Full wwPDB EM Validation Report ⓘ

Apr 20, 2024 – 01:15 PM EDT

PDB ID	:	8VAN
EMDB ID	:	EMD-43096
Title	:	Structure of the E. coli clamp loader bound to the beta clamp in an Initial-Binding conformation
Authors	:	Landeck, J.T.; Pajak, J.; Kelch, B.A.
Deposited on	:	2023-12-11
Resolution	:	7.70 Å(reported)
Based on initial models	:	3GLF, 2POL

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:

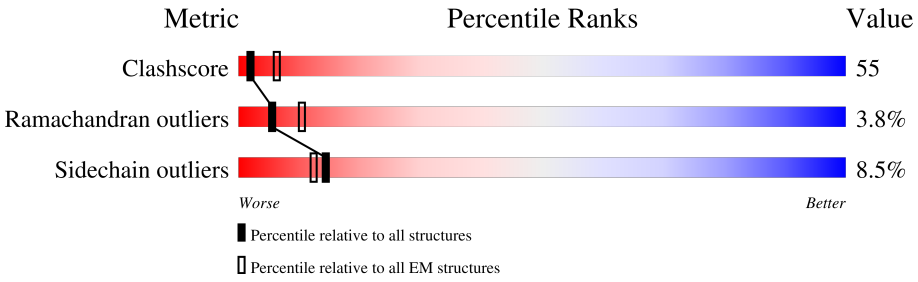
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 7.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	343	37% 42% 17% 5%
2	B	376	14% 49% 35% 10%
2	C	376	15% 44% 41% 11%
2	D	376	24% 50% 17% 5%
3	E	337	26% 44% 23% 7%
4	F	369	21% 43% 28% 7%
4	G	369	22% 44% 29%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19433 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 DNA polymerase III subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	343	Total	C	N	O	S	0	0
			2726	1728	493	495	10		

- Molecule 2 is a protein called DNA polymerase III subunit tau.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	360	Total	C	N	O	S	0	0
			2796	1757	505	518	16		
2	C	365	Total	C	N	O	S	0	0
			2835	1783	513	523	16		
2	D	359	Total	C	N	O	S	0	0
			2786	1752	503	516	15		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP P06710
B	-1	PRO	-	expression tag	UNP P06710
B	0	HIS	-	expression tag	UNP P06710
C	-2	GLY	-	expression tag	UNP P06710
C	-1	PRO	-	expression tag	UNP P06710
C	0	HIS	-	expression tag	UNP P06710
D	-2	GLY	-	expression tag	UNP P06710
D	-1	PRO	-	expression tag	UNP P06710
D	0	HIS	-	expression tag	UNP P06710

- Molecule 3 is a protein called DNA polymerase III subunit delta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	334	Total	C	N	O	S	0	0
			2602	1655	468	466	13		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	expression tag	UNP P28631
E	-1	PRO	-	expression tag	UNP P28631
E	0	HIS	-	expression tag	UNP P28631

- Molecule 4 is a protein called Beta sliding clamp.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	366	Total	C	N	O	S	0	0
			2844	1786	498	541	19		
4	G	366	Total	C	N	O	S	0	0
			2844	1786	498	541	19		

There are 6 discrepancies between the modelled and reference sequences:

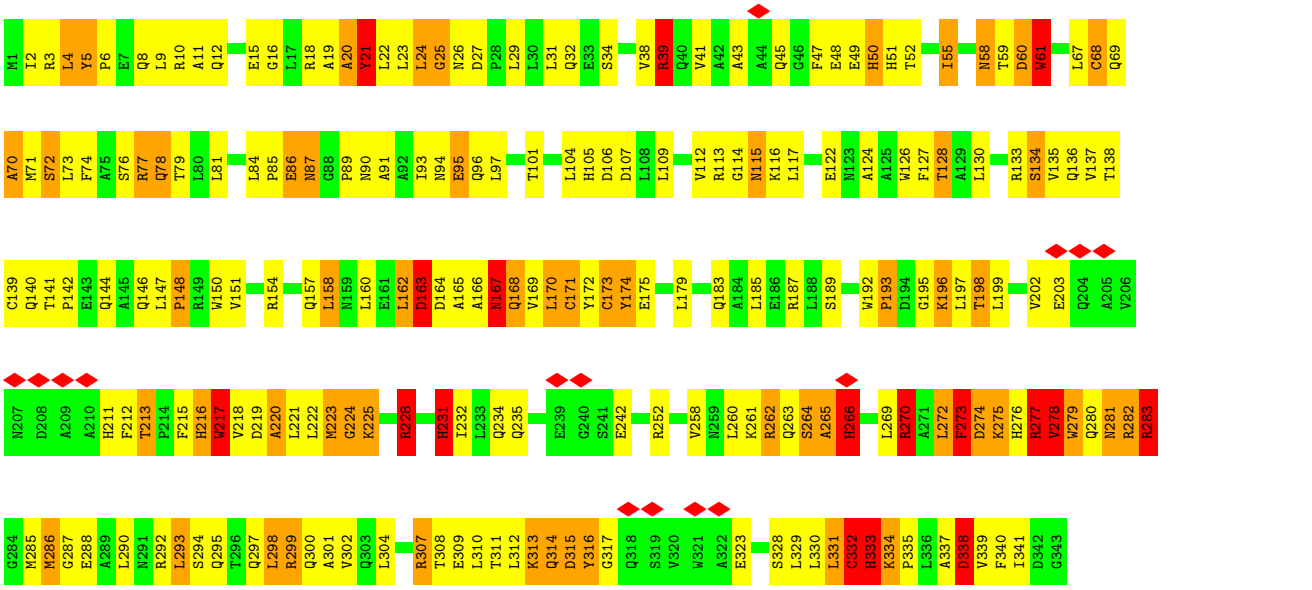
Chain	Residue	Modelled	Actual	Comment	Reference
F	-2	GLY	-	expression tag	UNP C3SLM2
F	-1	PRO	-	expression tag	UNP C3SLM2
F	0	HIS	-	expression tag	UNP C3SLM2
G	-2	GLY	-	expression tag	UNP C3SLM2
G	-1	PRO	-	expression tag	UNP C3SLM2
G	0	HIS	-	expression tag	UNP C3SLM2

3 Residue-property plots (i)

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

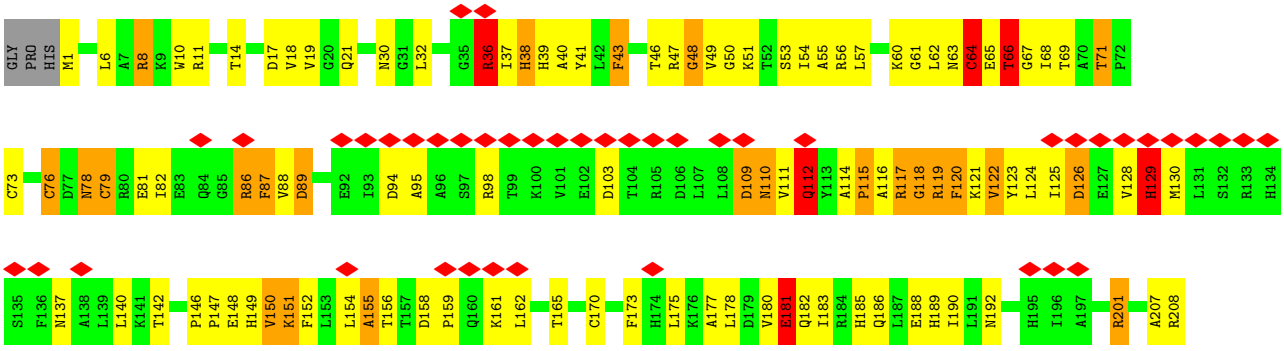
• Molecule 1: DNA polymerase III subunit delta

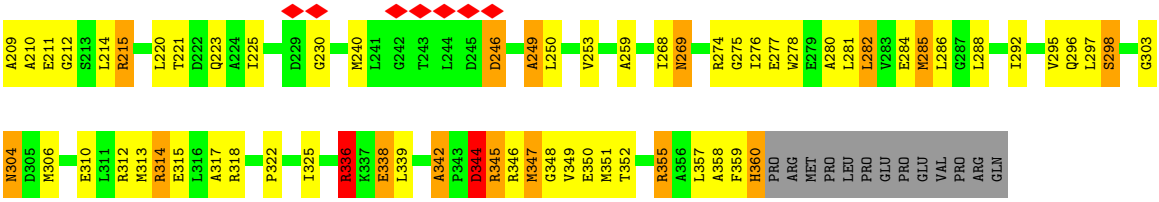
Chain A:

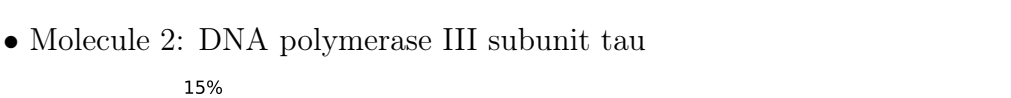


• Molecule 2: DNA polymerase III subunit tau

Chain B:

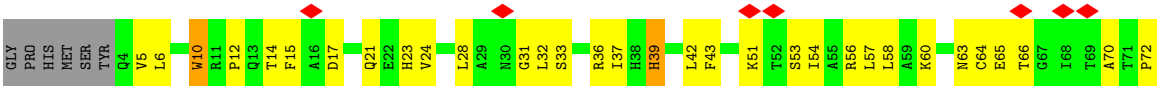


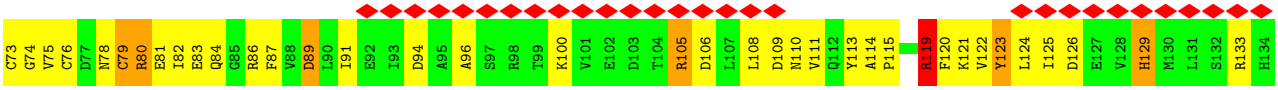


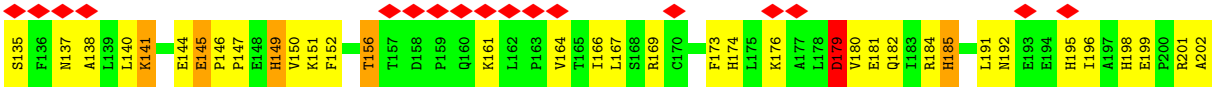


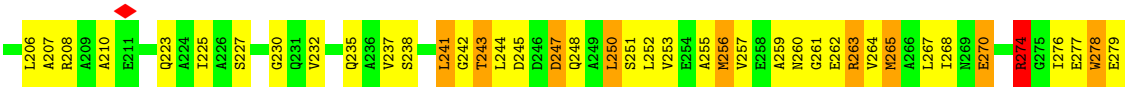
• Molecule 2: DNA polymerase III subunit tau

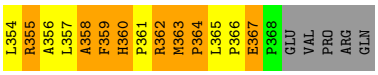
Chain C:





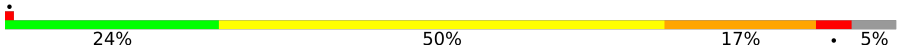


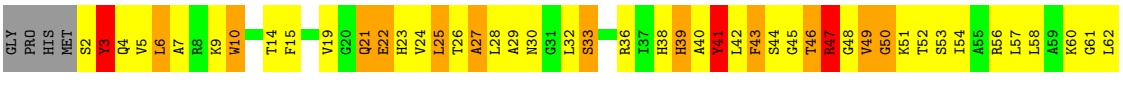


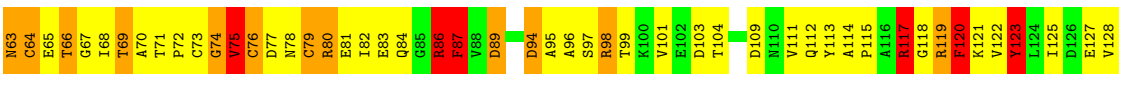


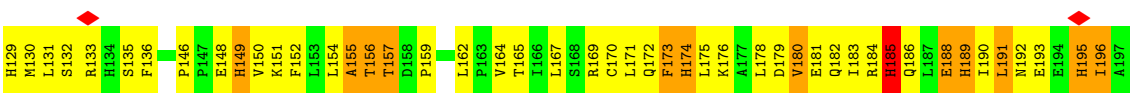
• Molecule 2: DNA polymerase III subunit tau

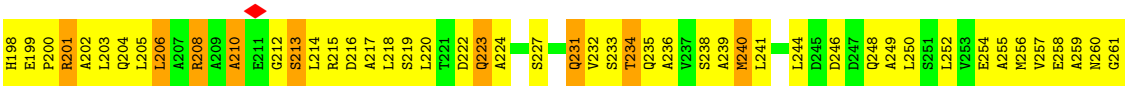
Chain D:

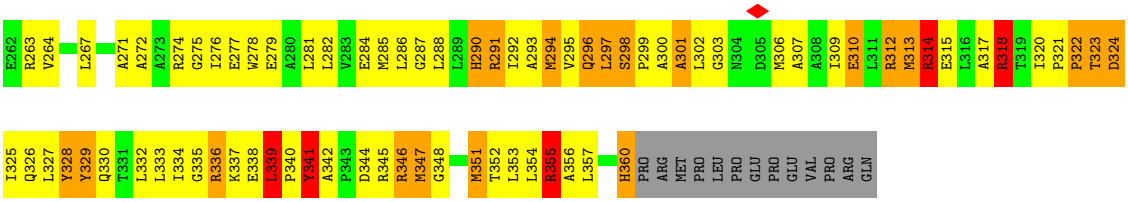






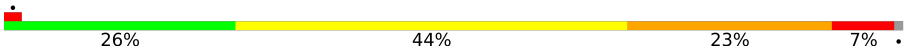


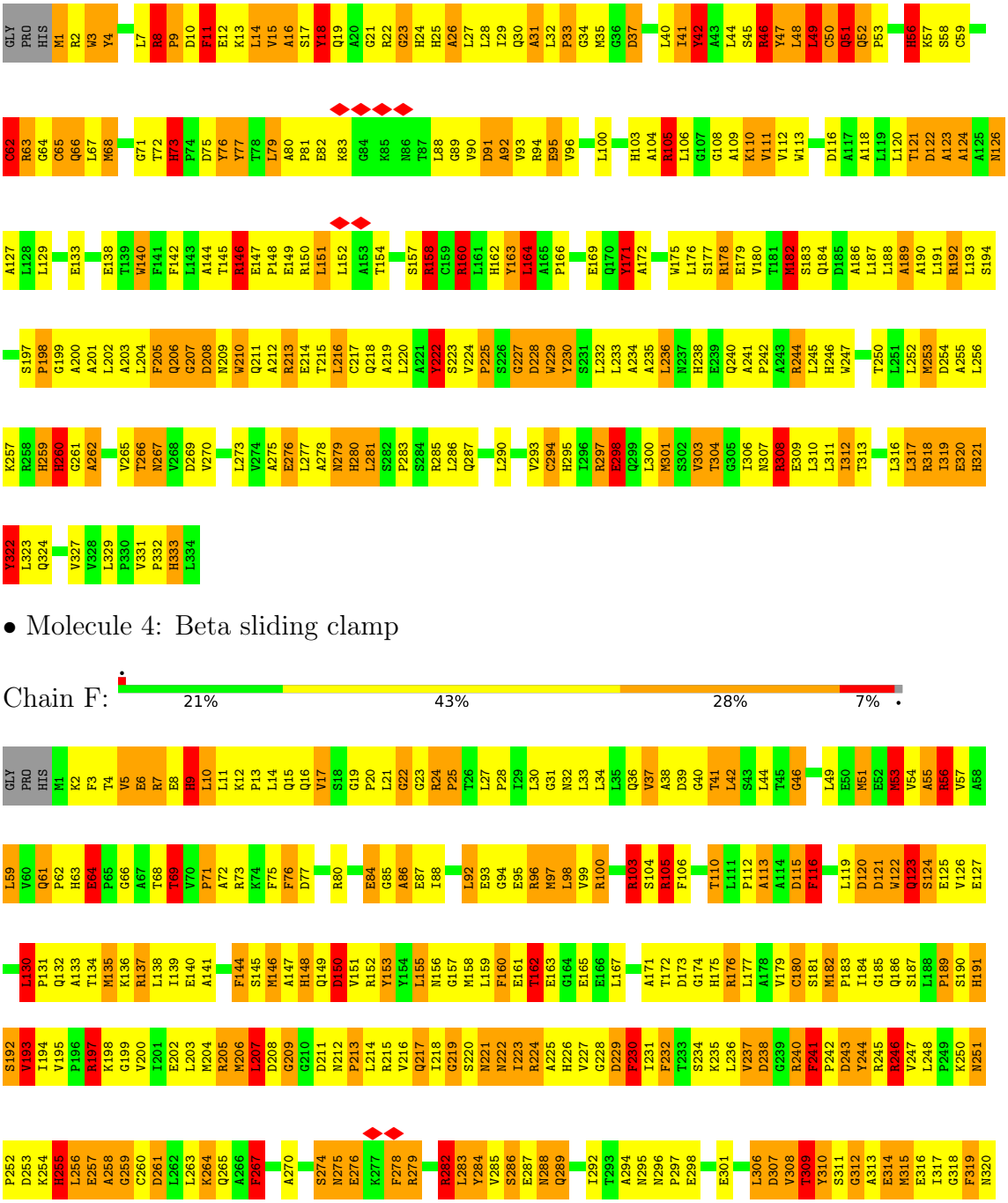




• Molecule 3: DNA polymerase III subunit delta'

Chain E:



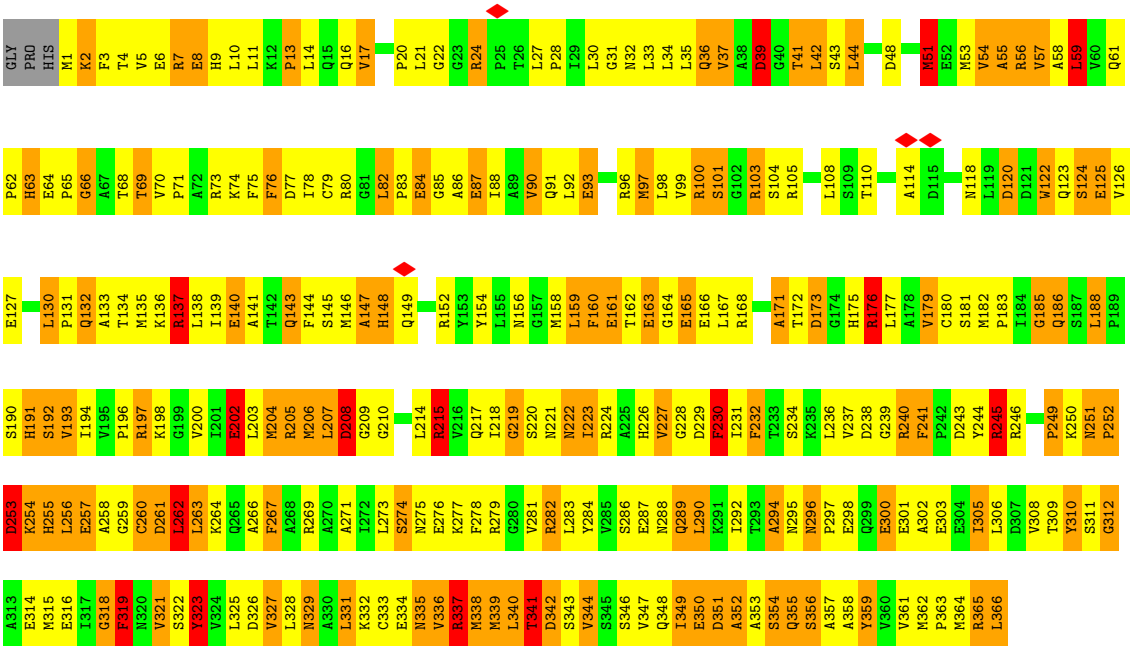


• Molecule 4: Beta sliding clamp

Chain F:

• Molecule 4: Beta sliding clamp

Chain G:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	44484	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	42.8	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.050	Depositor
Minimum map value	-0.238	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.084	Depositor
Recommended contour level	0.33	Depositor
Map size (Å)	261.0, 261.0, 261.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.87, 0.87, 0.87	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	1.61	17/2775 (0.6%)	1.92	89/3769 (2.4%)
2	B	1.38	7/2840 (0.2%)	1.70	61/3848 (1.6%)
2	C	1.45	8/2882 (0.3%)	1.77	55/3908 (1.4%)
2	D	1.63	17/2830 (0.6%)	2.00	89/3835 (2.3%)
3	E	1.72	35/2667 (1.3%)	2.14	119/3639 (3.3%)
4	F	1.92	55/2893 (1.9%)	2.28	161/3915 (4.1%)
4	G	1.83	40/2893 (1.4%)	2.16	136/3915 (3.5%)
All	All	1.66	179/19780 (0.9%)	2.01	710/26829 (2.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	16
2	B	0	9
2	C	0	8
2	D	0	12
3	E	0	16
4	F	0	14
4	G	0	8
All	All	0	83

