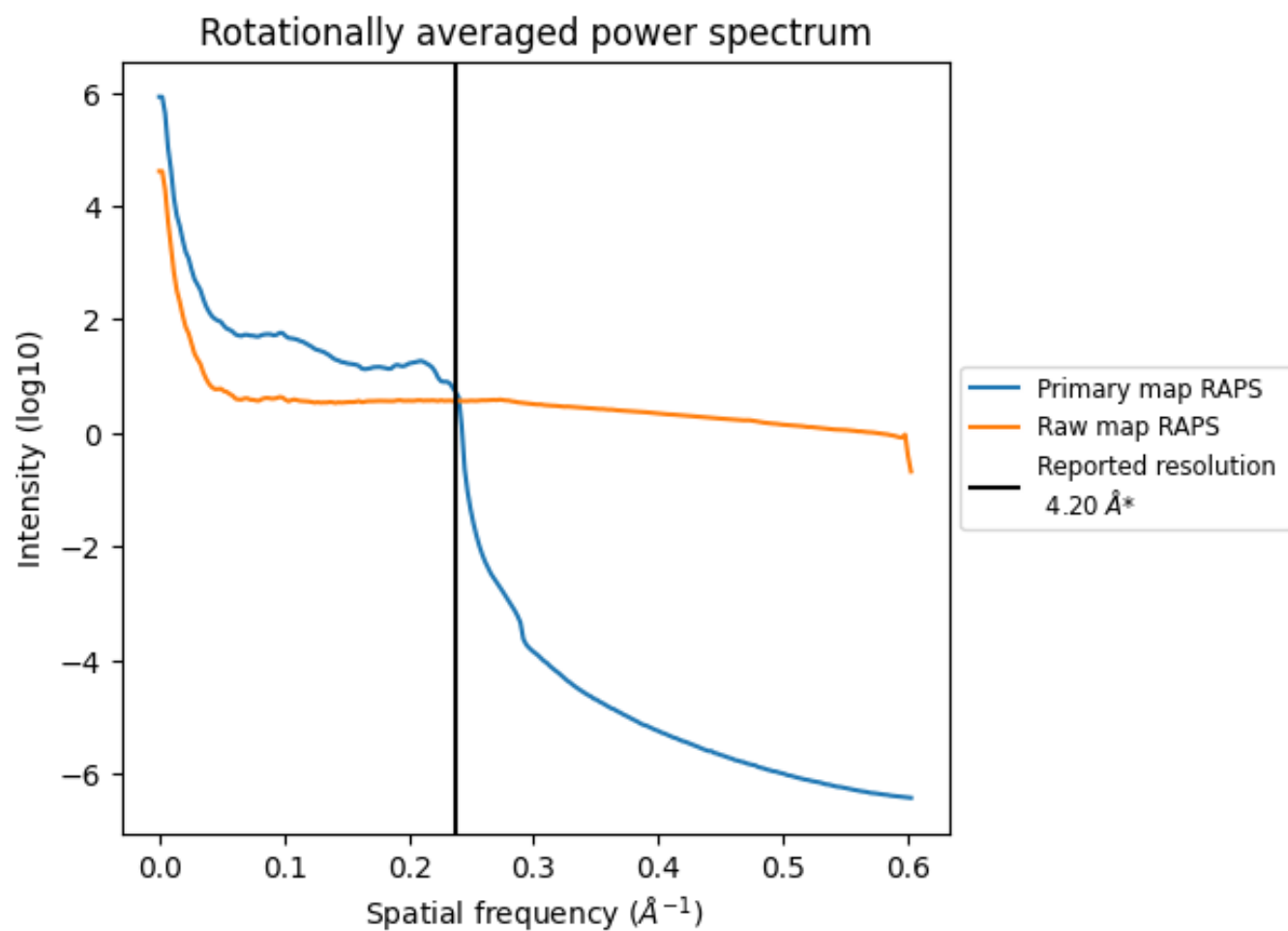
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 205 nm^3 ; this corresponds to an approximate mass of 185 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 ⓘ