All (179) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	64	CYS	CB-SG	-9.51	1.66	1.82
2	D	322	PRO	CA-C	-8.47	1.35	1.52
4	G	355	GLN	N-CA	-8.26	1.29	1.46
4	F	157	GLY	N-CA	-7.98	1.34	1.46
4	F	219	GLY	CA-C	-7.75	1.39	1.51
4	G	356	SER	N-CA	-7.75	1.30	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	267	PHE	CB-CG	-7.48	1.38	1.51
4	F	336	VAL	N-CA	-7.27	1.31	1.46
4	G	219	GLY	CA-C	-7.17	1.40	1.51
2	B	76	CYS	CB-SG	-7.02	1.70	1.82
4	F	122	TRP	CA-C	-7.00	1.34	1.52
2	C	341	TYR	CB-CG	-7.00	1.41	1.51
4	G	185	GLY	CA-C	-6.93	1.40	1.51
2	C	364	PRO	CA-C	-6.87	1.39	1.52
3	E	50	CYS	CB-SG	-6.82	1.70	1.82
4	F	42	LEU	N-CA	-6.78	1.32	1.46
3	E	73	HIS	N-CA	-6.75	1.32	1.46
3	E	76	TYR	CB-CG	-6.73	1.41	1.51
4	G	222	ASN	N-CA	-6.71	1.32	1.46
4	F	257	GLU	CA-C	-6.70	1.35	1.52
4	F	312	GLY	CA-C	-6.64	1.41	1.51
3	E	229	TRP	NE1-CE2	-6.61	1.28	1.37
4	F	10	LEU	N-CA	-6.57	1.33	1.46
4	G	350	GLU	N-CA	-6.51	1.33	1.46
4	F	223	ILE	N-CA	-6.50	1.33	1.46
4	G	336	VAL	N-CA	-6.45	1.33	1.46
1	A	313	LYS	CA-C	-6.44	1.36	1.52
4	F	55	ALA	CA-CB	-6.42	1.39	1.52
4	G	354	SER	CA-C	-6.42	1.36	1.52
3	E	281	LEU	N-CA	-6.39	1.33	1.46
4	G	290	LEU	N-CA	-6.34	1.33	1.46
2	D	323	THR	N-CA	-6.32	1.33	1.46
2	D	79	CYS	CB-SG	-6.30	1.71	1.82
4	G	262	LEU	CA-C	-6.28	1.36	1.52
2	D	66	THR	N-CA	-6.28	1.33	1.46
4	F	222	ASN	CA-C	-6.27	1.36	1.52
3	E	230	TYR	CB-CG	-6.27	1.42	1.51
4	G	36	GLN	N-CA	-6.27	1.33	1.46
4	G	219	GLY	N-CA	-6.24	1.36	1.46
4	F	123	GLN	N-CA	-6.24	1.33	1.46
2	C	367	GLU	N-CA	-6.19	1.33	1.46
3	E	280	HIS	CA-C	-6.19	1.36	1.52
4	F	308	VAL	N-CA	-6.15	1.34	1.46
4	F	146	MET	CA-C	-6.11	1.37	1.52
4	F	259	GLY	CA-C	-6.11	1.42	1.51
4	G	249	PRO	CA-C	-6.10	1.40	1.52
4	G	318	GLY	CA-C	-6.06	1.42	1.51
4	F	337	ARG	CA-CB	-6.01	1.40	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	337	ARG	N-CA	-6.01	1.34	1.46
4	F	122	TRP	N-CA	-6.00	1.34	1.46
4	F	56	ARG	CA-C	-6.00	1.37	1.52
3	E	73	HIS	CB-CG	-6.00	1.39	1.50
4	F	221	ASN	CA-C	-5.99	1.37	1.52
3	E	320	GLU	N-CA	-5.98	1.34	1.46
3	E	208	ASP	CA-C	-5.96	1.37	1.52
4	G	193	VAL	N-CA	-5.93	1.34	1.46
4	F	337	ARG	N-CA	-5.92	1.34	1.46
1	A	282	ARG	CA-C	-5.91	1.37	1.52
4	F	222	ASN	N-CA	-5.91	1.34	1.46
4	G	167	LEU	N-CA	-5.90	1.34	1.46
4	F	124	SER	N-CA	-5.90	1.34	1.46
4	F	288	ASN	N-CA	-5.90	1.34	1.46
4	G	223	ILE	N-CA	-5.89	1.34	1.46
1	A	286	MET	N-CA	-5.88	1.34	1.46
2	B	345	ARG	N-CA	-5.86	1.34	1.46
4	F	338	MET	CA-C	-5.83	1.37	1.52
3	E	76	TYR	N-CA	-5.82	1.34	1.46
4	G	338	MET	CA-C	-5.79	1.37	1.52
4	F	189	PRO	CA-C	-5.78	1.41	1.52
2	D	25	LEU	CA-C	-5.78	1.38	1.52
3	E	319	ILE	CA-C	-5.77	1.38	1.52
4	F	22	GLY	CA-C	-5.74	1.42	1.51
4	G	312	GLY	N-CA	-5.74	1.37	1.46
3	E	229	TRP	CA-C	-5.72	1.38	1.52
4	G	355	GLN	CA-C	-5.71	1.38	1.52
3	E	18	TYR	CA-C	-5.70	1.38	1.52
4	F	340	LEU	CA-C	-5.70	1.38	1.52
2	C	79	CYS	CB-SG	-5.69	1.72	1.81
4	F	25	PRO	CA-C	-5.67	1.41	1.52
4	F	337	ARG	CA-C	-5.67	1.38	1.52
4	G	134	THR	CA-C	-5.66	1.38	1.52
4	G	55	ALA	N-CA	-5.66	1.35	1.46
1	A	25	GLY	CA-C	-5.66	1.42	1.51
4	G	231	ILE	N-CA	-5.65	1.35	1.46
4	G	349	ILE	CA-C	-5.64	1.38	1.52
4	F	230	PHE	N-CA	-5.63	1.35	1.46
3	E	279	ASN	N-CA	-5.63	1.35	1.46
4	G	42	LEU	N-CA	-5.62	1.35	1.46
4	G	230	PHE	CA-C	-5.62	1.38	1.52
4	F	181	SER	N-CA	-5.62	1.35	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	318	ARG	N-CA	-5.62	1.35	1.46
4	F	46	GLY	N-CA	-5.61	1.37	1.46
3	E	18	TYR	CB-CG	-5.59	1.43	1.51
4	F	124	SER	CA-CB	-5.59	1.44	1.52
2	C	366	PRO	CA-C	-5.57	1.41	1.52
1	A	312	LEU	N-CA	-5.57	1.35	1.46
4	F	329	ASN	N-CA	-5.53	1.35	1.46
4	F	349	ILE	CA-CB	-5.53	1.42	1.54
4	F	256	LEU	CA-C	-5.52	1.38	1.52
1	A	78	GLN	N-CA	-5.50	1.35	1.46
4	F	55	ALA	N-CA	-5.49	1.35	1.46
4	G	352	ALA	N-CA	-5.48	1.35	1.46
4	G	263	LEU	N-CA	-5.47	1.35	1.46
1	A	278	VAL	CA-C	-5.45	1.38	1.52
3	E	23	GLY	CA-C	-5.44	1.43	1.51
2	D	291	ARG	CA-C	-5.42	1.38	1.52
4	G	56	ARG	N-CA	-5.42	1.35	1.46
4	F	230	PHE	CA-C	-5.42	1.38	1.52
4	F	6	GLU	CA-C	-5.40	1.39	1.52
4	F	345	SER	N-CA	-5.38	1.35	1.46
3	E	216	LEU	N-CA	-5.35	1.35	1.46
1	A	270	ARG	CA-C	-5.32	1.39	1.52
2	B	344	ASP	CA-C	-5.32	1.39	1.52
4	G	349	ILE	N-CA	-5.31	1.35	1.46
3	E	14	LEU	CA-C	-5.29	1.39	1.52
3	E	281	LEU	CA-C	-5.28	1.39	1.52
4	F	66	GLY	CA-C	-5.28	1.43	1.51
3	E	207	GLY	CA-C	-5.27	1.43	1.51
4	F	97	MET	N-CA	-5.27	1.35	1.46
3	E	229	TRP	CD1-NE1	-5.27	1.28	1.38
1	A	283	ARG	CA-CB	-5.26	1.42	1.53
2	B	118	GLY	CA-C	-5.26	1.43	1.51
4	G	63	HIS	N-CA	-5.26	1.35	1.46
4	F	335	ASN	CA-C	-5.26	1.39	1.52
2	C	330	GLN	N-CA	-5.23	1.35	1.46
4	F	121	ASP	CA-C	-5.23	1.39	1.52
4	F	358	ALA	CA-C	-5.23	1.39	1.52
4	F	41	THR	CA-C	-5.23	1.39	1.52
1	A	333	HIS	N-CA	-5.22	1.35	1.46
2	D	76	CYS	N-CA	-5.22	1.35	1.46
4	G	310	TYR	N-CA	-5.22	1.35	1.46
4	F	349	ILE	N-CA	-5.22	1.35	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	93	VAL	N-CA	-5.21	1.35	1.46
2	D	120	PHE	CA-C	-5.21	1.39	1.52
3	E	321	HIS	CB-CG	-5.21	1.40	1.50
3	E	33	PRO	N-CA	-5.20	1.38	1.47
2	B	64	CYS	CB-SG	-5.20	1.73	1.81
1	A	114	GLY	CA-C	-5.20	1.43	1.51
2	B	151	LYS	N-CA	-5.20	1.35	1.46
4	G	66	GLY	N-CA	-5.19	1.38	1.46
3	E	208	ASP	C-O	-5.19	1.13	1.23
1	A	270	ARG	N-CA	-5.18	1.35	1.46
2	C	347	MET	CA-C	-5.18	1.39	1.52
2	D	22	GLU	CA-C	-5.18	1.39	1.52
4	F	9	HIS	CA-C	-5.17	1.39	1.52
3	E	207	GLY	N-CA	-5.17	1.38	1.46
4	G	349	ILE	CA-CB	-5.17	1.43	1.54
1	A	293	LEU	CA-C	-5.16	1.39	1.52
2	D	64	CYS	CA-C	-5.15	1.39	1.52
4	F	350	GLU	N-CA	-5.15	1.36	1.46
4	G	350	GLU	CA-C	-5.15	1.39	1.52
3	E	16	ALA	CA-C	-5.14	1.39	1.52
4	F	148	HIS	CA-C	-5.14	1.39	1.52
4	G	356	SER	CA-C	-5.13	1.39	1.52
2	D	21	GLN	CA-C	-5.13	1.39	1.52
4	F	71	PRO	CA-C	-5.12	1.42	1.52
2	D	234	THR	CA-C	-5.12	1.39	1.52
2	B	48	GLY	CA-C	-5.11	1.43	1.51
2	D	200	PRO	CA-C	-5.11	1.42	1.52
3	E	298	GLU	CG-CD	5.11	1.59	1.51
2	D	162	LEU	N-CA	-5.10	1.36	1.46
1	A	198	THR	N-CA	-5.10	1.36	1.46
2	D	43	PHE	CA-C	-5.10	1.39	1.52
1	A	283	ARG	N-CA	-5.09	1.36	1.46
2	C	277	GLU	CB-CG	5.09	1.61	1.52
3	E	14	LEU	N-CA	-5.09	1.36	1.46
2	D	314	ARG	CA-C	-5.08	1.39	1.52
4	G	161	GLU	N-CA	-5.07	1.36	1.46
4	G	186	GLN	N-CA	-5.06	1.36	1.46
3	E	9	PRO	CA-C	-5.06	1.42	1.52
1	A	16	GLY	CA-C	-5.06	1.43	1.51
4	F	350	GLU	CA-CB	-5.04	1.42	1.53
4	F	350	GLU	CA-C	-5.04	1.39	1.52
4	F	192	SER	CA-C	-5.04	1.39	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	59	LEU	CA-C	-5.04	1.39	1.52
3	E	227	GLY	CA-C	-5.03	1.43	1.51
3	E	227	GLY	N-CA	-5.02	1.38	1.46
3	E	47	TYR	CB-CG	-5.01	1.44	1.51
1	A	115	ASN	CA-C	-5.00	1.40	1.52