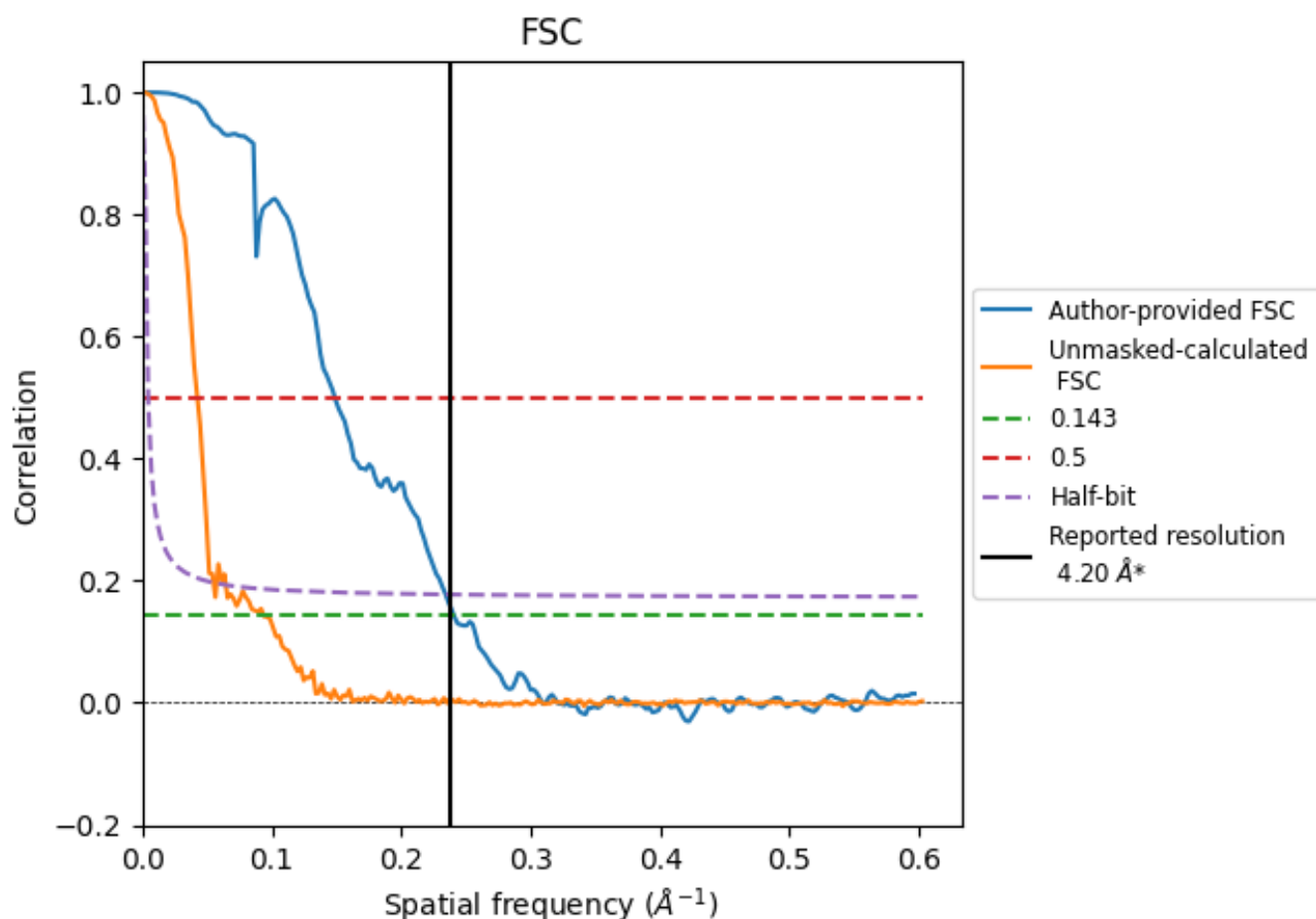


*Reported resolution corresponds to spatial frequency of 0.238 $\text{\AA}^{-1}$

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 0.238 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.15	6.72	4.27
Unmasked-calculated*	10.65	23.47	18.18

*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 10.65 differs from the reported value 4.2 by more than 10 %

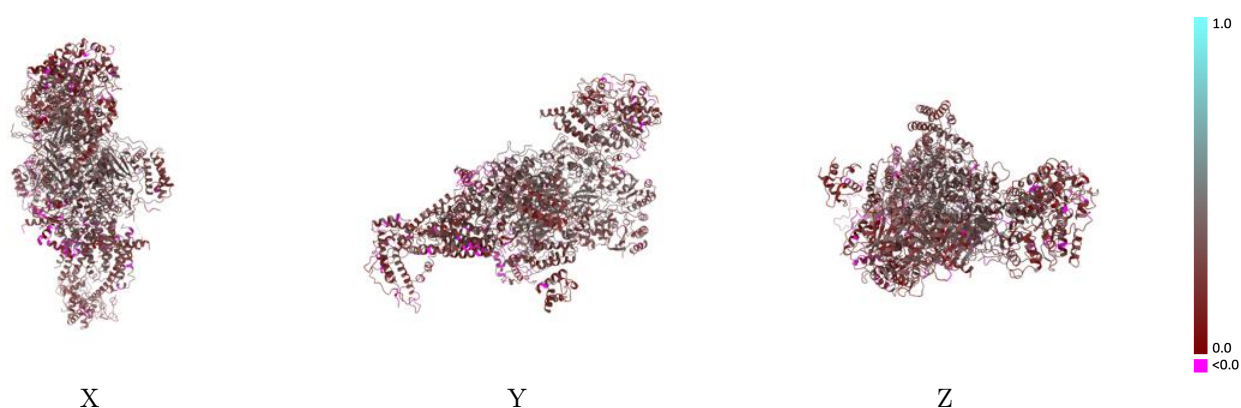
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-38521 and PDB model 8XO0. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)

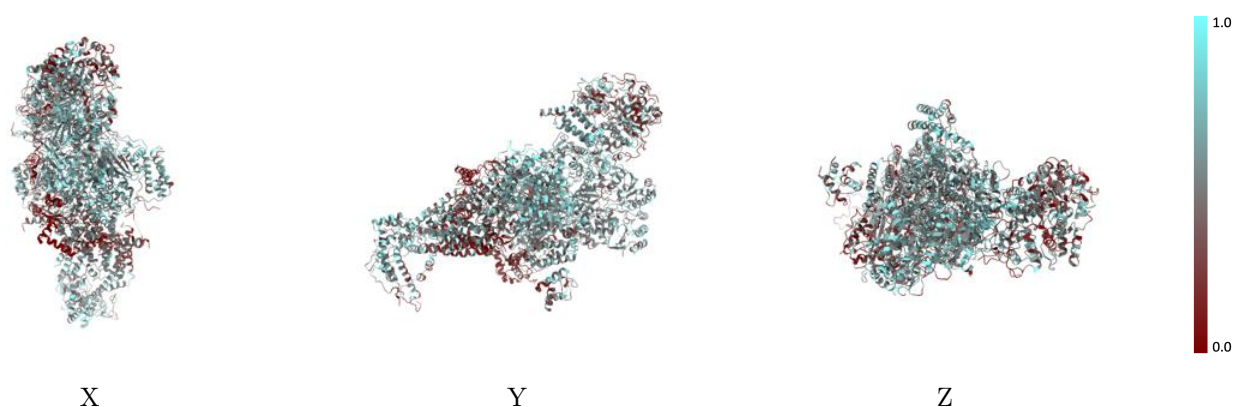
This section was not generated.