All (710) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	222	TYR	CB-CG-CD2	-25.40	105.76	121.00
3	E	158	ARG	NE-CZ-NH1	16.17	128.39	120.30
1	A	277	ARG	NE-CZ-NH2	-15.49	112.56	120.30
1	A	316	TYR	CB-CG-CD1	-15.17	111.90	121.00
4	F	176	ARG	NE-CZ-NH2	-14.99	112.81	120.30
4	F	224	ARG	NE-CZ-NH2	-13.35	113.63	120.30
1	A	273	PHE	CB-CG-CD2	-13.02	111.69	120.80
3	E	222	TYR	CB-CG-CD1	12.67	128.60	121.00
4	F	137	ARG	NE-CZ-NH2	-12.46	114.07	120.30
2	D	123	TYR	CB-CG-CD1	-12.06	113.76	121.00
4	F	24	ARG	NE-CZ-NH1	11.76	126.18	120.30
4	F	284	TYR	CB-CG-CD2	-11.59	114.05	121.00
2	D	263	ARG	NE-CZ-NH2	-11.50	114.55	120.30
4	F	100	ARG	NE-CZ-NH1	11.43	126.02	120.30
4	G	137	ARG	NE-CZ-NH1	11.30	125.95	120.30
4	F	100	ARG	NE-CZ-NH2	-11.21	114.69	120.30
2	B	120	PHE	CB-CG-CD2	11.20	128.64	120.80
2	B	342	ALA	N-CA-CB	11.18	125.75	110.10
2	C	351	MET	CG-SD-CE	-11.01	82.58	100.20
2	C	105	ARG	NE-CZ-NH2	-10.95	114.83	120.30
2	D	314	ARG	NE-CZ-NH1	10.78	125.69	120.30
3	E	192	ARG	NE-CZ-NH2	10.78	125.69	120.30
2	D	263	ARG	NE-CZ-NH1	10.70	125.65	120.30
2	D	336	ARG	NE-CZ-NH2	-10.63	114.98	120.30
2	C	274	ARG	NE-CZ-NH1	10.60	125.60	120.30
3	E	236	LEU	CB-CA-C	-10.53	90.20	110.20
3	E	297	ARG	NE-CZ-NH1	10.42	125.51	120.30
2	B	120	PHE	CB-CG-CD1	-10.40	113.52	120.80
2	C	362	ARG	N-CA-C	-10.29	83.22	111.00
4	G	232	PHE	CB-CG-CD2	10.27	127.99	120.80
2	D	341	TYR	CB-CG-CD2	-10.24	114.86	121.00
4	F	37	VAL	CA-CB-CG2	-10.05	95.82	110.90
2	D	3	TYR	CB-CG-CD1	-10.04	114.98	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	347	MET	CA-CB-CG	10.00	130.29	113.30
4	G	152	ARG	NE-CZ-NH1	9.97	125.28	120.30
2	D	98	ARG	NE-CZ-NH2	-9.93	115.34	120.30
3	E	62	CYS	N-CA-CB	9.75	128.15	110.60
2	C	367	GLU	N-CA-C	-9.73	84.74	111.00
4	F	157	GLY	N-CA-C	-9.70	88.85	113.10
4	F	323	TYR	CB-CG-CD2	-9.69	115.19	121.00
3	E	1	MET	CG-SD-CE	9.59	115.55	100.20
4	F	76	PHE	CB-CG-CD2	-9.53	114.13	120.80
2	D	76	CYS	N-CA-C	-9.41	85.59	111.00
4	G	274	SER	N-CA-CB	9.41	124.61	110.50
2	C	355	ARG	NE-CZ-NH2	-9.37	115.61	120.30
2	D	56	ARG	NE-CZ-NH2	9.36	124.98	120.30
4	G	339	MET	CG-SD-CE	-9.36	85.23	100.20
2	D	76	CYS	N-CA-CB	9.34	127.41	110.60
4	G	246	ARG	NE-CZ-NH2	9.34	124.97	120.30
2	C	256	MET	CG-SD-CE	-9.31	85.31	100.20
2	B	336	ARG	NE-CZ-NH1	9.29	124.95	120.30
4	G	356	SER	N-CA-C	-9.27	85.98	111.00
4	F	333	CYS	N-CA-CB	9.23	127.22	110.60
4	F	38	ALA	N-CA-C	-9.19	86.19	111.00
3	E	308	ARG	NE-CZ-NH2	-9.18	115.71	120.30
4	F	206	MET	CG-SD-CE	-9.14	85.57	100.20
2	D	341	TYR	CB-CG-CD1	9.13	126.48	121.00
3	E	229	TRP	CB-CG-CD2	-9.13	114.73	126.60
2	D	80	ARG	NE-CZ-NH2	-8.96	115.82	120.30
4	G	75	PHE	CB-CG-CD1	-8.90	114.57	120.80
2	B	47	ARG	NE-CZ-NH1	-8.89	115.85	120.30
4	F	182	MET	CG-SD-CE	-8.89	85.98	100.20
2	C	341	TYR	CB-CG-CD1	-8.88	115.67	121.00
3	E	178	ARG	NE-CZ-NH2	-8.84	115.88	120.30
2	B	306	MET	CG-SD-CE	-8.84	86.06	100.20
4	G	230	PHE	CB-CG-CD1	-8.80	114.64	120.80
2	C	355	ARG	NE-CZ-NH1	8.78	124.69	120.30
1	A	316	TYR	CB-CG-CD2	8.75	126.25	121.00
3	E	208	ASP	CB-CA-C	-8.75	92.90	110.40
3	E	3	TRP	CB-CG-CD2	-8.69	115.30	126.60
4	G	193	VAL	N-CA-C	-8.68	87.58	111.00
4	G	206	MET	CG-SD-CE	-8.62	86.42	100.20
4	G	39	ASP	N-CA-C	-8.61	87.76	111.00
3	E	205	PHE	CB-CG-CD1	-8.60	114.78	120.80
2	B	119	ARG	NE-CZ-NH2	-8.59	116.00	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	61	TRP	CB-CG-CD2	-8.54	115.50	126.60
4	F	76	PHE	CB-CG-CD1	8.54	126.78	120.80
1	A	228	ARG	NE-CZ-NH1	8.52	124.56	120.30
4	F	148	HIS	CA-CB-CG	-8.51	99.13	113.60
1	A	277	ARG	NE-CZ-NH1	8.51	124.55	120.30
2	D	346	ARG	NE-CZ-NH2	-8.48	116.06	120.30
4	G	147	ALA	N-CA-CB	8.42	121.89	110.10
4	F	335	ASN	CB-CA-C	-8.37	93.67	110.40
4	F	197	ARG	NE-CZ-NH2	-8.34	116.13	120.30
4	F	335	ASN	CA-C-N	-8.34	98.86	117.20
2	C	314	ARG	NE-CZ-NH1	8.33	124.46	120.30
4	G	222	ASN	N-CA-C	-8.28	88.64	111.00
4	F	310	TYR	CB-CG-CD1	-8.28	116.03	121.00
2	D	10	TRP	CB-CG-CD2	-8.25	115.88	126.60
3	E	322	TYR	CA-CB-CG	-8.23	97.76	113.40
1	A	283	ARG	NE-CZ-NH2	-8.23	116.19	120.30
4	G	124	SER	N-CA-C	-8.23	88.79	111.00
4	F	251	ASN	N-CA-CB	8.22	125.39	110.60
2	C	265	MET	CG-SD-CE	8.22	113.34	100.20
1	A	3	ARG	NE-CZ-NH1	8.21	124.41	120.30
4	F	53	MET	CG-SD-CE	-8.21	87.06	100.20
3	E	47	TYR	N-CA-CB	-8.16	95.91	110.60
4	F	279	ARG	NE-CZ-NH2	-8.12	116.24	120.30
4	F	336	VAL	CG1-CB-CG2	8.12	123.89	110.90
4	F	279	ARG	NE-CZ-NH1	8.10	124.35	120.30
4	F	38	ALA	N-CA-CB	8.08	121.42	110.10
4	F	261	ASP	CB-CA-C	8.08	126.56	110.40
4	G	137	ARG	NE-CZ-NH2	-8.06	116.27	120.30
4	G	296	ASN	N-CA-C	-7.99	89.44	111.00
2	D	294	MET	CG-SD-CE	-7.96	87.47	100.20
2	B	347	MET	CG-SD-CE	-7.95	87.48	100.20
4	G	240	ARG	NE-CZ-NH1	7.94	124.27	120.30
2	D	291	ARG	NE-CZ-NH1	-7.88	116.36	120.30
4	G	163	GLU	N-CA-C	-7.88	89.73	111.00
1	A	264	SER	N-CA-CB	7.85	122.28	110.50
4	G	207	LEU	CB-CG-CD1	-7.81	97.72	111.00
2	B	47	ARG	NE-CZ-NH2	7.80	124.20	120.30
4	F	113	ALA	CB-CA-C	-7.76	98.46	110.10
4	G	215	ARG	NE-CZ-NH2	-7.75	116.43	120.30
1	A	39	ARG	NE-CZ-NH2	-7.75	116.43	120.30
1	A	333	HIS	CB-CA-C	7.74	125.89	110.40
4	F	75	PHE	N-CA-CB	-7.73	96.69	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	219	GLY	N-CA-C	-7.72	93.80	113.10
1	A	273	PHE	CB-CG-CD1	7.70	126.19	120.80
2	D	313	MET	CG-SD-CE	-7.69	87.89	100.20
4	G	232	PHE	CB-CG-CD1	-7.68	115.42	120.80
3	E	322	TYR	CB-CG-CD2	-7.66	116.40	121.00
2	D	216	ASP	CB-CG-OD2	-7.65	111.42	118.30
4	F	335	ASN	N-CA-CB	7.64	124.35	110.60
4	F	207	LEU	CB-CG-CD2	7.63	123.97	111.00
4	G	161	GLU	CB-CG-CD	-7.62	93.61	114.20
1	A	223	MET	CG-SD-CE	7.62	112.39	100.20
3	E	163	TYR	CA-CB-CG	7.62	127.87	113.40
4	G	323	TYR	CB-CG-CD2	-7.62	116.43	121.00
2	D	98	ARG	NE-CZ-NH1	7.59	124.09	120.30
3	E	205	PHE	CB-CA-C	-7.59	95.22	110.40
4	F	135	MET	CG-SD-CE	-7.58	88.07	100.20
4	G	149	GLN	N-CA-CB	7.58	124.25	110.60
3	E	8	ARG	NE-CZ-NH1	7.58	124.09	120.30
2	D	351	MET	CG-SD-CE	-7.58	88.07	100.20
4	F	319	PHE	CB-CG-CD2	-7.58	115.50	120.80
3	E	8	ARG	NE-CZ-NH2	-7.56	116.52	120.30
2	D	80	ARG	NE-CZ-NH1	7.55	124.08	120.30
4	G	341	THR	CA-CB-CG2	-7.55	101.84	112.40
3	E	303	VAL	CA-CB-CG2	-7.54	99.59	110.90
2	B	338	GLU	CB-CA-C	-7.51	95.38	110.40
4	G	105	ARG	NE-CZ-NH1	7.51	124.06	120.30
3	E	49	LEU	CB-CG-CD1	-7.50	98.25	111.00
4	G	353	ALA	CB-CA-C	-7.49	98.86	110.10
2	C	89	ASP	CB-CG-OD2	-7.49	111.56	118.30
2	C	319	THR	CA-CB-CG2	-7.49	101.92	112.40
2	B	274	ARG	N-CA-C	-7.48	90.81	111.00
4	F	309	THR	CA-CB-CG2	-7.48	101.93	112.40
2	D	10	TRP	CB-CG-CD1	7.47	136.71	127.00
4	F	238	ASP	CB-CG-OD2	7.46	125.01	118.30
3	E	50	CYS	CA-CB-SG	-7.46	100.58	114.00
2	B	151	LYS	N-CA-C	-7.42	90.96	111.00
2	D	303	GLY	N-CA-C	-7.41	94.58	113.10
1	A	316	TYR	CA-CB-CG	-7.38	99.38	113.40
2	D	64	CYS	N-CA-C	-7.36	91.13	111.00
4	G	294	ALA	N-CA-CB	7.35	120.40	110.10
2	C	366	PRO	CA-C-N	-7.29	101.17	117.20
4	F	274	SER	CB-CA-C	-7.25	96.32	110.10
1	A	282	ARG	NE-CZ-NH1	-7.25	116.67	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	329	ASN	N-CA-CB	-7.24	97.57	110.60
2	D	123	TYR	CA-CB-CG	-7.22	99.67	113.40
4	G	207	LEU	CB-CA-C	-7.22	96.48	110.20
4	G	245	ARG	NE-CZ-NH2	-7.21	116.70	120.30
2	B	41	TYR	CB-CG-CD1	-7.20	116.68	121.00
4	G	54	VAL	CA-CB-CG2	-7.16	100.16	110.90
4	F	257	GLU	CA-CB-CG	-7.15	97.66	113.40
3	E	267	ASN	CA-CB-CG	-7.15	97.67	113.40
1	A	217	TRP	CB-CG-CD1	-7.14	117.71	127.00
3	E	22	ARG	N-CA-C	-7.14	91.72	111.00
3	E	294	CYS	CA-CB-SG	-7.14	101.15	114.00
2	D	336	ARG	NE-CZ-NH1	7.12	123.86	120.30
2	D	155	ALA	N-CA-CB	7.10	120.05	110.10
1	A	158	LEU	CB-CG-CD2	-7.07	98.98	111.00
2	D	208	ARG	NE-CZ-NH1	-7.07	116.77	120.30
2	C	278	TRP	CB-CA-C	-7.06	96.28	110.40
3	E	182	MET	N-CA-C	-7.05	91.95	111.00
3	E	192	ARG	NE-CZ-NH1	-7.03	116.79	120.30
2	D	297	LEU	N-CA-CB	7.01	124.42	110.40
3	E	121	THR	N-CA-CB	7.01	123.62	110.30
4	F	105	ARG	NE-CZ-NH1	7.01	123.80	120.30
3	E	73	HIS	CB-CA-C	7.01	124.41	110.40
4	F	278	PHE	CB-CG-CD1	7.00	125.70	120.80
1	A	228	ARG	NE-CZ-NH2	-7.00	116.80	120.30
4	F	230	PHE	CB-CG-CD2	-6.99	115.91	120.80
4	G	257	GLU	CA-CB-CG	-6.95	98.10	113.40
4	F	326	ASP	CB-CA-C	-6.95	96.50	110.40
2	D	36	ARG	NE-CZ-NH1	6.95	123.78	120.30
4	G	338	MET	N-CA-CB	6.95	123.10	110.60
4	F	180	CYS	N-CA-C	-6.94	92.27	111.00
4	G	41	THR	CA-CB-CG2	-6.93	102.70	112.40
3	E	301	MET	CG-SD-CE	-6.93	89.12	100.20
1	A	5	TYR	CB-CG-CD1	-6.92	116.85	121.00
2	D	213	SER	N-CA-CB	6.91	120.86	110.50
4	F	243	ASP	CB-CG-OD1	-6.90	112.09	118.30
1	A	292	ARG	NE-CZ-NH1	-6.89	116.86	120.30
2	D	297	LEU	CB-CG-CD1	6.88	122.69	111.00
3	E	182	MET	N-CA-CB	6.87	122.97	110.60
3	E	76	TYR	CB-CG-CD2	-6.86	116.88	121.00
4	G	84	GLU	CB-CG-CD	-6.86	95.69	114.20
4	G	103	ARG	NE-CZ-NH1	6.85	123.72	120.30
4	G	140	GLU	CB-CA-C	-6.85	96.70	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	335	ASN	N-CA-CB	6.85	122.93	110.60
2	D	298	SER	N-CA-C	-6.84	92.53	111.00
4	G	356	SER	CB-CA-C	6.82	123.05	110.10
2	C	277	GLU	N-CA-CB	-6.79	98.39	110.60
2	D	173	PHE	CB-CG-CD2	-6.78	116.06	120.80
4	F	93	GLU	N-CA-C	-6.74	92.80	111.00
4	F	120	ASP	CB-CG-OD2	6.73	124.36	118.30
4	F	336	VAL	CA-CB-CG2	-6.71	100.83	110.90
2	B	112	GLN	N-CA-CB	6.71	122.67	110.60
4	G	96	ARG	N-CA-C	-6.70	92.90	111.00
4	F	119	LEU	CB-CA-C	-6.69	97.50	110.20
4	F	223	ILE	N-CA-C	-6.67	92.98	111.00
4	F	337	ARG	NE-CZ-NH1	6.67	123.64	120.30
2	C	347	MET	CB-CA-C	-6.67	97.06	110.40
4	F	7	ARG	NE-CZ-NH1	6.67	123.63	120.30
4	F	110	THR	CA-CB-CG2	-6.66	103.08	112.40
1	A	61	TRP	CB-CG-CD1	6.65	135.64	127.00
3	E	122	ASP	CB-CA-C	-6.65	97.11	110.40
3	E	308	ARG	NE-CZ-NH1	6.63	123.61	120.30
4	G	366	LEU	N-CA-C	-6.62	93.12	111.00
2	B	155	ALA	N-CA-CB	6.62	119.37	110.10
2	D	274	ARG	NE-CZ-NH2	-6.62	116.99	120.30
2	D	155	ALA	N-CA-C	-6.62	93.14	111.00
3	E	3	TRP	CB-CG-CD1	6.61	135.59	127.00
1	A	55	ILE	N-CA-C	-6.60	93.19	111.00
3	E	208	ASP	CA-CB-CG	-6.58	98.92	113.40
3	E	329	LEU	CB-CA-C	-6.57	97.72	110.20
4	F	258	ALA	N-CA-CB	6.57	119.29	110.10
4	F	336	VAL	N-CA-C	-6.57	93.27	111.00
1	A	279	TRP	CB-CA-C	-6.56	97.28	110.40
1	A	274	ASP	CB-CG-OD1	6.55	124.19	118.30
4	F	122	TRP	CA-C-N	-6.55	102.79	117.20
3	E	92	ALA	N-CA-CB	6.54	119.26	110.10
2	B	123	TYR	CB-CG-CD2	-6.54	117.08	121.00
2	B	129	HIS	CA-CB-CG	6.54	124.72	113.60
4	G	191	HIS	N-CA-CB	6.54	122.38	110.60
4	G	305	ILE	N-CA-C	-6.54	93.34	111.00
3	E	111	VAL	N-CA-C	-6.54	93.34	111.00
4	F	224	ARG	NH1-CZ-NH2	6.54	126.59	119.40
2	B	56	ARG	NE-CZ-NH2	6.53	123.56	120.30
3	E	63	ARG	NE-CZ-NH1	6.53	123.56	120.30
4	F	338	MET	CA-CB-CG	-6.53	102.20	113.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	160	PHE	CA-CB-CG	-6.53	98.23	113.90
4	G	322	SER	N-CA-CB	6.53	120.29	110.50
2	C	36	ARG	NE-CZ-NH2	6.52	123.56	120.30
2	D	66	THR	N-CA-C	-6.51	93.42	111.00
3	E	62	CYS	CB-CA-C	-6.51	97.39	110.40
3	E	56	HIS	CA-CB-CG	-6.50	102.54	113.60
4	F	284	TYR	CB-CG-CD1	6.50	124.90	121.00
2	C	81	GLU	CB-CG-CD	-6.50	96.66	114.20
3	E	42	TYR	CB-CG-CD2	-6.49	117.11	121.00
4	G	124	SER	N-CA-CB	6.46	120.19	110.50
4	G	219	GLY	N-CA-C	-6.45	96.97	113.10
4	F	238	ASP	CB-CG-OD1	-6.45	112.50	118.30
4	F	213	PRO	N-CA-C	-6.44	95.36	112.10
2	B	347	MET	CB-CA-C	-6.44	97.52	110.40
4	F	267	PHE	CB-CA-C	-6.43	97.53	110.40
3	E	267	ASN	N-CA-C	-6.43	93.63	111.00
2	D	351	MET	CB-CA-C	-6.42	97.55	110.40
4	F	84	GLU	CA-CB-CG	-6.42	99.28	113.40
4	F	240	ARG	NE-CZ-NH2	-6.41	117.09	120.30
1	A	217	TRP	N-CA-CB	-6.41	99.06	110.60
2	B	201	ARG	NE-CZ-NH1	-6.41	117.10	120.30
3	E	116	ASP	N-CA-C	-6.40	93.71	111.00
2	C	105	ARG	NE-CZ-NH1	6.40	123.50	120.30
4	F	180	CYS	N-CA-CB	6.40	122.12	110.60
4	G	267	PHE	CB-CG-CD2	-6.39	116.33	120.80
1	A	282	ARG	CA-CB-CG	-6.39	99.35	113.40
2	B	344	ASP	N-CA-C	-6.39	93.76	111.00
4	F	306	LEU	N-CA-CB	6.38	123.16	110.40
4	F	341	THR	N-CA-C	-6.38	93.79	111.00
4	G	37	VAL	N-CA-C	-6.38	93.78	111.00
4	G	341	THR	N-CA-C	-6.37	93.79	111.00
4	F	204	MET	CG-SD-CE	-6.37	90.00	100.20
3	E	309	GLU	CB-CG-CD	-6.37	97.01	114.20
4	G	194	ILE	N-CA-C	-6.37	93.81	111.00
2	D	63	ASN	N-CA-CB	6.36	122.05	110.60
4	G	329	ASN	N-CA-CB	-6.36	99.16	110.60
3	E	73	HIS	CA-CB-CG	-6.35	102.80	113.60
2	B	342	ALA	CB-CA-C	-6.35	100.57	110.10
2	C	338	GLU	CB-CA-C	-6.35	97.70	110.40
2	D	120	PHE	N-CA-C	-6.35	93.86	111.00
2	C	336	ARG	NE-CZ-NH1	6.34	123.47	120.30
4	G	284	TYR	CA-CB-CG	-6.34	101.36	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	262	ARG	CB-CA-C	-6.33	97.73	110.40
4	F	181	SER	N-CA-C	-6.32	93.94	111.00
4	F	335	ASN	N-CA-C	-6.32	93.94	111.00
4	F	130	LEU	CB-CA-C	-6.30	98.23	110.20
1	A	242	GLU	CB-CG-CD	-6.29	97.20	114.20
4	G	336	VAL	N-CA-C	-6.29	94.01	111.00
2	D	173	PHE	N-CA-C	-6.28	94.04	111.00
4	F	197	ARG	NE-CZ-NH1	6.28	123.44	120.30
2	B	36	ARG	NE-CZ-NH2	6.28	123.44	120.30
4	G	215	ARG	NE-CZ-NH1	6.28	123.44	120.30
4	F	338	MET	CG-SD-CE	-6.27	90.17	100.20
2	D	123	TYR	CB-CG-CD2	6.26	124.76	121.00
4	F	350	GLU	CA-C-N	-6.25	103.44	117.20
2	B	351	MET	CG-SD-CE	6.25	110.20	100.20
1	A	187	ARG	NE-CZ-NH1	6.25	123.42	120.30
2	D	75	VAL	CA-C-N	-6.24	103.47	117.20
2	D	136	PHE	CB-CG-CD1	-6.24	116.43	120.80
4	G	114	ALA	CB-CA-C	-6.22	100.77	110.10
4	G	238	ASP	N-CA-C	-6.21	94.25	111.00
1	A	274	ASP	CB-CG-OD2	-6.20	112.72	118.30
2	C	39	HIS	CA-CB-CG	6.20	124.14	113.60
4	F	116	PHE	N-CA-C	-6.20	94.27	111.00
2	C	328	TYR	CB-CG-CD2	-6.19	117.28	121.00
4	G	36	GLN	N-CA-C	-6.19	94.29	111.00
1	A	333	HIS	N-CA-C	-6.18	94.31	111.00
1	A	225	LYS	CA-C-N	-6.18	103.60	117.20
4	F	319	PHE	CB-CA-C	-6.17	98.05	110.40
1	A	134	SER	N-CA-CB	-6.17	101.25	110.50
3	E	262	ALA	N-CA-CB	6.16	118.73	110.10
4	G	90	VAL	CB-CA-C	-6.16	99.70	111.40
1	A	3	ARG	NE-CZ-NH2	-6.16	117.22	120.30
4	G	355	GLN	N-CA-C	-6.15	94.40	111.00
3	E	152	LEU	N-CA-CB	6.15	122.70	110.40
3	E	236	LEU	CB-CG-CD2	-6.15	100.55	111.00
2	C	133	ARG	NE-CZ-NH1	6.14	123.37	120.30
4	F	17	VAL	CA-CB-CG2	-6.14	101.69	110.90
4	F	115	ASP	N-CA-C	-6.14	94.42	111.00
4	G	57	VAL	N-CA-C	-6.14	94.42	111.00
1	A	264	SER	CA-C-N	-6.13	103.71	117.20
4	G	127	GLU	N-CA-C	-6.12	94.46	111.00
1	A	25	GLY	N-CA-C	-6.12	97.79	113.10
3	E	26	ALA	N-CA-CB	6.12	118.67	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	317	GLY	N-CA-C	-6.11	97.82	113.10
4	F	44	LEU	CB-CG-CD1	-6.11	100.61	111.00
4	F	348	GLN	N-CA-CB	6.11	121.60	110.60
4	F	274	SER	N-CA-CB	6.11	119.66	110.50
3	E	266	THR	CA-CB-CG2	-6.09	103.87	112.40
4	F	193	VAL	CG1-CB-CG2	-6.09	101.15	110.90
4	G	104	SER	N-CA-CB	-6.08	101.38	110.50
3	E	68	MET	CB-CA-C	-6.08	98.25	110.40
4	G	59	LEU	CB-CG-CD2	6.07	121.32	111.00
4	G	100	ARG	NE-CZ-NH2	-6.07	117.26	120.30
1	A	48	GLU	CB-CG-CD	-6.07	97.81	114.20
4	G	239	GLY	N-CA-C	-6.07	97.93	113.10
2	C	366	PRO	N-CA-CB	6.07	110.58	103.30
4	G	338	MET	CB-CA-C	-6.05	98.29	110.40
4	G	197	ARG	NE-CZ-NH2	-6.05	117.28	120.30
3	E	158	ARG	NH1-CZ-NH2	-6.04	112.75	119.40
4	F	6	GLU	CA-CB-CG	-6.04	100.11	113.40
1	A	220	ALA	CB-CA-C	-6.04	101.05	110.10
2	B	119	ARG	NE-CZ-NH1	6.03	123.31	120.30
4	G	267	PHE	CB-CA-C	-6.03	98.34	110.40
2	C	328	TYR	CB-CG-CD1	6.01	124.61	121.00
4	F	319	PHE	N-CA-CB	6.01	121.41	110.60
4	G	231	ILE	N-CA-C	-6.01	94.78	111.00
2	B	78	ASN	N-CA-CB	6.00	121.40	110.60
2	B	86	ARG	NE-CZ-NH2	6.00	123.30	120.30
4	G	230	PHE	CA-C-N	-6.00	104.00	117.20
1	A	173	CYS	CB-CA-C	-6.00	98.41	110.40
2	B	359	PHE	CB-CA-C	-5.99	98.41	110.40
2	C	145	GLU	CB-CG-CD	-5.99	98.02	114.20
1	A	39	ARG	NE-CZ-NH1	5.99	123.29	120.30
3	E	230	TYR	CB-CG-CD2	-5.98	117.41	121.00
2	B	276	ILE	N-CA-C	-5.98	94.85	111.00
2	D	89	ASP	CB-CA-C	-5.98	98.44	110.40
2	D	156	THR	N-CA-C	-5.97	94.88	111.00
4	G	204	MET	CG-SD-CE	-5.97	90.64	100.20
2	C	341	TYR	CA-CB-CG	-5.97	102.06	113.40
4	F	36	GLN	CB-CG-CD	-5.97	96.09	111.60
4	F	176	ARG	NE-CZ-NH1	5.97	123.28	120.30
4	G	75	PHE	N-CA-CB	-5.97	99.86	110.60
4	F	289	GLN	N-CA-CB	5.96	121.33	110.60
4	F	310	TYR	CB-CG-CD2	5.96	124.58	121.00
4	G	160	PHE	CB-CA-C	-5.96	98.47	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	258	VAL	CA-CB-CG1	5.95	119.83	110.90
4	F	308	VAL	CA-CB-CG1	-5.95	101.97	110.90
4	F	294	ALA	N-CA-CB	5.94	118.42	110.10
4	F	122	TRP	CB-CG-CD1	-5.93	119.28	127.00
4	F	229	ASP	CB-CG-OD2	5.93	123.64	118.30
2	D	296	GLN	CB-CA-C	-5.93	98.54	110.40
3	E	66	GLN	N-CA-CB	5.93	121.28	110.60
4	F	275	ASN	N-CA-CB	-5.93	99.93	110.60
4	F	217	GLN	N-CA-C	-5.93	95.00	111.00
4	F	122	TRP	N-CA-C	-5.92	95.00	111.00
2	C	247	ASP	CA-CB-CG	-5.92	100.37	113.40
4	G	229	ASP	N-CA-CB	5.92	121.26	110.60
2	D	318	ARG	NE-CZ-NH2	5.92	123.26	120.30
2	B	109	ASP	N-CA-CB	5.92	121.26	110.60
2	B	360	HIS	CA-CB-CG	-5.92	103.55	113.60
3	E	42	TYR	N-CA-CB	-5.91	99.97	110.60
4	G	210	GLY	CA-C-N	-5.91	104.20	117.20
1	A	170	LEU	CB-CA-C	5.90	121.41	110.20
4	G	97	MET	CG-SD-CE	-5.90	90.76	100.20
2	D	117	ARG	NE-CZ-NH1	5.89	123.25	120.30
2	D	191	LEU	CB-CG-CD1	5.89	121.01	111.00
2	C	119	ARG	NE-CZ-NH2	5.88	123.24	120.30
4	F	162	THR	N-CA-C	-5.88	95.12	111.00
3	E	260	HIS	N-CA-CB	5.88	121.19	110.60
4	G	354	SER	N-CA-C	-5.88	95.13	111.00
2	D	301	ALA	N-CA-CB	5.87	118.32	110.10
4	F	246	ARG	NE-CZ-NH2	5.86	123.23	120.30
4	G	8	GLU	CB-CG-CD	-5.85	98.40	114.20
1	A	43	ALA	CB-CA-C	-5.85	101.33	110.10
4	F	256	LEU	N-CA-CB	5.84	122.08	110.40
4	G	56	ARG	N-CA-C	-5.84	95.24	111.00
4	F	222	ASN	CA-CB-CG	-5.83	100.56	113.40
4	F	338	MET	CB-CA-C	-5.83	98.73	110.40
2	C	210	ALA	CB-CA-C	-5.83	101.35	110.10
4	F	59	LEU	N-CA-CB	-5.83	98.74	110.40
2	C	274	ARG	NE-CZ-NH2	-5.82	117.39	120.30
2	D	133	ARG	NE-CZ-NH1	5.82	123.21	120.30
4	F	192	SER	N-CA-C	-5.82	95.28	111.00
3	E	207	GLY	CA-C-N	-5.82	104.40	117.20
4	G	331	LEU	N-CA-C	-5.82	95.29	111.00
1	A	277	ARG	N-CA-C	-5.81	95.31	111.00
3	E	37	ASP	N-CA-CB	-5.81	100.14	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	192	SER	N-CA-CB	5.81	119.22	110.50
2	D	64	CYS	CA-CB-SG	-5.80	103.55	114.00
1	A	282	ARG	CG-CD-NE	-5.80	99.62	111.80
4	G	276	GLU	CA-CB-CG	-5.80	100.64	113.40
2	D	291	ARG	CG-CD-NE	-5.80	99.63	111.80
2	C	235	GLN	CB-CG-CD	5.79	126.66	111.60
4	F	255	HIS	N-CA-C	-5.79	95.36	111.00
1	A	171	CYS	CA-CB-SG	-5.79	103.58	114.00
4	G	79	CYS	CB-CA-C	-5.79	98.82	110.40
2	D	346	ARG	N-CA-CB	-5.79	100.19	110.60
4	G	51	MET	CG-SD-CE	5.78	109.45	100.20
3	E	151	LEU	CB-CA-C	-5.78	99.22	110.20
4	G	188	LEU	N-CA-CB	5.77	121.95	110.40
4	G	251	ASN	CA-CB-CG	-5.77	100.70	113.40
3	E	23	GLY	CA-C-N	-5.76	104.53	117.20
4	F	209	GLY	N-CA-C	-5.76	98.70	113.10
4	G	205	ARG	NE-CZ-NH2	5.76	123.18	120.30
1	A	187	ARG	NE-CZ-NH2	-5.75	117.42	120.30
4	F	103	ARG	NE-CZ-NH1	5.75	123.17	120.30
3	E	253	MET	CG-SD-CE	5.75	109.40	100.20
4	G	263	LEU	N-CA-CB	-5.75	98.91	110.40
2	D	355	ARG	NE-CZ-NH2	5.74	123.17	120.30
3	E	4	TYR	N-CA-C	-5.74	95.52	111.00
4	F	245	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	A	298	LEU	CB-CA-C	5.72	121.07	110.20
2	D	157	THR	N-CA-C	-5.72	95.56	111.00
4	F	343	SER	CB-CA-C	-5.72	99.23	110.10
2	B	313	MET	CG-SD-CE	-5.71	91.06	100.20
4	F	148	HIS	O-C-N	5.71	131.84	122.70
3	E	94	ARG	O-C-N	-5.71	113.57	122.70
3	E	293	VAL	CA-CB-CG2	-5.70	102.35	110.90
4	G	354	SER	N-CA-CB	5.70	119.06	110.50
2	D	6	LEU	N-CA-CB	-5.70	99.00	110.40
2	B	221	THR	N-CA-CB	5.70	121.13	110.30
2	D	339	LEU	CB-CG-CD1	5.70	120.69	111.00
3	E	46	ARG	NE-CZ-NH1	5.70	123.15	120.30
3	E	83	LYS	CB-CA-C	-5.69	99.02	110.40
2	C	80	ARG	CG-CD-NE	-5.69	99.85	111.80
4	F	243	ASP	CB-CG-OD2	5.69	123.42	118.30
3	E	160	ARG	NE-CZ-NH2	5.69	123.14	120.30
4	F	6	GLU	N-CA-CB	5.69	120.84	110.60
3	E	189	ALA	N-CA-CB	5.69	118.06	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	22	ARG	N-CA-CB	5.68	120.83	110.60
4	F	350	GLU	N-CA-C	-5.68	95.66	111.00
4	G	222	ASN	CA-C-N	-5.68	104.70	117.20
1	A	302	VAL	CB-CA-C	-5.68	100.61	111.40
2	B	342	ALA	N-CA-C	-5.68	95.67	111.00
2	B	181	GLU	CB-CG-CD	-5.67	98.88	114.20
3	E	11	PHE	CB-CG-CD2	-5.67	116.83	120.80
3	E	280	HIS	CA-CB-CG	-5.67	103.96	113.60
4	F	245	ARG	NE-CZ-NH1	5.67	123.13	120.30
4	G	251	ASN	CB-CA-C	5.67	121.73	110.40
3	E	49	LEU	CB-CA-C	-5.66	99.44	110.20
2	D	347	MET	CB-CA-C	5.66	121.72	110.40
2	D	173	PHE	N-CA-CB	5.66	120.78	110.60
1	A	172	TYR	CB-CG-CD1	5.65	124.39	121.00
3	E	77	TYR	CB-CG-CD2	-5.65	117.61	121.00
3	E	267	ASN	CB-CG-OD1	-5.65	110.30	121.60
4	F	9	HIS	CA-C-N	-5.65	104.77	117.20
4	G	338	MET	CA-CB-CG	-5.65	103.70	113.30
4	F	237	VAL	N-CA-C	-5.65	95.75	111.00
4	F	182	MET	N-CA-C	-5.64	95.77	111.00
4	F	264	LYS	CB-CA-C	-5.64	99.12	110.40
2	B	89	ASP	CB-CG-OD2	-5.63	113.23	118.30
4	G	193	VAL	CA-CB-CG2	-5.63	102.45	110.90
1	A	279	TRP	C-N-CA	5.63	135.77	121.70
2	D	210	ALA	CB-CA-C	-5.62	101.67	110.10
1	A	281	ASN	N-CA-CB	-5.62	100.49	110.60
2	D	329	TYR	CB-CG-CD1	-5.61	117.63	121.00
2	D	174	HIS	CA-CB-CG	-5.61	104.07	113.60
3	E	4	TYR	N-CA-CB	5.61	120.69	110.60
2	D	277	GLU	CB-CG-CD	-5.60	99.07	114.20
1	A	270	ARG	N-CA-C	5.60	126.13	111.00
3	E	319	ILE	CB-CA-C	-5.60	100.40	111.60
4	G	101	SER	N-CA-C	-5.59	95.91	111.00
1	A	270	ARG	NE-CZ-NH2	-5.58	117.51	120.30
4	G	202	GLU	CB-CA-C	-5.58	99.23	110.40
2	B	79	CYS	CA-CB-SG	-5.57	103.97	114.00
4	F	276	GLU	CG-CD-OE2	5.56	129.43	118.30
3	E	164	LEU	N-CA-CB	5.56	121.52	110.40
1	A	59	THR	C-N-CA	5.56	135.60	121.70
4	G	241	PHE	N-CA-C	-5.56	96.00	111.00
2	B	120	PHE	CA-CB-CG	-5.55	100.57	113.90
2	D	324	ASP	CB-CA-C	-5.55	99.30	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	112	VAL	N-CA-C	-5.55	96.01	111.00
2	D	328	TYR	CB-CG-CD2	-5.55	117.67	121.00
4	F	319	PHE	CB-CG-CD1	5.55	124.68	120.80
2	B	246	ASP	CA-CB-CG	5.55	125.61	113.40
4	F	258	ALA	N-CA-C	-5.55	96.03	111.00
4	F	97	MET	N-CA-C	-5.54	96.03	111.00
2	D	254	GLU	CB-CG-CD	-5.54	99.25	114.20
4	F	86	ALA	N-CA-CB	5.54	117.85	110.10
4	G	57	VAL	CA-CB-CG1	5.54	119.20	110.90
2	C	241	LEU	CB-CA-C	-5.53	99.69	110.20
4	G	59	LEU	N-CA-C	-5.52	96.09	111.00
2	D	49	VAL	CA-CB-CG2	-5.51	102.63	110.90
3	E	260	HIS	CA-CB-CG	-5.51	104.23	113.60
4	F	345	SER	N-CA-C	-5.51	96.12	111.00
2	C	179	ASP	N-CA-CB	5.51	120.51	110.60
2	D	41	TYR	CB-CG-CD1	-5.49	117.70	121.00
3	E	146	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	A	224	GLY	N-CA-C	-5.49	99.37	113.10
1	A	4	LEU	N-CA-C	-5.49	96.18	111.00
4	G	208	ASP	CB-CG-OD1	5.49	123.24	118.30
2	B	249	ALA	CB-CA-C	-5.48	101.88	110.10
2	C	156	THR	N-CA-C	-5.48	96.21	111.00
2	C	257	VAL	CA-CB-CG1	5.47	119.11	110.90
2	D	324	ASP	CB-CG-OD1	5.47	123.22	118.30
2	C	314	ARG	NE-CZ-NH2	-5.47	117.57	120.30
3	E	230	TYR	CG-CD1-CE1	-5.46	116.93	121.30
2	D	345	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	A	70	ALA	CB-CA-C	-5.46	101.91	110.10
1	A	5	TYR	N-CA-C	-5.46	96.27	111.00
3	E	124	ALA	CB-CA-C	-5.45	101.92	110.10
4	F	66	GLY	N-CA-C	-5.45	99.47	113.10
4	F	99	VAL	N-CA-C	-5.45	96.28	111.00
4	F	216	VAL	CA-CB-CG2	-5.45	102.72	110.90
4	F	193	VAL	N-CA-C	-5.45	96.29	111.00
4	G	274	SER	N-CA-C	-5.44	96.30	111.00
4	F	309	THR	N-CA-C	-5.44	96.31	111.00
2	D	239	ALA	N-CA-CB	5.44	117.71	110.10
2	D	342	ALA	N-CA-CB	-5.43	102.50	110.10
2	C	309	ILE	C-N-CA	5.43	135.27	121.70
1	A	332	CYS	CA-C-N	-5.42	105.27	117.20
1	A	338	ASP	CB-CA-C	5.42	121.25	110.40
2	B	43	PHE	N-CA-CB	5.42	120.35	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	337	ARG	N-CA-C	-5.41	96.40	111.00
4	F	326	ASP	CB-CG-OD2	5.40	123.16	118.30
4	G	66	GLY	N-CA-C	-5.40	99.60	113.10
2	B	38	HIS	N-CA-CB	-5.39	100.90	110.60
4	G	252	PRO	N-CA-C	-5.39	98.09	112.10
1	A	168	GLN	CB-CG-CD	-5.39	97.59	111.60
2	B	338	GLU	N-CA-CB	5.38	120.29	110.60
3	E	15	VAL	N-CA-CB	-5.38	99.66	111.50
3	E	206	GLN	CA-C-N	-5.38	105.44	116.20
1	A	217	TRP	CB-CG-CD2	5.38	133.59	126.60
3	E	46	ARG	NE-CZ-NH2	-5.37	117.61	120.30
4	F	92	LEU	N-CA-C	-5.37	96.50	111.00
2	C	201	ARG	NE-CZ-NH1	-5.37	117.62	120.30
3	E	222	TYR	CG-CD1-CE1	-5.37	117.01	121.30
2	B	150	VAL	CA-CB-CG2	5.36	118.95	110.90
3	E	262	ALA	C-N-CA	5.36	135.10	121.70
4	F	122	TRP	CA-CB-CG	5.36	123.88	113.70
1	A	279	TRP	N-CA-CB	5.36	120.24	110.60
4	F	155	LEU	C-N-CA	5.36	135.09	121.70
1	A	58	ASN	N-CA-CB	5.35	120.23	110.60
2	D	312	ARG	NE-CZ-NH2	5.35	122.98	120.30
3	E	312	ILE	CA-CB-CG1	5.35	121.17	111.00
2	C	36	ARG	NE-CZ-NH1	-5.35	117.62	120.30
4	F	276	GLU	OE1-CD-OE2	-5.35	116.88	123.30
4	G	103	ARG	NE-CZ-NH2	-5.35	117.62	120.30
3	E	15	VAL	CB-CA-C	-5.35	101.24	111.40
4	F	96	ARG	N-CA-C	-5.35	96.56	111.00
4	F	345	SER	CA-C-N	-5.35	105.44	117.20
4	G	105	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	A	314	GLN	N-CA-CB	-5.34	100.98	110.60
2	D	87	PHE	N-CA-CB	5.34	120.21	110.60
2	D	185	HIS	N-CA-CB	-5.34	101.00	110.60
3	E	276	GLU	CB-CG-CD	-5.33	99.80	114.20
4	F	329	ASN	CB-CG-OD1	5.33	132.27	121.60
4	G	229	ASP	CB-CA-C	-5.33	99.74	110.40
2	D	49	VAL	CB-CA-C	-5.32	101.28	111.40
3	E	205	PHE	CA-CB-CG	-5.32	101.12	113.90
4	G	159	LEU	CB-CA-C	-5.32	100.09	110.20
1	A	10	ARG	NE-CZ-NH2	-5.32	117.64	120.30
4	F	160	PHE	CB-CG-CD2	-5.32	117.08	120.80
2	B	89	ASP	CB-CA-C	-5.31	99.77	110.40
4	G	171	ALA	N-CA-C	-5.31	96.65	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	289	GLN	N-CA-C	-5.31	96.65	111.00
3	E	308	ARG	CG-CD-NE	-5.31	100.65	111.80
4	F	37	VAL	N-CA-C	-5.31	96.67	111.00
1	A	124	ALA	N-CA-CB	5.30	117.53	110.10
4	F	124	SER	N-CA-CB	-5.30	102.55	110.50
2	C	362	ARG	CB-CA-C	5.30	120.99	110.40
4	F	332	LYS	N-CA-C	-5.30	96.70	111.00
4	G	311	SER	CA-C-N	-5.29	105.61	116.20
2	C	250	LEU	CB-CG-CD1	5.29	119.99	111.00
2	B	345	ARG	NE-CZ-NH1	-5.28	117.66	120.30
3	E	171	TYR	CB-CG-CD2	-5.28	117.83	121.00
3	E	123	ALA	CB-CA-C	5.28	118.02	110.10
4	F	191	HIS	N-CA-C	-5.28	96.75	111.00
2	B	282	LEU	CB-CA-C	-5.27	100.19	110.20
2	C	367	GLU	CA-CB-CG	-5.27	101.81	113.40
1	A	216	HIS	N-CA-CB	-5.26	101.12	110.60
2	D	27	ALA	N-CA-CB	5.26	117.47	110.10
3	E	95	GLU	N-CA-C	5.26	125.20	111.00
4	F	241	PHE	CB-CG-CD2	-5.26	117.12	120.80
3	E	73	HIS	N-CA-CB	-5.26	101.14	110.60
2	D	240	MET	N-CA-CB	5.25	120.06	110.60
4	F	246	ARG	CD-NE-CZ	-5.25	116.25	123.60
1	A	101	THR	CA-CB-CG2	-5.25	105.05	112.40
2	B	6	LEU	CB-CA-C	-5.25	100.23	110.20
2	D	227	SER	N-CA-CB	-5.24	102.63	110.50
3	E	198	PRO	N-CA-C	-5.24	98.47	112.10
1	A	183	GLN	CB-CA-C	-5.24	99.92	110.40
2	B	110	ASN	CB-CA-C	-5.24	99.93	110.40
4	G	355	GLN	CA-C-N	-5.24	105.68	117.20
3	E	244	ARG	NE-CZ-NH1	-5.23	117.69	120.30
1	A	198	THR	N-CA-C	-5.22	96.89	111.00
4	F	215	ARG	CG-CD-NE	-5.22	100.83	111.80
3	E	331	VAL	N-CA-C	-5.22	96.90	111.00
2	B	66	THR	N-CA-CB	5.22	120.22	110.30
2	C	362	ARG	NE-CZ-NH2	5.22	122.91	120.30
1	A	163	ASP	CB-CG-OD2	-5.21	113.61	118.30
2	D	36	ARG	NE-CZ-NH2	-5.21	117.70	120.30
3	E	18	TYR	CD1-CE1-CZ	-5.21	115.11	119.80
1	A	20	ALA	N-CA-CB	5.20	117.38	110.10
2	B	156	THR	N-CA-C	-5.20	96.95	111.00
1	A	225	LYS	O-C-N	5.20	131.02	122.70
2	C	151	LYS	N-CA-CB	5.20	119.96	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	167	ASN	CA-CB-CG	5.20	124.84	113.40
1	A	24	LEU	N-CA-C	-5.20	96.97	111.00
2	C	42	LEU	N-CA-CB	5.20	120.79	110.40
4	G	17	VAL	CG1-CB-CG2	5.19	119.20	110.90
4	G	43	SER	N-CA-C	-5.19	96.99	111.00
4	G	97	MET	N-CA-C	-5.19	96.99	111.00
1	A	231	HIS	CA-CB-CG	-5.18	104.79	113.60
4	G	335	ASN	N-CA-C	-5.18	97.00	111.00
4	G	319	PHE	CB-CG-CD2	-5.18	117.17	120.80
4	F	323	TYR	CB-CG-CD1	5.18	124.11	121.00
1	A	278	VAL	N-CA-CB	5.18	122.89	111.50
3	E	319	ILE	CA-CB-CG1	-5.18	101.16	111.00
4	G	39	ASP	N-CA-CB	5.18	119.92	110.60
4	F	335	ASN	CA-C-O	5.18	130.97	120.10
3	E	234	ALA	CB-CA-C	-5.18	102.33	110.10
2	C	316	LEU	CB-CA-C	5.17	120.03	110.20
4	F	64	GLU	N-CA-C	-5.17	97.03	111.00
4	F	6	GLU	N-CA-C	-5.17	97.05	111.00
4	G	35	LEU	CB-CA-C	-5.17	100.38	110.20
1	A	275	LYS	CB-CA-C	-5.17	100.07	110.40
1	A	172	TYR	CB-CG-CD2	-5.16	117.90	121.00
4	F	308	VAL	CA-C-N	-5.16	105.84	117.20
4	G	186	GLN	CA-C-N	-5.16	105.85	117.20
3	E	91	ASP	CB-CA-C	5.15	120.70	110.40
3	E	199	GLY	N-CA-C	-5.15	100.23	113.10
4	F	32	ASN	N-CA-C	-5.15	97.10	111.00
4	F	9	HIS	CA-CB-CG	-5.15	104.85	113.60
3	E	140	TRP	N-CA-C	-5.15	97.11	111.00
1	A	283	ARG	CG-CD-NE	-5.14	101.00	111.80
2	B	76	CYS	CB-CA-C	-5.14	100.11	110.40
4	F	191	HIS	N-CA-CB	5.14	119.86	110.60
2	C	358	ALA	CB-CA-C	-5.14	102.40	110.10
4	G	133	ALA	CB-CA-C	-5.13	102.40	110.10
2	D	77	ASP	CA-CB-CG	-5.13	102.11	113.40
4	G	57	VAL	CA-CB-CG2	-5.12	103.22	110.90
1	A	87	ASN	N-CA-CB	-5.12	101.39	110.60
3	E	322	TYR	N-CA-C	5.12	124.81	111.00
4	G	336	VAL	CA-C-N	-5.12	105.95	117.20
4	F	137	ARG	NE-CZ-NH1	5.11	122.86	120.30
3	E	298	GLU	CB-CA-C	-5.11	100.18	110.40
2	B	122	VAL	N-CA-C	-5.11	97.21	111.00
4	G	148	HIS	C-N-CA	5.11	134.46	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	170	CYS	CA-CB-SG	-5.10	104.82	114.00
2	B	285	MET	CA-CB-CG	-5.10	104.64	113.30
1	A	196	LYS	N-CA-CB	5.09	119.76	110.60
4	F	343	SER	N-CA-CB	5.09	118.14	110.50
2	B	66	THR	N-CA-C	-5.09	97.26	111.00
4	G	76	PHE	CB-CG-CD2	-5.09	117.24	120.80
4	G	44	LEU	CA-CB-CG	-5.08	103.61	115.30
2	D	173	PHE	CB-CG-CD1	5.08	124.36	120.80
4	G	152	ARG	CB-CG-CD	5.08	124.81	111.60
3	E	229	TRP	N-CA-CB	-5.08	101.46	110.60
1	A	265	ALA	N-CA-C	-5.08	97.30	111.00
4	F	69	THR	N-CA-CB	5.07	119.94	110.30
3	E	144	ALA	N-CA-CB	5.07	117.20	110.10
2	B	8	ARG	NE-CZ-NH2	5.06	122.83	120.30
3	E	48	LEU	CB-CG-CD1	5.06	119.61	111.00
2	C	135	SER	N-CA-CB	-5.06	102.91	110.50
4	G	82	LEU	CD1-CG-CD2	5.06	125.68	110.50
4	G	261	ASP	N-CA-CB	-5.06	101.49	110.60
4	G	24	ARG	NE-CZ-NH1	5.05	122.83	120.30
2	B	358	ALA	CB-CA-C	-5.05	102.53	110.10
3	E	91	ASP	CA-CB-CG	-5.05	102.29	113.40
2	C	207	ALA	N-CA-CB	5.04	117.16	110.10
2	C	313	MET	CG-SD-CE	-5.04	92.13	100.20
4	F	314	GLU	CB-CG-CD	-5.04	100.59	114.20
4	F	333	CYS	CA-C-N	-5.04	106.11	117.20
4	G	254	LYS	N-CA-C	-5.04	97.39	111.00
2	B	274	ARG	C-N-CA	5.04	132.87	122.30
3	E	192	ARG	CB-CA-C	-5.03	100.33	110.40
4	F	282	ARG	CD-NE-CZ	-5.03	116.55	123.60
4	G	147	ALA	N-CA-C	-5.03	97.41	111.00
3	E	4	TYR	CB-CG-CD1	-5.03	117.98	121.00
2	C	10	TRP	CB-CG-CD2	-5.03	120.06	126.60
3	E	129	LEU	CB-CA-C	-5.03	100.65	110.20
4	G	173	ASP	CB-CA-C	-5.03	100.35	110.40
1	A	21	TYR	N-CA-C	-5.02	97.44	111.00
2	B	209	ALA	N-CA-CB	5.02	117.13	110.10
4	F	176	ARG	CG-CD-NE	-5.02	101.25	111.80
4	F	207	LEU	CB-CA-C	-5.02	100.66	110.20
2	D	117	ARG	NE-CZ-NH2	-5.01	117.79	120.30
4	F	98	LEU	N-CA-C	-5.01	97.46	111.00
2	D	94	ASP	N-CA-CB	5.01	119.62	110.60
3	E	228	ASP	CB-CG-OD1	-5.01	113.79	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	340	PHE	CB-CG-CD2	-5.01	117.30	120.80
2	D	25	LEU	CB-CA-C	-5.00	100.69	110.20
2	B	173	PHE	CB-CA-C	-5.00	100.40	110.40
4	G	42	LEU	N-CA-C	-5.00	97.50	111.00
4	G	282	ARG	CB-CA-C	-5.00	100.40	110.40