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



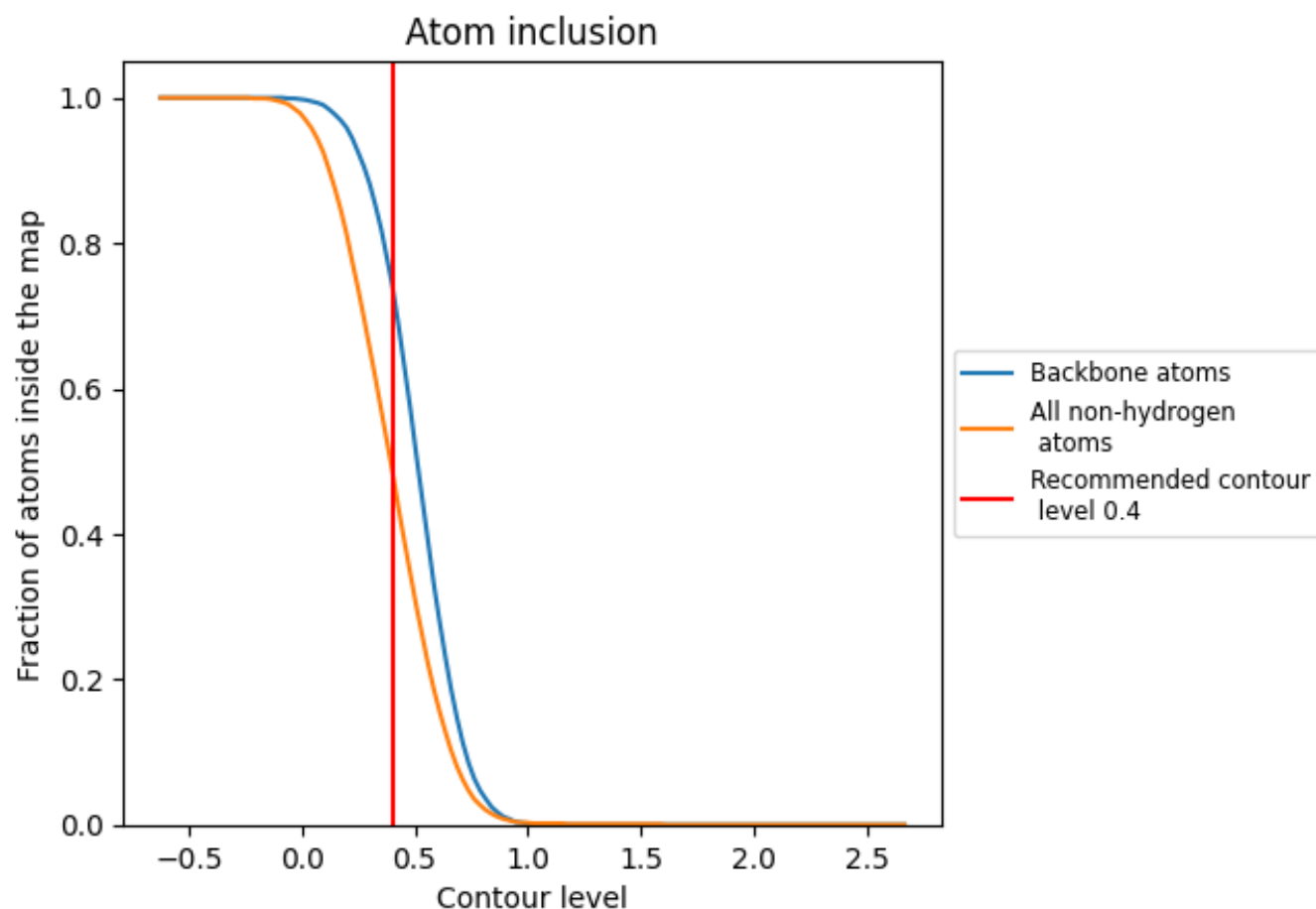
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 49% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4890	 0.2590
A	 0.3740	 0.1970
B	 0.5780	 0.3090
C	 0.5990	 0.3290
D	 0.5900	 0.3300
E	 0.4370	 0.2310
F	 0.4840	 0.2510
G	 0.5620	 0.2930
H	 0.4610	 0.2800
I	 0.6190	 0.3180
P	 0.3660	 0.2040
Q	 0.4320	 0.3000
R	 0.2740	 0.2010
S	 0.5560	 0.2570
T	 0.4470	 0.1740
V	 0.5710	 0.2460
W	 0.5250	 0.2630
X	 0.5420	 0.1810
Z	 0.5350	 0.2170
a	 0.5690	 0.2540
b	 0.4750	 0.2130
q	 0.0630	 0.1260
r	 0.1950	 0.1580
s	 0.1120	 0.1380