There are no chirality outliers.

All (83) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	174	TYR	Sidechain
1	A	21	TYR	Sidechain
1	A	228	ARG	Sidechain
1	A	231	HIS	Sidechain
1	A	252	ARG	Sidechain
1	A	266	HIS	Sidechain
1	A	270	ARG	Sidechain
1	A	273	PHE	Sidechain
1	A	277	ARG	Sidechain
1	A	283	ARG	Sidechain
1	A	299	ARG	Sidechain
1	A	307	ARG	Sidechain
1	A	316	TYR	Sidechain
1	A	333	HIS	Sidechain
1	A	39	ARG	Sidechain
1	A	77	ARG	Sidechain
2	B	11	ARG	Sidechain
2	B	137	ASN	Peptide
2	B	201	ARG	Sidechain
2	B	215	ARG	Sidechain
2	B	314	ARG	Sidechain,Mainchain
2	B	336	ARG	Sidechain
2	B	355	ARG	Sidechain
2	B	87	PHE	Sidechain
2	C	119	ARG	Sidechain
2	C	123	TYR	Sidechain
2	C	185	HIS	Sidechain
2	C	263	ARG	Sidechain
2	C	274	ARG	Sidechain
2	C	312	ARG	Sidechain
2	C	345	ARG	Sidechain
2	C	359	PHE	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	D	123	TYR	Sidechain
2	D	169	ARG	Sidechain
2	D	201	ARG	Sidechain
2	D	208	ARG	Sidechain
2	D	290	HIS	Sidechain
2	D	3	TYR	Sidechain
2	D	314	ARG	Sidechain
2	D	328	TYR	Sidechain
2	D	355	ARG	Sidechain
2	D	360	HIS	Sidechain
2	D	41	TYR	Sidechain
2	D	47	ARG	Sidechain
3	E	105	ARG	Sidechain
3	E	146	ARG	Sidechain
3	E	158	ARG	Sidechain
3	E	163	TYR	Sidechain
3	E	171	TYR	Sidechain
3	E	18	TYR	Sidechain
3	E	222	TYR	Sidechain
3	E	259	HIS	Sidechain
3	E	260	HIS	Sidechain
3	E	308	ARG	Sidechain
3	E	322	TYR	Sidechain
3	E	42	TYR	Sidechain
3	E	46	ARG	Sidechain
3	E	73	HIS	Sidechain
3	E	77	TYR	Sidechain
3	E	8	ARG	Sidechain
4	F	105	ARG	Sidechain
4	F	197	ARG	Sidechain
4	F	205	ARG	Sidechain
4	F	230	PHE	Sidechain
4	F	241	PHE	Sidechain
4	F	244	TYR	Sidechain
4	F	246	ARG	Sidechain
4	F	267	PHE	Sidechain
4	F	282	ARG	Sidechain
4	F	284	TYR	Sidechain
4	F	323	TYR	Sidechain
4	F	359	TYR	Sidechain
4	F	56	ARG	Sidechain
4	F	9	HIS	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
4	G	137	ARG	Sidechain
4	G	230	PHE	Sidechain
4	G	240	ARG	Sidechain
4	G	244	TYR	Sidechain
4	G	255	HIS	Sidechain
4	G	323	TYR	Sidechain
4	G	337	ARG	Sidechain
4	G	359	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2726	0	2779	311	0
2	B	2796	0	2846	165	0
2	C	2835	0	2889	228	0
2	D	2786	0	2832	354	0
3	E	2602	0	2607	431	0
4	F	2844	0	2861	440	0
4	G	2844	0	2861	346	0
All	All	19433	0	19675	2150	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 55.

All (2150) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:LEU:HD11	4:F:176:ARG:C	1.48	1.33
1:A:73:LEU:CD2	4:F:177:LEU:HB2	1.65	1.26
1:A:73:LEU:HD21	4:F:177:LEU:CB	1.77	1.14
1:A:73:LEU:HD13	4:F:172:THR:OG1	1.49	1.10
1:A:73:LEU:HD22	4:F:177:LEU:HB2	1.32	1.07
1:A:73:LEU:CD2	4:F:177:LEU:CB	2.31	1.06
1:A:73:LEU:CD1	4:F:176:ARG:C	2.24	1.05
1:A:73:LEU:HD21	4:F:177:LEU:HB3	1.37	1.02

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:354:SER:HA	4:F:357:ALA:HB3	1.41	1.00
2:D:295:VAL:HG11	2:D:314:ARG:HA	1.44	0.97
1:A:72:SER:OG	4:F:362:MET:SD	2.21	0.97
1:A:73:LEU:HD13	4:F:172:THR:HG1	1.26	0.94
1:A:73:LEU:HD11	4:F:177:LEU:N	1.84	0.91
4:G:207:LEU:HD21	4:G:214:LEU:HB2	1.51	0.90
3:E:146:ARG:HB3	3:E:150:ARG:HE	1.38	0.89
3:E:33:PRO:HD3	3:E:146:ARG:HA	1.55	0.89
4:F:193:VAL:HG21	4:F:236:LEU:HD13	1.59	0.84
2:B:129:HIS:CD2	2:B:158:ASP:HB3	2.13	0.83
1:A:73:LEU:CD1	4:F:176:ARG:O	2.27	0.83
2:B:286:LEU:HD13	2:B:336:ARG:HH11	1.44	0.82
4:G:17:VAL:HA	4:G:53:MET:HB3	1.60	0.82
1:A:263:GLN:HA	1:A:266:HIS:CE1	2.15	0.81
2:D:201:ARG:HG2	2:D:234:THR:HG23	1.60	0.81
1:A:220:ALA:HB1	1:A:228:ARG:HG3	1.62	0.81
4:F:121:ASP:HA	4:F:224:ARG:HH22	1.45	0.81
1:A:300:GLN:HE21	1:A:330:LEU:HD11	1.45	0.81
4:F:53:MET:CE	4:F:230:PHE:HB3	2.11	0.81
4:G:206:MET:HB3	4:G:227:VAL:HB	1.62	0.81
2:D:121:LYS:H	2:D:149:HIS:HB2	1.44	0.80
4:G:132:GLN:HB3	4:G:207:LEU:HD22	1.62	0.80
1:A:73:LEU:HD12	4:F:175:HIS:N	1.97	0.79
2:C:357:LEU:O	2:C:364:PRO:HA	1.82	0.79
3:E:229:TRP:HD1	3:E:320:GLU:HG2	1.45	0.79
1:A:69:GLN:HE21	4:F:362:MET:CE	1.96	0.79
4:F:122:TRP:CE3	4:F:222:ASN:HB2	2.17	0.79
1:A:220:ALA:CB	1:A:228:ARG:HG3	2.13	0.78
4:G:77:ASP:HA	4:G:80:ARG:HE	1.46	0.78
1:A:69:GLN:HE21	4:F:362:MET:HE1	1.49	0.78
2:D:67:GLY:HA2	2:D:119:ARG:HH12	1.48	0.78
2:C:15:PHE:CD1	2:C:72:PRO:HA	2.18	0.78
1:A:73:LEU:HD12	4:F:176:ARG:N	1.99	0.78
2:B:315:GLU:HA	2:B:318:ARG:HE	1.48	0.78
2:C:347:MET:SD	2:D:287:GLY:HA2	2.23	0.78
2:D:201:ARG:CG	2:D:234:THR:HG23	2.14	0.77
1:A:220:ALA:HA	1:A:223:MET:SD	2.25	0.77
2:B:292:ILE:HG23	2:B:317:ALA:HA	1.65	0.77
2:D:25:LEU:HD23	2:D:54:ILE:HD11	1.67	0.77
1:A:73:LEU:HD23	4:F:247:VAL:HG21	1.67	0.77
3:E:118:ALA:HB1	3:E:150:ARG:HB3	1.67	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:21:GLN:HA	2:D:23:HIS:CE1	2.19	0.77
2:D:122:VAL:HG22	2:D:151:LYS:HG3	1.66	0.77
4:F:100:ARG:HH11	4:F:105:ARG:HG2	1.47	0.77
2:D:23:HIS:CD2	2:D:24:VAL:HG23	2.21	0.76
1:A:330:LEU:O	1:A:333:HIS:CE1	2.38	0.76
2:B:259:ALA:HB2	2:B:360:HIS:HA	1.65	0.76
3:E:176:LEU:HD11	3:E:202:LEU:HA	1.68	0.76
4:F:317:ILE:HD12	4:F:343:SER:HA	1.68	0.76
4:G:132:GLN:CB	4:G:207:LEU:HD22	2.16	0.76
1:A:269:LEU:H	1:A:269:LEU:HD22	1.51	0.76
3:E:212:ALA:HA	3:E:215:THR:OG1	1.86	0.75
4:F:121:ASP:HA	4:F:224:ARG:NH2	2.01	0.75
3:E:75:ASP:HB3	3:E:110:LYS:HA	1.67	0.74
4:G:9:HIS:CG	4:G:57:VAL:HG13	2.22	0.74
4:F:193:VAL:HG23	4:F:238:ASP:CG	2.07	0.74
3:E:31:ALA:HB1	3:E:35:MET:SD	2.27	0.74
4:G:9:HIS:CD2	4:G:57:VAL:HG13	2.23	0.74
4:G:258:ALA:HB2	4:G:308:VAL:HG22	1.70	0.74
1:A:78:GLN:H	1:A:107:ASP:HA	1.53	0.74
4:F:146:MET:CA	4:F:171:ALA:HB1	2.19	0.73
1:A:73:LEU:HD22	4:F:177:LEU:CD1	2.18	0.73
4:G:3:PHE:HB3	4:G:63:HIS:HA	1.71	0.73
3:E:48:LEU:HD22	3:E:140:TRP:CG	2.23	0.73
3:E:180:VAL:HG21	3:E:205:PHE:CD2	2.23	0.73
2:D:3:TYR:HB2	3:E:21:GLY:HA2	1.71	0.73
3:E:10:ASP:HA	3:E:162:HIS:CE1	2.24	0.73
4:F:103:ARG:HE	4:G:305:ILE:HB	1.54	0.73
2:C:191:LEU:HD22	2:C:196:ILE:HB	1.70	0.73
1:A:154:ARG:HA	1:A:157:GLN:HG2	1.70	0.73
3:E:11:PHE:CD1	3:E:56:HIS:HE1	2.06	0.73
4:F:137:ARG:HE	4:F:332:LYS:HE3	1.53	0.73
1:A:77:ARG:HE	1:A:107:ASP:H	1.35	0.73
2:D:288:LEU:HA	2:D:306:MET:SD	2.29	0.73
3:E:297:ARG:O	3:E:301:MET:HG2	1.89	0.73
3:E:227:GLY:HA2	3:E:323:LEU:CD1	2.19	0.72
3:E:18:TYR:HB2	3:E:52:GLN:HE22	1.55	0.72
4:G:3:PHE:CB	4:G:63:HIS:HA	2.20	0.72
4:G:296:ASN:HD21	4:G:298:GLU:HB3	1.55	0.72
2:D:120:PHE:HD1	2:D:149:HIS:HA	1.55	0.72
4:G:162:THR:H	4:G:190:SER:HB3	1.55	0.72
4:F:56:ARG:H	4:F:229:ASP:HB3	1.55	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:181:SER:O	4:G:356:SER:HA	1.90	0.71
2:D:2:SER:CA	3:E:25:HIS:HB3	2.20	0.71
3:E:180:VAL:HG11	3:E:205:PHE:HB2	1.72	0.71
4:G:82:LEU:HD13	4:G:101:SER:HB3	1.72	0.71
2:C:255:ALA:HB2	2:C:263:ARG:NE	2.06	0.71
3:E:90:VAL:HA	3:E:124:ALA:HA	1.70	0.71
3:E:48:LEU:O	3:E:109:ALA:HB3	1.91	0.71
2:C:75:VAL:H	2:C:79:CYS:HB2	1.56	0.71
1:A:73:LEU:HD11	4:F:176:ARG:CA	2.21	0.70
4:G:203:LEU:HD21	4:G:232:PHE:CD1	2.25	0.70
2:C:227:SER:HA	2:D:27:ALA:CB	2.21	0.70
1:A:73:LEU:HD22	4:F:177:LEU:CB	2.08	0.70
3:E:295:HIS:HA	3:E:298:GLU:HG2	1.74	0.70
1:A:272:LEU:HD21	1:A:273:PHE:CZ	2.26	0.70
1:A:231:HIS:CE1	1:A:235:GLN:HE21	2.10	0.70
4:F:59:LEU:HD21	4:F:63:HIS:HB3	1.74	0.70
2:D:114:ALA:HB2	4:G:366:LEU:HD21	1.73	0.70
3:E:229:TRP:CD1	3:E:320:GLU:HG2	2.26	0.70
4:F:202:GLU:HB2	4:F:205:ARG:HH21	1.57	0.70
3:E:14:LEU:HD22	3:E:27:LEU:HD13	1.74	0.70
4:F:256:LEU:HB3	4:F:338:MET:SD	2.31	0.70
4:G:177:LEU:HD21	4:G:179:VAL:HG13	1.74	0.70
1:A:148:PRO:HB3	1:A:167:ASN:HD21	1.57	0.70
3:E:146:ARG:HD2	3:E:150:ARG:HH21	1.55	0.70
4:G:206:MET:O	4:G:207:LEU:HD23	1.92	0.69
3:E:14:LEU:HD21	3:E:162:HIS:CD2	2.27	0.69
2:C:114:ALA:HA	2:C:149:HIS:CD2	2.27	0.69
1:A:166:ALA:HA	1:A:199:LEU:HD13	1.74	0.69
4:F:255:HIS:CG	4:F:256:LEU:N	2.60	0.69
1:A:23:LEU:HD22	1:A:34:SER:HB3	1.73	0.69
1:A:73:LEU:HD23	4:F:247:VAL:CG2	2.23	0.69
3:E:118:ALA:CB	3:E:150:ARG:HB3	2.22	0.69
3:E:182:MET:SD	3:E:205:PHE:CD1	2.85	0.69
3:E:224:VAL:HA	3:E:229:TRP:CZ2	2.27	0.69
4:F:337:ARG:HH12	4:F:352:ALA:HA	1.57	0.69
4:G:193:VAL:HG21	4:G:218:ILE:HG13	1.73	0.69
1:A:234:GLN:HE21	2:B:303:GLY:HA3	1.58	0.69
1:A:333:HIS:HB3	1:A:338:ASP:H	1.59	0.68
2:C:359:PHE:CE1	2:D:323:THR:HA	2.28	0.68
3:E:48:LEU:HD13	3:E:142:PHE:CZ	2.28	0.68
4:G:260:CYS:HB3	4:G:334:GLU:HA	1.76	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:SER:HA	1:A:195:GLY:HA2	1.75	0.68
2:C:364:PRO:HG2	2:C:367:GLU:CD	2.13	0.68
4:F:182:MET:HA	4:F:355:GLN:HB2	1.75	0.68
3:E:281:LEU:HA	3:E:285:ARG:HE	1.58	0.68
1:A:297:GLN:HB2	1:A:333:HIS:CE1	2.28	0.68
2:C:244:LEU:HD13	2:C:274:ARG:HH11	1.58	0.68
2:C:199:GLU:HG3	2:C:202:ALA:H	1.59	0.68
1:A:73:LEU:CD1	4:F:176:ARG:N	2.56	0.68
2:C:225:ILE:HG23	2:C:230:GLY:HA2	1.76	0.68
3:E:33:PRO:CD	3:E:146:ARG:HA	2.24	0.68
4:F:146:MET:HA	4:F:171:ALA:HB1	1.76	0.68
4:F:159:LEU:CD1	4:F:240:ARG:HA	2.24	0.68
4:F:321:VAL:O	4:F:324:VAL:HG22	1.93	0.68
1:A:77:ARG:HA	1:A:107:ASP:HA	1.75	0.67
2:D:2:SER:HA	3:E:25:HIS:HB3	1.75	0.67
2:D:310:GLU:HG3	2:D:314:ARG:HD3	1.76	0.67
4:F:317:ILE:CD1	4:F:343:SER:HA	2.24	0.67
4:G:193:VAL:HA	4:G:236:LEU:HD22	1.77	0.67
2:B:69:THR:HB	2:B:71:THR:H	1.59	0.67
2:D:210:ALA:HB1	2:D:217:ALA:HB2	1.77	0.67
4:G:331:LEU:HD11	4:G:333:CYS:HB3	1.75	0.67
3:E:191:LEU:CD1	3:E:201:ALA:HB2	2.25	0.67
4:G:357:ALA:HB1	4:G:359:TYR:CE2	2.30	0.67
3:E:32:LEU:HD13	3:E:35:MET:HE3	1.77	0.67
3:E:48:LEU:HD22	3:E:140:TRP:CD2	2.30	0.67
4:F:121:ASP:CA	4:F:224:ARG:HH22	2.07	0.67
3:E:25:HIS:HA	3:E:140:TRP:CZ3	2.30	0.67
3:E:92:ALA:HA	3:E:95:GLU:OE2	1.95	0.67
4:F:357:ALA:HB1	4:F:359:TYR:CZ	2.29	0.67
4:F:223:ILE:HB	4:F:236:LEU:HD11	1.77	0.66
4:F:254:LYS:HB2	4:F:340:LEU:HB2	1.77	0.66
4:G:315:MET:HA	4:G:342:ASP:CB	2.25	0.66
1:A:270:ARG:HA	1:A:273:PHE:CD2	2.31	0.66
4:F:8:GLU:HA	4:F:11:LEU:HB2	1.77	0.66
4:G:92:LEU:HA	4:G:97:MET:SD	2.36	0.66
1:A:331:LEU:O	1:A:333:HIS:CD2	2.48	0.66
2:C:355:ARG:HG3	2:C:359:PHE:CE2	2.30	0.66
2:B:111:VAL:HG11	2:B:147:PRO:HG2	1.77	0.66
3:E:49:LEU:HD21	3:E:73:HIS:CE1	2.31	0.66
4:G:245:ARG:HA	4:G:245:ARG:HE	1.61	0.66
2:C:289:LEU:HD13	2:C:329:TYR:CA	2.25	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:31:GLY:CA	4:G:73:ARG:HH12	2.08	0.66
1:A:192:TRP:HB2	1:A:195:GLY:H	1.60	0.66
2:C:358:ALA:HB3	2:D:326:GLN:HG3	1.78	0.66
2:D:256:MET:HG2	2:D:357:LEU:HA	1.78	0.66
3:E:11:PHE:CD1	3:E:56:HIS:CE1	2.83	0.66
3:E:33:PRO:HA	3:E:37:ASP:HB2	1.76	0.66
4:F:135:MET:HG3	4:F:207:LEU:HD12	1.78	0.66
4:F:259:GLY:HA2	4:F:334:GLU:OE1	1.96	0.66
3:E:49:LEU:HD22	3:E:68:MET:HG3	1.78	0.65
2:B:73:CYS:HB3	2:B:76:CYS:SG	2.37	0.65
4:F:51:MET:HB2	4:F:232:PHE:CE2	2.32	0.65
1:A:273:PHE:CD2	1:A:283:ARG:HA	2.31	0.65
2:B:64:CYS:HB3	2:B:79:CYS:SG	2.36	0.65
2:D:346:ARG:HH22	3:E:192:ARG:HD2	1.60	0.65
3:E:33:PRO:HD3	3:E:146:ARG:CA	2.25	0.65
3:E:140:TRP:HB3	3:E:142:PHE:CZ	2.31	0.65
1:A:158:LEU:HD13	1:A:185:LEU:HD13	1.78	0.65
2:C:15:PHE:CE1	2:C:57:LEU:HB3	2.32	0.65
2:D:261:GLY:HA2	2:D:357:LEU:HD21	1.78	0.65
3:E:31:ALA:HB1	3:E:35:MET:CG	2.26	0.65
4:F:6:GLU:OE2	4:F:9:HIS:CE1	2.50	0.65
4:G:191:HIS:CD2	4:G:218:ILE:HG12	2.32	0.65
4:F:12:LYS:HZ2	4:F:16:GLN:HG3	1.59	0.65
4:F:162:THR:O	4:F:190:SER:HA	1.96	0.65
4:G:206:MET:HB3	4:G:227:VAL:CB	2.25	0.65
2:D:62:LEU:HD23	2:D:68:ILE:HG22	1.78	0.65
2:D:79:CYS:HA	2:D:82:ILE:HD12	1.79	0.65
4:G:5:VAL:HA	4:G:59:LEU:HD12	1.79	0.65
2:D:195:HIS:CD2	2:D:196:ILE:H	2.15	0.65
3:E:27:LEU:HA	3:E:160:ARG:O	1.98	0.64
3:E:278:ALA:HA	3:E:286:LEU:HD11	1.79	0.64
4:G:9:HIS:CE1	4:G:58:ALA:O	2.50	0.64
4:F:212:ASN:HB3	4:F:227:VAL:HG13	1.78	0.64
3:E:18:TYR:CG	3:E:140:TRP:CZ3	2.85	0.64
4:F:255:HIS:CE1	4:F:257:GLU:H	2.14	0.64
2:D:121:LYS:O	2:D:150:VAL:HA	1.97	0.64
2:D:224:ALA:HA	2:D:240:MET:SD	2.37	0.64
2:D:296:GLN:HG2	2:D:317:ALA:O	1.96	0.64
3:E:47:TYR:HE2	3:E:52:GLN:HE21	1.44	0.64
4:G:78:ILE:HG21	4:G:99:VAL:HG11	1.79	0.64
4:F:24:ARG:HH22	4:F:73:ARG:HG2	1.62	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:53:MET:HE1	4:F:206:MET:SD	2.37	0.64
2:C:252:LEU:O	2:C:255:ALA:HB3	1.97	0.64
2:D:7:ALA:HA	2:D:218:LEU:HD13	1.80	0.64
2:C:179:ASP:HB2	2:C:182:GLN:H	1.62	0.64
2:C:282:LEU:HA	2:C:285:MET:HE3	1.80	0.64
2:D:39:HIS:HB2	2:D:151:LYS:HA	1.80	0.64
4:G:357:ALA:HB1	4:G:359:TYR:CZ	2.32	0.64
3:E:3:TRP:HA	3:E:7:LEU:HD12	1.80	0.64
4:F:122:TRP:NE1	4:F:219:GLY:HA3	2.12	0.64
4:F:137:ARG:HE	4:F:332:LYS:CE	2.11	0.64
1:A:189:SER:HA	1:A:195:GLY:CA	2.28	0.64
2:C:341:TYR:HB2	2:D:333:LEU:CD1	2.28	0.64
2:C:338:GLU:HB3	2:D:333:LEU:HD21	1.79	0.63
2:C:358:ALA:HB1	2:D:322:PRO:HB2	1.79	0.63
3:E:35:MET:SD	3:E:166:PRO:HA	2.38	0.63
4:F:124:SER:CB	4:F:217:GLN:HB3	2.28	0.63
4:F:354:SER:CA	4:F:357:ALA:HB3	2.22	0.63
3:E:158:ARG:H	3:E:158:ARG:HD2	1.64	0.63
3:E:25:HIS:HA	3:E:140:TRP:CE3	2.33	0.63
2:C:111:VAL:O	2:C:150:VAL:HG21	1.97	0.63
2:D:42:LEU:HD21	2:D:159:PRO:HB3	1.79	0.63
2:D:298:SER:HB2	2:D:301:ALA:H	1.62	0.63
3:E:88:LEU:HB3	3:E:120:LEU:HA	1.80	0.63
4:F:317:ILE:HA	4:F:343:SER:HB2	1.81	0.63
4:G:131:PRO:O	4:G:135:MET:HB2	1.99	0.63
2:D:324:ASP:HA	2:D:327:LEU:HD12	1.79	0.63
3:E:254:ASP:HB3	3:E:265:VAL:HG12	1.81	0.63
4:G:146:MET:HB3	4:G:156:ASN:HA	1.80	0.63
1:A:61:TRP:HE1	1:A:93:ILE:HA	1.64	0.63
3:E:280:HIS:HB2	3:E:281:LEU:HD12	1.81	0.63
4:F:59:LEU:HD21	4:F:63:HIS:CB	2.28	0.63
4:F:132:GLN:O	4:F:135:MET:HB3	1.98	0.63
4:G:137:ARG:HH11	4:G:357:ALA:CB	2.12	0.63
2:D:14:THR:CA	2:D:57:LEU:HD21	2.29	0.63
1:A:273:PHE:HB3	1:A:278:VAL:HB	1.81	0.63
4:F:121:ASP:HA	4:F:224:ARG:CZ	2.29	0.63
4:G:146:MET:CB	4:G:156:ASN:HA	2.29	0.63
3:E:203:ALA:HA	3:E:206:GLN:OE1	1.99	0.62
4:F:276:GLU:OE1	4:F:276:GLU:HA	1.98	0.62
4:G:351:ASP:HB2	4:G:354:SER:H	1.64	0.62
1:A:171:CYS:O	1:A:175:GLU:HA	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:96:ALA:HA	2:D:130:MET:HG3	1.81	0.62
3:E:180:VAL:HG21	3:E:205:PHE:CG	2.34	0.62
3:E:241:ALA:HB3	3:E:242:PRO:HD3	1.82	0.62
3:E:252:LEU:HB2	3:E:290:LEU:HD13	1.81	0.62
2:C:278:TRP:HB3	2:C:349:VAL:HG21	1.82	0.62
2:D:131:LEU:HB3	2:D:135:SER:CB	2.29	0.62
2:D:249:ALA:CB	2:D:284:GLU:HG3	2.30	0.62
3:E:32:LEU:HB3	3:E:34:GLY:H	1.64	0.62
3:E:216:LEU:HD13	3:E:235:ALA:HB3	1.82	0.62
4:F:13:PRO:HG2	4:F:57:VAL:CG2	2.29	0.62
2:C:365:LEU:O	2:C:367:GLU:HG2	2.00	0.62
2:B:339:LEU:HB3	2:B:345:ARG:HE	1.62	0.62
2:D:60:LYS:HB2	2:D:72:PRO:CB	2.29	0.62
2:D:338:GLU:HA	2:D:341:TYR:CE2	2.34	0.62
3:E:27:LEU:HD11	3:E:162:HIS:CB	2.30	0.62
2:D:297:LEU:HD12	2:D:298:SER:N	2.15	0.62
2:D:64:CYS:HA	2:D:79:CYS:SG	2.40	0.62
2:D:348:GLY:HA2	2:D:351:MET:SD	2.40	0.62
3:E:109:ALA:HA	3:E:138:GLU:HB3	1.82	0.62
4:F:123:GLN:OE1	4:F:123:GLN:HA	1.99	0.62
1:A:72:SER:OG	4:F:362:MET:CG	2.47	0.62
1:A:273:PHE:CE1	1:A:286:MET:HG3	2.35	0.62
3:E:244:ARG:HA	3:E:247:TRP:CD2	2.34	0.62
4:F:11:LEU:HA	4:F:14:LEU:HB2	1.82	0.62
4:G:22:GLY:HA2	4:G:30:LEU:HB3	1.80	0.62
4:F:218:ILE:HG22	4:F:219:GLY:O	2.00	0.61
4:G:159:LEU:HB2	4:G:241:PHE:CB	2.30	0.61
2:D:4:GLN:HE21	2:D:5:VAL:HG22	1.65	0.61
4:F:13:PRO:HB3	4:F:55:ALA:HB3	1.81	0.61
4:F:121:ASP:HA	4:F:224:ARG:NH1	2.15	0.61
4:G:191:HIS:CD2	4:G:218:ILE:O	2.53	0.61
2:B:180:VAL:O	2:B:207:ALA:HB1	2.00	0.61
3:E:229:TRP:CD1	3:E:320:GLU:CG	2.84	0.61
4:G:6:GLU:CG	4:G:9:HIS:HB2	2.30	0.61
2:C:227:SER:HA	2:D:27:ALA:HB1	1.81	0.61
1:A:211:HIS:CD2	1:A:213:THR:HA	2.36	0.61
1:A:329:LEU:HB3	1:A:334:LYS:NZ	2.16	0.61
4:F:87:GLU:HA	4:F:87:GLU:OE2	2.00	0.61
4:G:14:LEU:HA	4:G:44:LEU:HD21	1.82	0.61
2:C:341:TYR:HB2	2:D:333:LEU:HD12	1.81	0.61
2:D:3:TYR:CD1	3:E:21:GLY:O	2.54	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:154:LEU:HD12	2:D:170:CYS:SG	2.40	0.61
2:D:338:GLU:HA	2:D:341:TYR:CZ	2.35	0.61
4:G:7:ARG:CZ	4:G:84:GLU:HB3	2.30	0.61
4:G:42:LEU:O	4:G:56:ARG:HA	2.00	0.61
4:G:148:HIS:CE1	4:G:156:ASN:HB2	2.36	0.61
4:G:274:SER:HA	4:G:294:ALA:HB1	1.83	0.61
3:E:46:ARG:HE	3:E:65:CYS:HB2	1.66	0.61
3:E:176:LEU:CD1	3:E:202:LEU:HA	2.30	0.61
4:F:144:PHE:CE2	4:F:176:ARG:HD2	2.35	0.61
4:G:254:LYS:HB3	4:G:310:TYR:CE1	2.35	0.61
1:A:148:PRO:CB	1:A:167:ASN:HD21	2.14	0.61
3:E:17:SER:CB	3:E:23:GLY:HA3	2.31	0.61
3:E:24:HIS:CE1	3:E:26:ALA:HB3	2.36	0.61
4:F:243:ASP:H	4:F:246:ARG:NH2	1.99	0.61
2:B:19:VAL:HG21	2:B:185:HIS:CD2	2.36	0.61
1:A:18:ARG:HA	1:A:133:ARG:O	2.00	0.60
1:A:47:PHE:CE2	1:A:77:ARG:HB3	2.36	0.60
2:D:184:ARG:HD3	2:D:204:GLN:HG2	1.82	0.60
3:E:48:LEU:HG	3:E:52:GLN:HG2	1.83	0.60
4:F:22:GLY:HA2	4:F:72:ALA:HB3	1.83	0.60
1:A:73:LEU:CD2	4:F:247:VAL:HG21	2.31	0.60
3:E:82:GLU:CG	3:E:92:ALA:HB2	2.31	0.60
3:E:14:LEU:HD13	3:E:27:LEU:HD21	1.81	0.60
3:E:176:LEU:O	3:E:179:GLU:HG2	2.02	0.60
3:E:187:LEU:HA	3:E:205:PHE:CZ	2.36	0.60
3:E:213:ARG:HA	3:E:247:TRP:CE3	2.36	0.60
3:E:255:ALA:HB2	3:E:277:LEU:HB2	1.84	0.60
4:F:54:VAL:O	4:F:230:PHE:HA	2.01	0.60
4:F:150:ASP:OD2	4:F:155:LEU:HD12	2.01	0.60
4:G:31:GLY:HA2	4:G:73:ARG:HH12	1.64	0.60
2:D:298:SER:CB	2:D:301:ALA:H	2.15	0.60
4:F:121:ASP:HA	4:F:224:ARG:HH12	1.65	0.60
4:G:137:ARG:HA	4:G:332:LYS:HD2	1.83	0.60
2:C:355:ARG:HG3	2:C:359:PHE:CD2	2.37	0.60
3:E:81:PRO:HA	3:E:88:LEU:HA	1.82	0.60
3:E:213:ARG:HD2	3:E:247:TRP:HB3	1.83	0.60
3:E:259:HIS:HE2	3:E:286:LEU:HD12	1.66	0.60
4:F:24:ARG:HA	4:F:31:GLY:HA3	1.83	0.60
4:F:315:MET:SD	4:F:342:ASP:HA	2.40	0.60
4:G:16:GLN:HG3	4:G:230:PHE:CE2	2.37	0.60
1:A:269:LEU:HB3	1:A:287:GLY:HA3	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:45:SER:HA	3:E:111:VAL:HG11	1.84	0.60
4:F:161:GLU:HA	4:F:192:SER:HA	1.84	0.60
1:A:199:LEU:HA	1:A:202:VAL:HG12	1.84	0.60
2:B:54:ILE:HG13	2:B:175:LEU:HD11	1.82	0.60
2:D:307:ALA:HA	2:D:310:GLU:HB2	1.83	0.60
3:E:244:ARG:HG2	3:E:247:TRP:CH2	2.36	0.60
3:E:316:LEU:O	3:E:320:GLU:HG3	2.02	0.60
4:F:182:MET:HA	4:F:355:GLN:CB	2.32	0.60
4:G:219:GLY:H	4:G:223:ILE:HG22	1.67	0.60
1:A:158:LEU:CD2	1:A:185:LEU:HB3	2.31	0.60
2:B:63:ASN:CB	2:B:118:GLY:HA3	2.32	0.60
1:A:295:GLN:HA	1:A:298:LEU:HD23	1.83	0.60
3:E:259:HIS:NE2	3:E:286:LEU:HD12	2.16	0.60
3:E:318:ARG:HA	3:E:321:HIS:HB2	1.83	0.60
2:C:57:LEU:HA	2:C:60:LYS:HZ2	1.66	0.59
3:E:90:VAL:HG13	3:E:91:ASP:OD2	2.02	0.59
4:F:21:LEU:HD21	4:F:46:GLY:HA2	1.82	0.59
3:E:47:TYR:HA	3:E:59:CYS:SG	2.42	0.59
1:A:225:LYS:NZ	1:A:228:ARG:HG2	2.17	0.59
2:D:115:PRO:HB2	2:D:118:GLY:H	1.67	0.59
2:D:339:LEU:O	2:D:348:GLY:HA3	2.02	0.59
3:E:223:SER:HA	3:E:228:ASP:O	2.02	0.59
4:F:256:LEU:HD11	4:F:308:VAL:HG11	1.83	0.59
4:G:1:MET:N	4:G:66:GLY:HA3	2.17	0.59
3:E:180:VAL:HG11	3:E:205:PHE:CB	2.32	0.59
1:A:51:HIS:HE1	1:A:78:GLN:HB2	1.67	0.59
3:E:209:ASN:O	3:E:213:ARG:N	2.32	0.59
4:F:135:MET:HG3	4:F:207:LEU:CD1	2.32	0.59
4:G:315:MET:HA	4:G:342:ASP:HB3	1.84	0.59
4:F:132:GLN:HG3	4:F:214:LEU:HD11	1.84	0.59
4:G:82:LEU:CD1	4:G:101:SER:HB3	2.33	0.59
4:G:120:ASP:HA	4:G:122:TRP:CZ2	2.38	0.59
4:G:257:GLU:HG2	4:G:337:ARG:HA	1.84	0.59
1:A:72:SER:HG	4:F:362:MET:CG	2.15	0.59
2:B:82:ILE:HD11	2:B:87:PHE:CD2	2.38	0.59
2:D:75:VAL:HA	2:D:80:ARG:CD	2.32	0.59
1:A:231:HIS:C	1:A:231:HIS:CD2	2.76	0.59
2:C:351:MET:SD	2:D:290:HIS:HA	2.43	0.59
4:F:126:VAL:HG22	4:F:191:HIS:HE1	1.68	0.59
4:F:150:ASP:CG	4:F:155:LEU:HD12	2.23	0.59
1:A:223:MET:HA	1:A:288:GLU:OE1	2.03	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:172:GLN:HB3	2:D:174:HIS:CE1	2.38	0.59
3:E:276:GLU:HA	3:E:279:ASN:CB	2.33	0.59
4:F:130:LEU:HB3	4:F:132:GLN:H	1.68	0.59
3:E:246:HIS:HB2	3:E:297:ARG:NH1	2.18	0.59
4:F:5:VAL:HG11	4:F:57:VAL:HG11	1.85	0.59
4:G:135:MET:HB3	4:G:207:LEU:HD13	1.85	0.59
1:A:314:GLN:CD	3:E:303:VAL:HG22	2.24	0.58
2:C:289:LEU:HD13	2:C:329:TYR:HA	1.84	0.58
4:F:159:LEU:HD22	4:F:241:PHE:H	1.68	0.58
4:G:191:HIS:CD2	4:G:218:ILE:HG23	2.38	0.58
2:B:63:ASN:HB3	2:B:87:PHE:CE2	2.37	0.58
2:B:63:ASN:O	2:B:78:ASN:HB3	2.04	0.58
2:B:339:LEU:HD22	2:B:345:ARG:HA	1.84	0.58
2:D:172:GLN:CB	2:D:174:HIS:CE1	2.86	0.58
4:F:267:PHE:HB2	4:F:325:LEU:HD11	1.83	0.58
2:B:10:TRP:CD2	2:B:190:ILE:HG21	2.38	0.58
2:C:121:LYS:HG2	2:C:123:TYR:CZ	2.38	0.58
3:E:228:ASP:OD1	3:E:230:TYR:HB3	2.02	0.58
4:G:202:GLU:O	4:G:205:ARG:HB2	2.03	0.58
4:G:286:SER:HA	4:G:314:GLU:OE1	2.03	0.58
1:A:273:PHE:HD2	1:A:283:ARG:CA	2.16	0.58
1:A:273:PHE:HB2	1:A:283:ARG:HD2	1.84	0.58
2:C:12:PRO:HA	2:C:17:ASP:HB3	1.83	0.58
2:D:75:VAL:HG23	2:D:80:ARG:CG	2.33	0.58
4:F:17:VAL:HG21	4:F:55:ALA:CB	2.34	0.58
2:B:249:ALA:HB1	2:B:285:MET:HG2	1.85	0.58
2:D:22:GLU:OE2	2:D:25:LEU:HD12	2.03	0.58
4:F:147:ALA:HB1	4:F:149:GLN:O	2.02	0.58
4:G:82:LEU:HD13	4:G:101:SER:CB	2.33	0.58
4:G:93:GLU:OE2	4:G:98:LEU:HD13	2.04	0.58
4:F:135:MET:CG	4:F:207:LEU:HD12	2.34	0.58
4:F:282:ARG:HB3	4:F:316:GLU:OE1	2.03	0.58
2:B:277:GLU:HG2	2:B:280:ALA:H	1.69	0.58
2:D:120:PHE:CD1	2:D:149:HIS:HA	2.37	0.58
4:F:122:TRP:CE2	4:F:219:GLY:HA3	2.38	0.58
4:G:17:VAL:HG13	4:G:53:MET:O	2.04	0.58
1:A:18:ARG:HB2	1:A:21:TYR:CE2	2.38	0.58
1:A:24:LEU:HD22	1:A:115:ASN:O	2.04	0.58
1:A:163:ASP:OD2	1:A:199:LEU:HB2	2.04	0.58
3:E:10:ASP:CA	3:E:162:HIS:CE1	2.87	0.58
3:E:186:ALA:HB1	3:E:210:TRP:CD1	2.38	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:276:GLU:CG	4:F:298:GLU:OE1	2.51	0.58
4:F:340:LEU:N	4:F:340:LEU:HD12	2.19	0.58
4:G:192:SER:O	4:G:220:SER:HA	2.04	0.58
4:G:282:ARG:HA	4:G:318:GLY:HA3	1.84	0.58
2:B:183:ILE:HD11	2:B:211:GLU:HA	1.86	0.58
2:D:164:VAL:HG23	2:D:165:THR:HG23	1.85	0.58
3:E:67:LEU:C	3:E:73:HIS:HB2	2.24	0.58
4:G:361:VAL:HG22	4:G:362:MET:H	1.68	0.58
1:A:264:SER:HB3	1:A:290:LEU:HD13	1.86	0.57
4:G:132:GLN:O	4:G:136:LYS:HB2	2.04	0.57
1:A:25:GLY:HA3	1:A:139:CYS:H	1.68	0.57
3:E:49:LEU:HB3	3:E:68:MET:SD	2.43	0.57
3:E:73:HIS:HB3	3:E:76:TYR:CB	2.34	0.57
3:E:204:LEU:O	3:E:210:TRP:HB2	2.04	0.57
4:G:132:GLN:HG3	4:G:209:GLY:C	2.24	0.57
4:G:144:PHE:CZ	4:G:327:VAL:HG12	2.39	0.57
2:B:62:LEU:HD22	2:B:120:PHE:CD2	2.39	0.57
2:C:279:GLU:OE2	2:C:336:ARG:HA	2.03	0.57
4:F:25:PRO:HD2	4:F:31:GLY:HA2	1.87	0.57
4:G:8:GLU:HA	4:G:11:LEU:HB2	1.86	0.57
4:G:139:ILE:O	4:G:143:GLN:HG3	2.05	0.57
1:A:55:ILE:HG12	1:A:93:ILE:HG23	1.85	0.57
1:A:273:PHE:HB3	1:A:283:ARG:HG2	1.86	0.57
1:A:311:THR:HA	1:A:315:ASP:OD2	2.03	0.57
3:E:190:ALA:HB1	3:E:204:LEU:CD1	2.33	0.57
4:F:351:ASP:HB3	4:F:354:SER:CA	2.34	0.57
4:G:254:LYS:HB3	4:G:310:TYR:HE1	1.68	0.57
1:A:273:PHE:CD2	1:A:283:ARG:O	2.57	0.57
2:C:256:MET:SD	2:C:356:ALA:HB3	2.44	0.57
3:E:32:LEU:HA	3:E:146:ARG:O	2.05	0.57
3:E:259:HIS:CD2	3:E:286:LEU:HD12	2.39	0.57
3:E:276:GLU:HA	3:E:279:ASN:HB2	1.86	0.57
4:F:251:ASN:HB3	4:F:253:ASP:OD1	2.04	0.57
4:G:1:MET:H1	4:G:66:GLY:HA3	1.69	0.57
3:E:33:PRO:HA	3:E:37:ASP:CB	2.34	0.57
3:E:256:LEU:HD21	3:E:286:LEU:HB2	1.86	0.57
4:F:145:SER:HB3	4:F:172:THR:HA	1.86	0.57
4:G:148:HIS:CE1	4:G:156:ASN:CB	2.88	0.57
2:C:32:LEU:HD13	2:C:70:ALA:HA	1.86	0.57
3:E:147:GLU:HA	3:E:147:GLU:OE2	2.03	0.57
4:G:215:ARG:HD3	4:G:226:HIS:HB2	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:60:LYS:HD2	2:C:73:CYS:C	2.25	0.57
3:E:210:TRP:HA	3:E:213:ARG:HB3	1.87	0.57
3:E:238:HIS:H	3:E:241:ALA:HB2	1.69	0.57
4:F:6:GLU:O	4:F:10:LEU:HB2	2.04	0.57
4:F:267:PHE:CB	4:F:325:LEU:HD11	2.34	0.57
1:A:334:LYS:HZ3	1:A:338:ASP:CG	2.07	0.56
2:C:23:HIS:CE1	2:C:24:VAL:HG23	2.40	0.56
2:D:205:LEU:HD13	2:D:238:SER:HA	1.86	0.56
3:E:176:LEU:HD22	3:E:201:ALA:HB1	1.87	0.56
3:E:230:TYR:CE1	3:E:313:THR:HG23	2.39	0.56
4:F:122:TRP:CZ2	4:F:124:SER:HA	2.40	0.56
4:F:163:GLU:HA	4:F:190:SER:OG	2.05	0.56
4:G:154:TYR:CD1	4:G:237:VAL:HG21	2.40	0.56
1:A:217:TRP:O	1:A:220:ALA:HB3	2.05	0.56
2:B:65:GLU:HB2	2:B:76:CYS:SG	2.45	0.56
2:D:111:VAL:HB	2:D:150:VAL:CG2	2.36	0.56
3:E:81:PRO:HA	3:E:88:LEU:HB2	1.87	0.56
4:F:12:LYS:HD2	4:F:16:GLN:HG2	1.86	0.56
4:F:133:ALA:HA	4:F:136:LYS:CE	2.35	0.56
1:A:70:ALA:HB1	4:F:175:HIS:ND1	2.21	0.56
1:A:223:MET:HA	1:A:288:GLU:CD	2.26	0.56
2:C:252:LEU:HA	2:C:267:LEU:HD12	1.88	0.56
2:D:2:SER:HA	3:E:25:HIS:CB	2.35	0.56
3:E:12:GLU:HA	3:E:56:HIS:CE1	2.40	0.56
3:E:51:GLN:HB2	3:E:108:GLY:HA2	1.87	0.56
3:E:80:ALA:O	3:E:88:LEU:HD13	2.05	0.56
4:F:159:LEU:HD11	4:F:240:ARG:HA	1.86	0.56
4:G:41:THR:HB	4:G:56:ARG:HB2	1.87	0.56
4:G:154:TYR:O	4:G:241:PHE:CZ	2.58	0.56
2:D:252:LEU:HD21	2:D:267:LEU:HD23	1.88	0.56
3:E:175:TRP:CZ3	3:E:198:PRO:HB2	2.40	0.56
3:E:179:GLU:CD	3:E:202:LEU:HD23	2.25	0.56
2:B:64:CYS:CB	2:B:79:CYS:SG	2.94	0.56
3:E:15:VAL:HG23	3:E:44:LEU:HD23	1.87	0.56
3:E:103:HIS:CG	3:E:104:ALA:H	2.24	0.56
3:E:229:TRP:CD1	3:E:229:TRP:N	2.69	0.56
4:G:137:ARG:HH11	4:G:357:ALA:HB2	1.69	0.56
1:A:329:LEU:HB3	1:A:334:LYS:HZ1	1.71	0.56
2:D:42:LEU:HA	2:D:154:LEU:HB2	1.88	0.56
3:E:49:LEU:HD11	3:E:76:TYR:HB2	1.87	0.56
3:E:310:LEU:HG	3:E:311:LEU:HD12	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:6:GLU:HG3	4:G:9:HIS:HB2	1.87	0.56
4:G:22:GLY:CA	4:G:30:LEU:HB3	2.36	0.56
2:C:252:LEU:HD12	2:C:267:LEU:CB	2.35	0.56
2:C:358:ALA:HB3	2:D:326:GLN:CG	2.35	0.56
2:C:365:LEU:H	2:C:365:LEU:HD22	1.70	0.56
2:D:80:ARG:NE	2:D:80:ARG:HA	2.21	0.56
3:E:27:LEU:HD11	3:E:162:HIS:HB2	1.87	0.56
3:E:68:MET:HE3	3:E:76:TYR:CE1	2.40	0.56
3:E:259:HIS:CD2	3:E:283:PRO:HB3	2.40	0.56
4:F:55:ALA:HB1	4:F:230:PHE:HE1	1.71	0.56
4:G:84:GLU:C	4:G:86:ALA:H	2.07	0.56
2:B:64:CYS:HB2	2:B:66:THR:H	1.71	0.56
2:B:111:VAL:HG11	2:B:147:PRO:CG	2.36	0.56
2:B:142:THR:O	2:B:146:PRO:HA	2.06	0.56
2:D:244:LEU:HD21	2:D:276:ILE:HG21	1.86	0.56
4:G:264:LYS:HE2	4:G:328:LEU:HB3	1.86	0.56
2:B:98:ARG:HA	2:B:103:ASP:HB3	1.88	0.56
2:B:178:LEU:HB3	2:B:183:ILE:HG13	1.87	0.56
3:E:89:GLY:C	3:E:124:ALA:HB2	2.25	0.56
3:E:332:PRO:O	3:E:333:HIS:CG	2.59	0.56
4:F:207:LEU:HD23	4:F:208:ASP:O	2.06	0.56
4:G:36:GLN:O	4:G:42:LEU:HA	2.06	0.56
4:F:21:LEU:CD2	4:F:46:GLY:HA2	2.36	0.56
4:F:260:CYS:HB2	4:F:334:GLU:O	2.06	0.56
1:A:269:LEU:C	1:A:270:ARG:HG2	2.26	0.55
2:B:38:HIS:HD2	2:B:40:ALA:H	1.52	0.55
3:E:256:LEU:HD11	3:E:287:GLN:HA	1.88	0.55
4:F:315:MET:HG2	4:F:342:ASP:HA	1.88	0.55
2:D:10:TRP:HA	2:D:10:TRP:CE3	2.40	0.55
3:E:16:ALA:HA	3:E:19:GLN:OE1	2.07	0.55
3:E:208:ASP:HA	3:E:211:GLN:CD	2.25	0.55
4:F:15:GLN:HG3	4:F:16:GLN:N	2.21	0.55
4:F:237:VAL:HG12	4:F:238:ASP:O	2.06	0.55
4:G:255:HIS:O	4:G:255:HIS:CG	2.58	0.55
1:A:217:TRP:HB2	1:A:232:ILE:HB	1.89	0.55
3:E:18:TYR:HB3	3:E:140:TRP:CH2	2.41	0.55
3:E:216:LEU:HA	3:E:235:ALA:HB1	1.87	0.55
4:F:98:LEU:HD13	4:F:105:ARG:NH2	2.20	0.55
4:F:224:ARG:HG2	4:F:226:HIS:CE1	2.41	0.55
1:A:163:ASP:CB	1:A:198:THR:HA	2.37	0.55
1:A:262:ARG:HH22	3:E:317:LEU:CD1	2.20	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:PHE:CB	1:A:278:VAL:HB	2.36	0.55
1:A:333:HIS:ND1	1:A:339:VAL:HB	2.22	0.55
2:D:64:CYS:SG	2:D:73:CYS:HB2	2.46	0.55
3:E:50:CYS:SG	3:E:65:CYS:N	2.79	0.55
4:G:254:LYS:HZ1	4:G:342:ASP:CG	2.09	0.55
1:A:73:LEU:HB2	4:F:174:GLY:C	2.27	0.55
3:E:7:LEU:O	3:E:40:LEU:HD13	2.06	0.55
3:E:193:LEU:HD11	3:E:247:TRP:HA	1.89	0.55
1:A:77:ARG:NE	1:A:107:ASP:H	2.03	0.55
2:B:62:LEU:O	2:B:119:ARG:HD3	2.07	0.55
2:D:148:GLU:O	2:D:150:VAL:N	2.34	0.55
2:D:334:ILE:HG22	2:D:338:GLU:OE2	2.05	0.55
3:E:24:HIS:CE1	3:E:26:ALA:CB	2.89	0.55
4:G:78:ILE:CG2	4:G:99:VAL:HG11	2.37	0.55
1:A:199:LEU:HD12	1:A:203:GLU:OE1	2.06	0.55
1:A:333:HIS:CB	1:A:337:ALA:HA	2.36	0.55
2:D:23:HIS:O	2:D:27:ALA:HB2	2.06	0.55
3:E:32:LEU:CD1	3:E:35:MET:HE3	2.36	0.55
4:F:354:SER:HB2	4:F:357:ALA:H	1.72	0.55
4:G:16:GLN:HB2	4:G:230:PHE:CE1	2.41	0.55
1:A:78:GLN:HG3	1:A:107:ASP:HB3	1.88	0.55
1:A:142:PRO:HA	1:A:146:GLN:HE21	1.72	0.55
3:E:32:LEU:HD21	3:E:200:ALA:HB2	1.88	0.55
2:C:199:GLU:CG	2:C:202:ALA:H	2.20	0.55
2:D:32:LEU:HD11	2:D:58:LEU:HA	1.89	0.55
2:D:41:TYR:HB3	2:D:43:PHE:CZ	2.42	0.55
4:F:251:ASN:N	4:F:341:THR:HG23	2.22	0.55
1:A:144:GLN:HA	1:A:175:GLU:OE1	2.07	0.55
2:B:149:HIS:CD2	2:B:150:VAL:HG13	2.42	0.55
2:D:24:VAL:HA	2:D:27:ALA:HB3	1.89	0.55
3:E:179:GLU:OE1	3:E:202:LEU:HD23	2.06	0.55
4:F:17:VAL:HG21	4:F:55:ALA:HB3	1.89	0.55
4:F:92:LEU:HA	4:F:97:MET:HE3	1.89	0.55
4:F:354:SER:HA	4:F:357:ALA:CB	2.26	0.55
4:G:37:VAL:HG12	4:G:39:ASP:HA	1.89	0.55
4:G:206:MET:CB	4:G:227:VAL:HG21	2.37	0.55
2:D:76:CYS:HB2	2:D:79:CYS:H	1.72	0.54
2:D:296:GLN:OE1	2:D:322:PRO:HA	2.06	0.54
3:E:46:ARG:O	3:E:50:CYS:SG	2.64	0.54
4:F:255:HIS:HE1	4:F:309:THR:HB	1.72	0.54
4:F:341:THR:HG22	4:F:342:ASP:OD2	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:130:LEU:HD11	4:G:185:GLY:HA2	1.89	0.54
1:A:47:PHE:CD2	1:A:77:ARG:HB3	2.42	0.54
2:B:149:HIS:CE1	2:B:150:VAL:HG13	2.42	0.54
2:D:51:LYS:HA	2:D:175:LEU:CD1	2.37	0.54
2:D:61:GLY:HA2	2:D:64:CYS:HB2	1.90	0.54
2:D:191:LEU:HD23	2:D:198:HIS:HB2	1.89	0.54
2:D:257:VAL:HA	2:D:360:HIS:CD2	2.42	0.54
2:D:295:VAL:HG23	2:D:302:LEU:HD21	1.89	0.54
2:D:357:LEU:HA	2:D:360:HIS:O	2.06	0.54
3:E:12:GLU:HG2	3:E:56:HIS:CD2	2.42	0.54
1:A:162:LEU:HA	1:A:197:LEU:HB2	1.89	0.54
1:A:274:ASP:OD1	1:A:283:ARG:HD3	2.08	0.54
2:D:191:LEU:HG	2:D:198:HIS:CB	2.37	0.54
2:D:198:HIS:HD2	2:D:203:LEU:CD1	2.20	0.54
2:D:206:LEU:HD12	2:D:241:LEU:HD11	1.89	0.54
3:E:4:TYR:H	3:E:7:LEU:HD12	1.72	0.54
3:E:92:ALA:CA	3:E:95:GLU:OE2	2.54	0.54
4:F:317:ILE:HD12	4:F:343:SER:CA	2.37	0.54
1:A:32:GLN:HA	1:A:113:ARG:NH1	2.23	0.54
2:B:129:HIS:CB	2:B:161:LYS:HB2	2.38	0.54
2:D:250:LEU:HD13	2:D:288:LEU:HD13	1.88	0.54
3:E:51:GLN:HA	3:E:109:ALA:H	1.72	0.54
3:E:73:HIS:HB3	3:E:76:TYR:HB2	1.90	0.54
4:F:13:PRO:HB3	4:F:55:ALA:CB	2.38	0.54
4:G:340:LEU:HB3	4:G:347:VAL:HG13	1.89	0.54
2:B:149:HIS:CG	2:B:150:VAL:N	2.75	0.54
2:C:149:HIS:CD2	2:C:150:VAL:HG23	2.43	0.54
2:C:341:TYR:CD1	2:D:337:LYS:HA	2.42	0.54
2:D:355:ARG:HD2	3:E:333:HIS:CE1	2.42	0.54
3:E:14:LEU:O	3:E:18:TYR:CG	2.60	0.54
4:F:17:VAL:CG2	4:F:55:ALA:HB2	2.38	0.54
4:F:148:HIS:O	4:F:156:ASN:HB3	2.07	0.54
4:G:217:GLN:O	4:G:223:ILE:HA	2.07	0.54
1:A:164:ASP:HA	1:A:167:ASN:HB3	1.90	0.54
1:A:211:HIS:CG	1:A:212:PHE:N	2.76	0.54
1:A:299:ARG:CZ	3:E:320:GLU:HB3	2.37	0.54
2:C:10:TRP:HA	2:C:10:TRP:CE3	2.41	0.54
2:C:259:ALA:HA	2:C:357:LEU:CD2	2.38	0.54
2:D:2:SER:O	3:E:140:TRP:CH2	2.61	0.54
2:D:95:ALA:O	2:D:130:MET:HB2	2.08	0.54
3:E:109:ALA:HB1	3:E:138:GLU:O	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:365:ARG:N	4:F:365:ARG:HD2	2.23	0.54
3:E:227:GLY:HA2	3:E:323:LEU:HD11	1.90	0.54
4:F:12:LYS:NZ	4:F:16:GLN:HG3	2.23	0.54
4:F:328:LEU:HB3	4:F:329:ASN:OD1	2.07	0.54
4:G:256:LEU:HG	4:G:338:MET:HE3	1.89	0.54
1:A:47:PHE:CE2	1:A:109:LEU:HB2	2.43	0.54
2:B:65:GLU:CD	2:B:78:ASN:H	2.11	0.54
2:D:98:ARG:HD3	2:D:103:ASP:HB3	1.90	0.54
2:D:172:GLN:HB2	2:D:174:HIS:NE2	2.23	0.54
4:F:104:SER:HA	4:G:303:GLU:O	2.08	0.54
1:A:144:GLN:HA	1:A:175:GLU:CD	2.28	0.54
1:A:219:ASP:OD1	1:A:285:MET:HG3	2.08	0.54
2:B:46:THR:O	2:B:49:VAL:HG22	2.08	0.54
3:E:30:GLN:HG3	3:E:148:PRO:HD3	1.90	0.54
4:F:103:ARG:HH11	4:G:305:ILE:HG22	1.71	0.54
4:F:137:ARG:HA	4:F:332:LYS:NZ	2.23	0.54
4:F:158:MET:SD	4:F:171:ALA:HB2	2.48	0.54
4:F:229:ASP:HB2	4:F:230:PHE:CZ	2.43	0.54
4:F:251:ASN:H	4:F:341:THR:HG23	1.71	0.54
4:G:135:MET:O	4:G:139:ILE:HG13	2.08	0.54
4:G:275:ASN:HD21	4:G:278:PHE:H	1.56	0.54
2:D:38:HIS:CE1	2:D:40:ALA:HB3	2.43	0.53
3:E:177:SER:HB3	3:E:184:GLN:HE22	1.72	0.53
4:F:7:ARG:HB2	4:F:88:ILE:HD11	1.89	0.53
4:F:138:LEU:CD2	4:F:182:MET:HG2	2.39	0.53
4:F:354:SER:HB3	4:F:357:ALA:O	2.07	0.53
1:A:263:GLN:HA	1:A:266:HIS:HE1	1.70	0.53
4:F:137:ARG:HG2	4:F:182:MET:CE	2.39	0.53
4:G:215:ARG:CD	4:G:226:HIS:HB2	2.39	0.53
1:A:122:GLU:HA	1:A:127:PHE:CD2	2.44	0.53
1:A:231:HIS:HE1	1:A:235:GLN:HE21	1.51	0.53
1:A:261:LYS:HE2	1:A:290:LEU:O	2.08	0.53
2:D:64:CYS:C	2:D:66:THR:H	2.09	0.53
3:E:191:LEU:HD12	3:E:201:ALA:HB2	1.89	0.53
3:E:241:ALA:HB3	3:E:308:ARG:HH11	1.74	0.53
4:G:83:PRO:O	4:G:86:ALA:HB3	2.09	0.53
1:A:73:LEU:HD13	4:F:176:ARG:O	2.04	0.53
2:D:131:LEU:HB3	2:D:135:SER:HB2	1.89	0.53
2:D:201:ARG:HD2	2:D:205:LEU:HD21	1.90	0.53
4:F:97:MET:HB2	4:F:110:THR:HG21	1.91	0.53
4:G:6:GLU:HB3	4:G:9:HIS:CB	2.38	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:266:ALA:HA	4:G:269:ARG:HE	1.74	0.53
4:G:283:LEU:O	4:G:316:GLU:HA	2.08	0.53
4:G:348:GLN:C	4:G:349:ILE:HG13	2.29	0.53
3:E:48:LEU:CD2	3:E:140:TRP:CD2	2.91	0.53
4:F:122:TRP:CH2	4:F:124:SER:HB2	2.44	0.53
4:F:224:ARG:CZ	4:F:224:ARG:HB2	2.38	0.53
4:G:37:VAL:HA	4:G:42:LEU:HB3	1.89	0.53
4:G:202:GLU:O	4:G:206:MET:HG2	2.08	0.53
1:A:334:LYS:HG2	1:A:338:ASP:HB3	1.90	0.53
2:B:30:ASN:HB3	2:B:36:ARG:HH11	1.72	0.53
2:C:252:LEU:HD12	2:C:267:LEU:HB2	1.89	0.53
2:D:236:ALA:O	2:D:240:MET:HB2	2.08	0.53
3:E:18:TYR:N	3:E:18:TYR:CD1	2.75	0.53
1:A:220:ALA:HB1	1:A:228:ARG:CG	2.36	0.53
2:B:63:ASN:HB3	2:B:118:GLY:HA3	1.91	0.53
2:D:191:LEU:CD2	2:D:198:HIS:HA	2.38	0.53
3:E:222:TYR:OH	3:E:228:ASP:HB3	2.08	0.53
4:F:2:LYS:O	4:F:37:VAL:HG21	2.09	0.53
4:G:139:ILE:CD1	4:G:204:MET:HA	2.39	0.53
2:D:42:LEU:HD11	2:D:156:THR:CG2	2.39	0.53
2:D:146:PRO:HB3	2:D:152:PHE:CE2	2.43	0.53
3:E:79:LEU:HD22	3:E:96:VAL:HG21	1.91	0.53
3:E:81:PRO:HA	3:E:88:LEU:CA	2.38	0.53
4:G:132:GLN:HA	4:G:207:LEU:HD13	1.91	0.53
4:G:135:MET:CG	4:G:207:LEU:HD11	2.38	0.53
4:G:340:LEU:HD13	4:G:342:ASP:CA	2.39	0.53
1:A:231:HIS:HE1	1:A:235:GLN:NE2	2.07	0.53
1:A:314:GLN:HB2	3:E:303:VAL:HG13	1.90	0.53
1:A:328:SER:O	1:A:332:CYS:HB2	2.08	0.53
2:B:61:GLY:O	2:B:68:ILE:HA	2.08	0.53
3:E:202:LEU:O	3:E:202:LEU:HD22	2.09	0.53
3:E:246:HIS:HB2	3:E:297:ARG:HH11	1.74	0.53
4:F:267:PHE:HB3	4:F:325:LEU:HD21	1.91	0.53
4:F:276:GLU:OE1	4:F:276:GLU:CA	2.56	0.53
4:G:7:ARG:CG	4:G:88:ILE:HD11	2.39	0.53
2:C:144:GLU:HA	2:C:169:ARG:CZ	2.39	0.53
4:F:13:PRO:HG2	4:F:57:VAL:HG22	1.90	0.53
1:A:6:PRO:HD3	1:A:138:THR:O	2.09	0.52
1:A:333:HIS:HB2	1:A:337:ALA:HA	1.90	0.52
2:B:87:PHE:CZ	2:B:117:ARG:HB2	2.45	0.52
2:D:19:VAL:HG13	2:D:178:LEU:HD22	1.89	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:97:SER:HA	3:E:127:ALA:HB2	1.91	0.52
3:E:46:ARG:HA	3:E:68:MET:CE	2.39	0.52
3:E:49:LEU:HA	3:E:111:VAL:HG23	1.91	0.52
1:A:220:ALA:HB2	1:A:228:ARG:HG3	1.90	0.52
2:B:189:HIS:CE1	2:B:190:ILE:HG12	2.44	0.52
3:E:190:ALA:HB1	3:E:204:LEU:HD12	1.92	0.52
3:E:223:SER:CA	3:E:228:ASP:O	2.58	0.52
4:F:258:ALA:C	4:F:335:ASN:HD22	2.12	0.52
4:G:2:LYS:HA	4:G:90:VAL:O	2.10	0.52
4:G:5:VAL:HA	4:G:59:LEU:CD1	2.38	0.52
1:A:270:ARG:N	1:A:273:PHE:CE2	2.73	0.52
2:D:3:TYR:HB2	3:E:21:GLY:CA	2.39	0.52
2:D:24:VAL:HG13	2:D:173:PHE:HB3	1.90	0.52
2:D:172:GLN:HB2	2:D:174:HIS:CE1	2.45	0.52
2:D:196:ILE:HB	2:D:231:GLN:HA	1.90	0.52
2:D:261:GLY:HA2	2:D:357:LEU:CD2	2.38	0.52
3:E:32:LEU:HA	3:E:146:ARG:HA	1.91	0.52
1:A:234:GLN:HG2	2:B:304:ASN:OD1	2.10	0.52
2:C:227:SER:O	2:D:27:ALA:HA	2.09	0.52
2:D:15:PHE:HA	2:D:57:LEU:HD11	1.91	0.52
2:D:190:ILE:HA	2:D:193:GLU:OE2	2.09	0.52
4:F:34:LEU:HA	4:F:69:THR:HG22	1.90	0.52
4:F:132:GLN:HG2	4:F:207:LEU:HD21	1.92	0.52
4:G:143:GLN:HA	4:G:158:MET:HE2	1.91	0.52
4:G:250:LYS:O	4:G:341:THR:HG21	2.09	0.52
4:G:337:ARG:CZ	4:G:337:ARG:HB3	2.39	0.52
1:A:138:THR:HG23	1:A:140:GLN:HG2	1.91	0.52
1:A:333:HIS:HA	1:A:338:ASP:O	2.09	0.52
2:C:28:LEU:HD22	2:C:58:LEU:HD13	1.92	0.52
3:E:15:VAL:HG12	3:E:19:GLN:OE1	2.09	0.52
4:F:257:GLU:HG2	4:F:337:ARG:HA	1.91	0.52
2:C:250:LEU:CD2	2:C:312:ARG:HE	2.23	0.52
2:C:259:ALA:HA	2:C:357:LEU:HD21	1.91	0.52
2:C:292:ILE:CG2	2:C:317:ALA:HA	2.40	0.52
4:F:103:ARG:NH1	4:G:305:ILE:HG22	2.25	0.52
4:F:259:GLY:O	4:F:263:LEU:HB2	2.10	0.52
4:G:264:LYS:HB2	4:G:328:LEU:HD13	1.91	0.52
2:B:63:ASN:HA	2:B:119:ARG:H	1.74	0.52
2:B:87:PHE:CZ	2:B:117:ARG:CB	2.92	0.52
2:D:271:ALA:HB1	2:D:276:ILE:HB	1.90	0.52
2:D:295:VAL:CG1	2:D:314:ARG:HA	2.28	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:5:VAL:HG12	4:F:6:GLU:H	1.75	0.52
4:F:132:GLN:CG	4:F:214:LEU:HD11	2.39	0.52
4:G:59:LEU:HD12	4:G:61:GLN:HB2	1.92	0.52
4:G:132:GLN:HB2	4:G:207:LEU:HB3	1.92	0.52
3:E:45:SER:CA	3:E:111:VAL:HG11	2.40	0.52
3:E:294:CYS:O	3:E:298:GLU:OE2	2.27	0.52
4:F:53:MET:SD	4:F:230:PHE:HB3	2.49	0.52
4:G:255:HIS:O	4:G:255:HIS:CD2	2.62	0.52
1:A:223:MET:HA	1:A:288:GLU:OE2	2.10	0.52
2:C:292:ILE:HG23	2:C:317:ALA:HA	1.91	0.52
2:D:60:LYS:CB	2:D:72:PRO:HB2	2.39	0.52
2:D:179:ASP:H	2:D:182:GLN:HE21	1.58	0.52
2:D:276:ILE:O	2:D:278:TRP:CE2	2.63	0.52
3:E:118:ALA:CB	3:E:150:ARG:CB	2.88	0.52
4:F:206:MET:SD	4:F:232:PHE:CB	2.98	0.52
4:G:37:VAL:HG12	4:G:39:ASP:CA	2.39	0.52
4:G:130:LEU:CD1	4:G:185:GLY:HA2	2.40	0.52
1:A:47:PHE:HB3	1:A:79:THR:OG1	2.10	0.52
1:A:73:LEU:CD1	4:F:177:LEU:HB2	2.40	0.51
1:A:309:GLU:OE1	3:E:306:ILE:HD12	2.10	0.51
3:E:175:TRP:CE3	3:E:198:PRO:HB2	2.45	0.51
4:F:3:PHE:CB	4:F:59:LEU:HD21	2.40	0.51
4:F:7:ARG:HD3	4:F:84:GLU:HA	1.91	0.51
4:F:126:VAL:CG2	4:F:191:HIS:HE1	2.23	0.51
4:F:137:ARG:HH22	4:F:141:ALA:HB2	1.74	0.51
4:G:191:HIS:HD2	4:G:218:ILE:HG12	1.74	0.51
1:A:32:GLN:HE22	2:B:165:THR:HG23	1.74	0.51
2:B:39:HIS:CE1	2:B:147:PRO:O	2.63	0.51
2:B:269:ASN:CA	2:B:346:ARG:HH21	2.24	0.51
2:B:278:TRP:CE2	2:B:346:ARG:HB2	2.45	0.51
2:C:84:GLN:CB	2:C:86:ARG:HG2	2.39	0.51
2:C:179:ASP:CG	2:C:182:GLN:HE21	2.13	0.51
2:C:346:ARG:O	2:C:350:GLU:HG3	2.11	0.51
2:D:121:LYS:HG3	2:D:123:TYR:CZ	2.46	0.51
3:E:145:THR:HG21	3:E:151:LEU:HG	1.92	0.51
3:E:222:TYR:CE1	3:E:223:SER:HA	2.45	0.51
3:E:244:ARG:HA	3:E:247:TRP:CE3	2.45	0.51
4:F:207:LEU:O	4:F:214:LEU:HD21	2.11	0.51
4:F:228:GLY:C	4:F:230:PHE:H	2.14	0.51
4:G:6:GLU:HB3	4:G:9:HIS:HB2	1.92	0.51
4:G:264:LYS:HE2	4:G:328:LEU:CB	2.39	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:GLN:CD	1:A:333:HIS:CD2	2.84	0.51
2:B:63:ASN:HA	2:B:118:GLY:CA	2.40	0.51
2:C:341:TYR:CE1	2:D:337:LYS:HA	2.46	0.51
2:D:112:GLN:HG3	2:D:113:TYR:N	2.24	0.51
3:E:11:PHE:CG	3:E:56:HIS:CE1	2.98	0.51
3:E:18:TYR:CB	3:E:140:TRP:CZ3	2.93	0.51
3:E:27:LEU:CD1	3:E:162:HIS:HB2	2.40	0.51
4:G:166:GLU:HA	4:G:183:PRO:O	2.11	0.51
1:A:51:HIS:HE1	1:A:78:GLN:CB	2.22	0.51
1:A:269:LEU:H	1:A:269:LEU:CD2	2.21	0.51
1:A:277:ARG:HE	1:A:278:VAL:H	1.57	0.51
1:A:334:LYS:HB3	1:A:335:PRO:HD2	1.91	0.51
2:B:286:LEU:CD1	2:B:336:ARG:HH11	2.17	0.51
2:C:12:PRO:HA	2:C:17:ASP:CB	2.40	0.51
2:D:46:THR:HB	2:D:49:VAL:HG23	1.92	0.51
3:E:48:LEU:HD23	3:E:52:GLN:CG	2.41	0.51
3:E:176:LEU:HA	3:E:179:GLU:OE1	2.09	0.51
3:E:233:LEU:HD12	3:E:312:ILE:CG2	2.41	0.51
4:F:17:VAL:HG23	4:F:55:ALA:HB2	1.91	0.51
4:F:39:ASP:CG	4:F:40:GLY:H	2.13	0.51
4:F:274:SER:C	4:F:296:ASN:HB3	2.29	0.51
4:G:256:LEU:HD13	4:G:310:TYR:CG	2.46	0.51
4:G:350:GLU:HB2	4:G:355:GLN:NE2	2.25	0.51
1:A:61:TRP:CD1	1:A:96:GLN:HB2	2.45	0.51
1:A:73:LEU:HD22	4:F:177:LEU:HD13	1.91	0.51
1:A:162:LEU:HD13	1:A:163:ASP:O	2.11	0.51
1:A:262:ARG:HH22	3:E:317:LEU:HD13	1.75	0.51
2:D:74:GLY:C	2:D:80:ARG:HH11	2.14	0.51
3:E:14:LEU:HB3	3:E:18:TYR:CE2	2.46	0.51
3:E:245:LEU:HD13	3:E:297:ARG:CA	2.40	0.51
4:F:16:GLN:HB3	4:F:53:MET:HG2	1.92	0.51
4:F:17:VAL:CG2	4:F:55:ALA:CB	2.88	0.51
4:F:130:LEU:O	4:F:213:PRO:HA	2.11	0.51
1:A:278:VAL:HG21	1:A:286:MET:HG2	1.92	0.51
1:A:333:HIS:HB3	1:A:338:ASP:N	2.24	0.51
2:B:94:ASP:O	2:B:125:ILE:HG23	2.11	0.51
2:D:78:ASN:O	2:D:82:ILE:HG13	2.11	0.51
2:D:295:VAL:CG2	2:D:302:LEU:HD21	2.40	0.51
4:G:87:GLU:OE1	4:G:87:GLU:HA	2.10	0.51
4:G:132:GLN:CA	4:G:207:LEU:HD22	2.40	0.51
1:A:270:ARG:CB	1:A:283:ARG:HB3	2.40	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:347:MET:SD	2:C:290:HIS:CD2	3.04	0.51
2:D:199:GLU:HG3	2:D:202:ALA:H	1.75	0.51
3:E:18:TYR:HB2	3:E:52:GLN:NE2	2.24	0.51
4:F:13:PRO:HA	4:F:55:ALA:CB	2.40	0.51
4:F:217:GLN:CD	4:F:226:HIS:HE1	2.14	0.51
1:A:22:LEU:HA	1:A:112:VAL:O	2.11	0.51
1:A:104:LEU:HB2	1:A:106:ASP:HB2	1.92	0.51
1:A:171:CYS:O	1:A:175:GLU:CA	2.59	0.51
2:C:250:LEU:HD23	2:C:309:ILE:HG21	1.93	0.51
2:C:288:LEU:HA	2:C:291:ARG:HE	1.75	0.51
2:C:358:ALA:CB	2:D:326:GLN:CG	2.89	0.51
2:D:205:LEU:HD13	2:D:238:SER:CA	2.40	0.51
3:E:11:PHE:CE1	3:E:44:LEU:HA	2.46	0.51
3:E:18:TYR:CD1	3:E:140:TRP:CZ3	2.98	0.51
3:E:320:GLU:O	3:E:324:GLN:HG2	2.11	0.51
4:G:163:GLU:OE1	4:G:168:ARG:CB	2.59	0.51
4:G:257:GLU:OE1	4:G:352:ALA:HB1	2.11	0.51
1:A:301:ALA:HA	1:A:330:LEU:HD23	1.93	0.51
1:A:313:LYS:HB3	3:E:304:THR:O	2.11	0.51
2:B:87:PHE:CE2	2:B:117:ARG:HB2	2.46	0.51
2:D:188:GLU:OE1	2:D:203:LEU:HD13	2.10	0.51
3:E:227:GLY:HA2	3:E:229:TRP:HE1	1.76	0.51
4:F:86:ALA:O	4:F:88:ILE:HG13	2.11	0.51
4:F:176:ARG:HB3	4:F:361:VAL:HG12	1.93	0.51
4:G:176:ARG:HB3	4:G:361:VAL:HG23	1.93	0.51
1:A:147:LEU:O	1:A:151:VAL:HG23	2.10	0.51
2:C:156:THR:HG21	2:C:161:LYS:HB2	1.93	0.51
2:D:279:GLU:OE2	2:D:282:LEU:HD12	2.10	0.51
2:D:292:ILE:HG12	2:D:313:MET:HA	1.92	0.51
3:E:49:LEU:HD22	3:E:68:MET:CG	2.41	0.51
3:E:145:THR:HB	3:E:147:GLU:O	2.11	0.51
4:G:10:LEU:HA	4:G:57:VAL:CG2	2.41	0.51
4:G:249:PRO:HA	4:G:346:SER:HB2	1.92	0.51
4:G:251:ASN:HB3	4:G:253:ASP:OD2	2.11	0.51
1:A:77:ARG:HH12	1:A:105:HIS:CD2	2.29	0.50
3:E:17:SER:HB2	3:E:23:GLY:CA	2.41	0.50
3:E:32:LEU:H	3:E:35:MET:HE3	1.76	0.50
3:E:259:HIS:NE2	3:E:278:ALA:HA	2.26	0.50
4:F:77:ASP:CG	4:F:80:ARG:HH21	2.13	0.50
4:F:133:ALA:HA	4:F:136:LYS:HE3	1.93	0.50
4:F:159:LEU:HD13	4:F:240:ARG:HA	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:LEU:HD21	1:A:185:LEU:HB3	1.93	0.50
1:A:223:MET:HG2	1:A:285:MET:SD	2.52	0.50
2:D:41:TYR:CE2	2:D:58:LEU:HD21	2.46	0.50
2:D:290:HIS:CD2	2:D:290:HIS:C	2.83	0.50
3:E:210:TRP:O	3:E:213:ARG:HB3	2.11	0.50
3:E:332:PRO:O	3:E:333:HIS:CD2	2.65	0.50
4:G:331:LEU:CD1	4:G:333:CYS:HB3	2.40	0.50
1:A:49:GLU:O	1:A:78:GLN:HA	2.11	0.50
1:A:84:LEU:HD22	1:A:89:PRO:HD3	1.93	0.50
2:D:75:VAL:HG23	2:D:80:ARG:HG3	1.93	0.50
3:E:63:ARG:HA	3:E:66:GLN:HG2	1.92	0.50
3:E:81:PRO:HA	3:E:88:LEU:CB	2.42	0.50
4:F:137:ARG:HH22	4:F:141:ALA:CB	2.24	0.50
4:G:132:GLN:HG3	4:G:209:GLY:O	2.11	0.50
1:A:29:LEU:HD13	1:A:179:LEU:HA	1.94	0.50
1:A:297:GLN:OE1	1:A:333:HIS:CD2	2.64	0.50
2:B:62:LEU:HB3	2:B:120:PHE:HD2	1.77	0.50
2:C:367:GLU:HA	2:D:322:PRO:HD3	1.93	0.50
2:D:111:VAL:HB	2:D:150:VAL:HG22	1.94	0.50
2:D:276:ILE:O	2:D:278:TRP:CD2	2.65	0.50
3:E:230:TYR:HA	3:E:316:LEU:HD13	1.92	0.50
4:F:126:VAL:HG22	4:F:191:HIS:CE1	2.46	0.50
4:G:146:MET:SD	4:G:171:ALA:HB1	2.52	0.50
1:A:91:ALA:HA	1:A:95:GLU:OE1	2.11	0.50
1:A:304:LEU:O	1:A:307:ARG:HB3	2.12	0.50
2:B:249:ALA:O	2:B:253:VAL:HG23	2.12	0.50
2:C:15:PHE:CD1	2:C:57:LEU:HD13	2.46	0.50
2:C:333:LEU:O	2:C:336:ARG:HB2	2.12	0.50
2:D:214:LEU:O	2:D:218:LEU:HG	2.10	0.50
2:D:315:GLU:HA	2:D:318:ARG:CZ	2.41	0.50
3:E:32:LEU:HD13	3:E:35:MET:CE	2.39	0.50
3:E:236:LEU:O	3:E:241:ALA:HA	2.12	0.50
3:E:242:PRO:HB3	3:E:297:ARG:HG3	1.93	0.50
4:G:147:ALA:HB2	4:G:173:ASP:HA	1.93	0.50
2:B:109:ASP:O	2:B:112:GLN:HG2	2.11	0.50
2:B:268:ILE:HD13	2:B:350:GLU:HB2	1.93	0.50
2:C:359:PHE:CZ	2:D:326:GLN:HB2	2.47	0.50
2:D:146:PRO:HB3	2:D:152:PHE:HE2	1.77	0.50
4:F:307:ASP:O	4:F:308:VAL:HG13	2.11	0.50
4:G:186:GLN:HB3	4:G:188:LEU:H	1.77	0.50
4:G:339:MET:HG2	4:G:350:GLU:OE1	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:LYS:HZ3	1:A:228:ARG:HG2	1.76	0.50
2:B:49:VAL:CG2	2:B:175:LEU:HD13	2.42	0.50
2:D:195:HIS:CG	2:D:196:ILE:N	2.79	0.50
2:D:249:ALA:HB1	2:D:285:MET:HG3	1.92	0.50
4:F:115:ASP:O	4:F:116:PHE:CB	2.60	0.50
4:F:193:VAL:HG13	4:F:236:LEU:HD22	1.94	0.50
4:G:222:ASN:HA	4:G:234:SER:O	2.12	0.50
1:A:215:PHE:HA	1:A:218:VAL:HG12	1.92	0.50
1:A:270:ARG:CA	1:A:273:PHE:CD2	2.94	0.50
2:B:67:GLY:HA2	2:B:119:ARG:HE	1.77	0.50
2:D:60:LYS:CE	2:D:83:GLU:OE1	2.59	0.50
2:D:183:ILE:HD11	2:D:212:GLY:HA2	1.93	0.50
3:E:10:ASP:O	3:E:14:LEU:HG	2.12	0.50
4:F:331:LEU:HD21	4:F:351:ASP:HA	1.94	0.50
4:G:36:GLN:HG3	4:G:63:HIS:CE1	2.46	0.50
4:G:260:CYS:SG	4:G:328:LEU:O	2.69	0.50
4:G:290:LEU:HD21	4:G:292:ILE:HG13	1.94	0.50
1:A:55:ILE:CG2	1:A:85:PRO:HD3	2.42	0.50
1:A:225:LYS:HE2	1:A:228:ARG:HB2	1.94	0.50
2:B:65:GLU:HG2	2:B:78:ASN:CG	2.32	0.50
3:E:14:LEU:HD22	3:E:27:LEU:CD1	2.41	0.50
4:F:12:LYS:NZ	4:F:230:PHE:CD2	2.80	0.50
4:F:53:MET:HE3	4:F:230:PHE:HB3	1.89	0.50
4:F:96:ARG:CZ	4:G:300:GLU:H	2.24	0.50
1:A:166:ALA:O	1:A:170:LEU:HG	2.11	0.49
2:B:345:ARG:O	2:B:349:VAL:HG23	2.12	0.49
2:C:21:GLN:NE2	2:C:23:HIS:CE1	2.80	0.49
2:C:56:ARG:O	2:C:60:LYS:HB3	2.12	0.49
2:D:32:LEU:HB3	2:D:70:ALA:HA	1.93	0.49
2:D:60:LYS:HB2	2:D:72:PRO:HB3	1.92	0.49
2:D:255:ALA:HA	2:D:258:GLU:CD	2.32	0.49
3:E:24:HIS:ND1	3:E:26:ALA:HB3	2.27	0.49
3:E:48:LEU:CD2	3:E:140:TRP:CG	2.95	0.49
3:E:68:MET:HE3	3:E:76:TYR:CD1	2.47	0.49
3:E:223:SER:OG	3:E:232:LEU:HD21	2.12	0.49
4:F:176:ARG:CB	4:F:361:VAL:HG12	2.42	0.49
4:F:255:HIS:CE1	4:F:309:THR:O	2.65	0.49
4:G:245:ARG:HE	4:G:245:ARG:CA	2.24	0.49
4:G:249:PRO:HB3	4:G:346:SER:O	2.12	0.49
4:G:340:LEU:HD13	4:G:342:ASP:HA	1.93	0.49
1:A:225:LYS:HB3	1:A:228:ARG:HB3	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:LYS:CG	1:A:338:ASP:HB3	2.42	0.49
2:C:105:ARG:HA	2:C:108:LEU:HD12	1.94	0.49
3:E:15:VAL:HG11	3:E:56:HIS:ND1	2.27	0.49
3:E:18:TYR:CG	3:E:140:TRP:CE3	3.00	0.49
3:E:188:LEU:HA	3:E:191:LEU:HB3	1.95	0.49
3:E:191:LEU:HD13	3:E:201:ALA:HB2	1.92	0.49
4:F:122:TRP:CZ2	4:F:124:SER:CB	2.96	0.49
4:F:193:VAL:HG23	4:F:238:ASP:OD2	2.13	0.49
2:B:98:ARG:HA	2:B:103:ASP:CB	2.42	0.49
2:D:290:HIS:HB2	2:D:329:TYR:CE1	2.47	0.49
2:D:291:ARG:CB	2:D:313:MET:SD	3.01	0.49
2:D:320:ILE:O	2:D:325:ILE:HD11	2.12	0.49
3:E:8:ARG:HD2	3:E:12:GLU:OE1	2.12	0.49
4:G:17:VAL:HG22	4:G:53:MET:O	2.12	0.49
4:G:206:MET:CB	4:G:227:VAL:CG2	2.90	0.49
4:G:255:HIS:CD2	4:G:255:HIS:H	2.30	0.49
2:C:288:LEU:HG	2:C:291:ARG:HH21	1.77	0.49
2:C:358:ALA:CB	2:D:322:PRO:HB2	2.42	0.49
2:D:60:LYS:HB2	2:D:72:PRO:HB2	1.95	0.49
2:D:181:GLU:O	2:D:185:HIS:HB3	2.12	0.49
2:D:302:LEU:HD12	2:D:302:LEU:H	1.78	0.49
3:E:146:ARG:HB3	3:E:150:ARG:NE	2.18	0.49
3:E:223:SER:HB3	3:E:229:TRP:HA	1.95	0.49
3:E:244:ARG:HD3	3:E:247:TRP:CZ3	2.46	0.49
4:F:34:LEU:HB2	4:F:116:PHE:CD2	2.47	0.49
4:F:295:ASN:HA	4:F:301:GLU:HG2	1.92	0.49
4:G:55:ALA:HB2	4:G:230:PHE:CE1	2.48	0.49
4:G:271:ALA:HB2	4:G:321:VAL:HG11	1.94	0.49
2:D:185:HIS:CG	2:D:186:GLN:N	2.80	0.49
4:F:125:GLU:OE1	4:F:191:HIS:CE1	2.65	0.49
4:F:256:LEU:HD12	4:F:310:TYR:HD1	1.77	0.49
4:G:123:GLN:HA	4:G:224:ARG:HD3	1.95	0.49
4:G:355:GLN:NE2	4:G:355:GLN:HA	2.19	0.49
1:A:20:ALA:O	1:A:134:SER:HB3	2.13	0.49
2:C:261:GLY:HA2	2:C:264:VAL:CG2	2.42	0.49
2:C:293:ALA:HB2	2:C:325:ILE:HG21	1.95	0.49
2:D:291:ARG:HB2	2:D:313:MET:SD	2.53	0.49
3:E:73:HIS:CE1	3:E:75:ASP:HB2	2.47	0.49
4:F:122:TRP:CD2	4:F:222:ASN:HB2	2.47	0.49
4:F:260:CYS:HB3	4:F:261:ASP:OD2	2.12	0.49
4:F:320:ASN:OD1	4:F:323:TYR:CD1	2.66	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:123:GLN:HA	4:G:224:ARG:CD	2.42	0.49
4:G:144:PHE:CE1	4:G:327:VAL:HG12	2.48	0.49
1:A:158:LEU:HD22	1:A:185:LEU:HB3	1.94	0.49
2:B:314:ARG:HG2	2:B:314:ARG:HH21	1.77	0.49
2:C:256:MET:HG3	2:C:357:LEU:HD21	1.93	0.49
2:C:351:MET:HB2	2:D:290:HIS:CD2	2.48	0.49
3:E:10:ASP:HB3	3:E:162:HIS:CE1	2.47	0.49
3:E:11:PHE:CD1	3:E:44:LEU:HG	2.48	0.49
3:E:12:GLU:HA	3:E:56:HIS:ND1	2.27	0.49
3:E:210:TRP:CH2	3:E:213:ARG:HD3	2.48	0.49
4:F:51:MET:HG2	4:F:198:LYS:HG2	1.95	0.49
4:F:243:ASP:H	4:F:246:ARG:HH21	1.60	0.49
4:F:315:MET:SD	4:F:342:ASP:O	2.70	0.49
4:G:135:MET:HG3	4:G:207:LEU:HD11	1.95	0.49
1:A:261:LYS:HD3	1:A:293:LEU:O	2.12	0.49
3:E:133:GLU:CD	3:E:158:ARG:HH21	2.16	0.49
4:G:4:THR:HB	4:G:61:GLN:HB3	1.95	0.49
4:G:206:MET:HB3	4:G:227:VAL:CG2	2.42	0.49
4:G:350:GLU:HG2	4:G:351:ASP:O	2.12	0.49
1:A:94:ASN:O	1:A:126:TRP:HB3	2.13	0.49
1:A:295:GLN:HA	1:A:298:LEU:HB3	1.95	0.49
2:B:269:ASN:HA	2:B:346:ARG:HH21	1.77	0.49
2:C:39:HIS:CD2	2:C:146:PRO:HG3	2.48	0.49
2:C:252:LEU:HA	2:C:267:LEU:CD1	2.43	0.49
2:C:261:GLY:CA	2:C:264:VAL:HG22	2.43	0.49
2:C:289:LEU:CD1	2:C:329:TYR:HA	2.43	0.49
4:F:3:PHE:HA	4:F:63:HIS:HA	1.95	0.49
4:F:92:LEU:HD11	4:F:94:GLY:O	2.13	0.49
4:F:202:GLU:HA	4:F:205:ARG:HE	1.78	0.49
4:G:273:LEU:HD22	4:G:300:GLU:HB3	1.95	0.49
2:C:245:ASP:O	2:C:248:GLN:HG2	2.13	0.49
2:C:255:ALA:HA	2:C:260:ASN:OD1	2.12	0.49
2:D:47:ARG:HG2	2:D:215:ARG:HD2	1.95	0.49
3:E:242:PRO:HG2	3:E:301:MET:SD	2.53	0.49
3:E:255:ALA:CB	3:E:277:LEU:HB2	2.42	0.49
4:F:33:LEU:O	4:F:69:THR:HA	2.13	0.49
4:F:159:LEU:HD11	4:F:192:SER:HB3	1.95	0.49
4:F:308:VAL:HG23	4:F:310:TYR:HB2	1.94	0.49
4:G:190:SER:HA	4:G:218:ILE:HD13	1.95	0.49
4:G:223:ILE:HG23	4:G:236:LEU:HD11	1.94	0.49
2:B:250:LEU:HA	2:B:288:LEU:HD13	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:262:GLU:N	2:C:262:GLU:CD	2.66	0.48
2:D:299:PRO:HB2	2:D:314:ARG:HE	1.78	0.48
3:E:207:GLY:C	3:E:209:ASN:H	2.15	0.48
3:E:229:TRP:CD2	3:E:319:ILE:HG21	2.47	0.48
3:E:259:HIS:CE1	3:E:283:PRO:HD3	2.47	0.48
2:B:183:ILE:CD1	2:B:211:GLU:HA	2.42	0.48
2:C:367:GLU:OE2	2:D:322:PRO:HD2	2.13	0.48
2:D:310:GLU:HG3	2:D:314:ARG:CD	2.43	0.48
4:F:125:GLU:HG2	4:F:218:ILE:O	2.12	0.48
4:F:275:ASN:HA	4:F:296:ASN:HA	1.96	0.48
4:F:308:VAL:CG2	4:F:310:TYR:HB2	2.43	0.48
4:G:3:PHE:HA	4:G:63:HIS:HA	1.94	0.48
4:G:139:ILE:HD13	4:G:204:MET:HA	1.95	0.48
4:G:256:LEU:HD13	4:G:310:TYR:HB2	1.94	0.48
1:A:41:VAL:O	1:A:45:GLN:HG3	2.13	0.48
2:C:164:VAL:HA	2:C:167:LEU:HB3	1.95	0.48
2:D:95:ALA:HB1	2:D:131:LEU:HG	1.96	0.48
3:E:15:VAL:HG13	3:E:47:TYR:CE2	2.48	0.48
3:E:147:GLU:H	3:E:150:ARG:HG2	1.78	0.48
4:F:285:VAL:O	4:F:314:GLU:HB3	2.14	0.48
4:F:296:ASN:HB2	4:F:297:PRO:HD2	1.94	0.48
4:G:92:LEU:CA	4:G:97:MET:SD	3.00	0.48
4:G:350:GLU:HB2	4:G:355:GLN:CD	2.33	0.48
1:A:280:GLN:CA	1:A:283:ARG:HG3	2.43	0.48
1:A:300:GLN:NE2	1:A:330:LEU:HD11	2.23	0.48
2:B:89:ASP:OD2	2:B:115:PRO:HB3	2.13	0.48
2:C:248:GLN:HG3	2:C:274:ARG:NH1	2.28	0.48
2:C:350:GLU:HB3	2:D:290:HIS:NE2	2.28	0.48
2:C:365:LEU:HB2	2:D:322:PRO:HG3	1.95	0.48
2:D:191:LEU:HD21	2:D:198:HIS:HA	1.94	0.48
2:D:335:GLY:HA3	2:D:352:THR:HG23	1.94	0.48
3:E:30:GLN:HG2	3:E:31:ALA:N	2.29	0.48
3:E:75:ASP:HA	3:E:105:ARG:NH2	2.28	0.48
3:E:229:TRP:HD1	3:E:320:GLU:CG	2.17	0.48
4:G:3:PHE:HA	4:G:62:PRO:O	2.13	0.48
4:G:8:GLU:C	4:G:11:LEU:H	2.17	0.48
4:G:145:SER:O	4:G:172:THR:N	2.47	0.48
4:F:6:GLU:CD	4:F:9:HIS:CG	2.87	0.48
4:G:55:ALA:HB2	4:G:230:PHE:HE1	1.78	0.48
4:G:124:SER:O	4:G:217:GLN:HB3	2.14	0.48
4:G:340:LEU:CB	4:G:347:VAL:HG22	2.43	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:GLY:HA3	1:A:335:PRO:HA	1.96	0.48
2:C:89:ASP:HB2	2:C:122:VAL:HG22	1.93	0.48
2:C:364:PRO:HG2	2:C:367:GLU:OE2	2.13	0.48
3:E:4:TYR:H	3:E:7:LEU:CD1	2.26	0.48
3:E:82:GLU:HG2	3:E:92:ALA:HB2	1.94	0.48
3:E:253:MET:HE3	3:E:266:THR:HG21	1.96	0.48
4:F:103:ARG:HE	4:G:305:ILE:CB	2.24	0.48
4:F:176:ARG:HD3	4:F:323:TYR:CE1	2.48	0.48
4:G:355:GLN:NE2	4:G:358:ALA:HB2	2.29	0.48
1:A:158:LEU:HD21	1:A:185:LEU:CB	2.44	0.48
1:A:270:ARG:HA	1:A:273:PHE:H	1.78	0.48
1:A:329:LEU:O	1:A:338:ASP:O	2.31	0.48
2:C:181:GLU:OE1	2:C:185:HIS:HB2	2.13	0.48
2:C:355:ARG:HD3	2:D:330:GLN:OE1	2.13	0.48
2:C:360:HIS:C	2:C:362:ARG:H	2.17	0.48
3:E:76:TYR:HE1	3:E:113:TRP:HE1	1.62	0.48
4:F:256:LEU:HD12	4:F:310:TYR:CD1	2.49	0.48
1:A:218:VAL:O	1:A:221:LEU:HB3	2.14	0.48
2:C:357:LEU:HD23	2:C:360:HIS:CG	2.49	0.48
2:D:4:GLN:NE2	2:D:5:VAL:HG22	2.28	0.48
3:E:176:LEU:HD12	3:E:179:GLU:OE1	2.14	0.48
4:F:16:GLN:HB3	4:F:53:MET:CG	2.43	0.48
4:F:97:MET:SD	4:F:110:THR:HG21	2.53	0.48
4:F:180:CYS:HA	4:F:357:ALA:HA	1.94	0.48
4:G:254:LYS:NZ	4:G:312:GLY:HA3	2.28	0.48
1:A:71:MET:SD	4:F:175:HIS:CE1	3.07	0.48
2:B:259:ALA:HB2	2:B:360:HIS:CA	2.40	0.48
2:B:339:LEU:HB2	2:B:345:ARG:HH21	1.78	0.48
2:C:15:PHE:CE1	2:C:72:PRO:HA	2.48	0.48
2:C:278:TRP:CD1	2:C:345:ARG:HB2	2.49	0.48
3:E:51:GLN:O	3:E:52:GLN:HB2	2.14	0.48
3:E:208:ASP:O	3:E:212:ALA:N	2.40	0.48
4:F:138:LEU:HD21	4:F:182:MET:HG2	1.95	0.48
4:F:282:ARG:HH21	4:F:318:GLY:N	2.12	0.48
4:G:161:GLU:HA	4:G:190:SER:CB	2.44	0.48
4:G:165:GLU:HA	4:G:186:GLN:C	2.34	0.48
1:A:47:PHE:CE2	1:A:77:ARG:CB	2.96	0.48
2:C:192:ASN:O	2:C:195:HIS:CE1	2.67	0.48
2:D:15:PHE:CE2	2:D:28:LEU:HD23	2.49	0.48
2:D:272:ALA:C	2:D:275:GLY:H	2.17	0.48
4:F:220:SER:C	4:F:236:LEU:HD12	2.33	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:315:MET:CG	4:F:342:ASP:HA	2.44	0.48
2:B:38:HIS:CD2	2:B:40:ALA:O	2.67	0.47
2:B:82:ILE:CD1	2:B:87:PHE:CD2	2.97	0.47
2:C:362:ARG:HB3	2:C:363:MET:SD	2.53	0.47
2:D:294:MET:HB2	2:D:302:LEU:HD23	1.96	0.47
2:D:297:LEU:HD12	2:D:298:SER:H	1.79	0.47
3:E:49:LEU:CA	3:E:111:VAL:HG23	2.43	0.47
4:F:17:VAL:HG13	4:F:46:GLY:N	2.28	0.47
4:F:146:MET:N	4:F:171:ALA:HB1	2.29	0.47
4:F:173:ASP:OD1	4:F:176:ARG:HG3	2.14	0.47
1:A:310:LEU:CD2	3:E:303:VAL:HG21	2.43	0.47
2:D:95:ALA:HB3	2:D:128:VAL:HA	1.96	0.47
2:D:202:ALA:HA	2:D:205:LEU:HB2	1.96	0.47
2:D:252:LEU:CD2	2:D:264:VAL:HA	2.44	0.47
2:D:352:THR:CA	2:D:355:ARG:HH21	2.27	0.47
4:F:103:ARG:HH11	4:G:305:ILE:CG2	2.27	0.47
4:F:319:PHE:N	4:F:364:MET:O	2.47	0.47
4:F:351:ASP:HB2	4:F:359:TYR:HE2	1.78	0.47
4:F:357:ALA:HB1	4:F:359:TYR:OH	2.15	0.47
4:G:74:LYS:HB2	4:G:108:LEU:HD23	1.96	0.47
4:G:207:LEU:HD11	4:G:214:LEU:HD13	1.94	0.47
1:A:332:CYS:HB3	1:A:334:LYS:O	2.14	0.47
2:B:120:PHE:CD1	2:B:151:LYS:NZ	2.83	0.47
2:C:363:MET:SD	2:C:363:MET:N	2.88	0.47
2:D:96:ALA:HA	2:D:130:MET:CG	2.44	0.47
3:E:45:SER:CB	3:E:111:VAL:HG11	2.43	0.47
3:E:214:GLU:HA	3:E:217:CYS:SG	2.54	0.47
4:F:7:ARG:CB	4:F:88:ILE:HD11	2.45	0.47
4:F:221:ASN:O	4:F:235:LYS:HA	2.14	0.47
4:G:259:GLY:HA2	4:G:334:GLU:O	2.14	0.47
1:A:163:ASP:HB2	1:A:198:THR:HA	1.94	0.47
1:A:219:ASP:O	1:A:223:MET:SD	2.73	0.47
2:B:322:PRO:HA	2:B:325:ILE:CG1	2.44	0.47
2:C:31:GLY:O	2:C:37:ILE:HG23	2.15	0.47
2:C:356:ALA:O	2:C:360:HIS:HA	2.13	0.47
2:D:3:TYR:CG	3:E:21:GLY:O	2.68	0.47
2:D:38:HIS:O	2:D:41:TYR:CE2	2.67	0.47
2:D:296:GLN:CG	2:D:317:ALA:O	2.62	0.47
3:E:242:PRO:CG	3:E:301:MET:SD	3.02	0.47
3:E:245:LEU:CD1	3:E:297:ARG:HA	2.44	0.47
4:F:68:THR:HA	4:F:112:PRO:HA	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:37:VAL:HG13	4:G:59:LEU:HD21	1.97	0.47
4:G:137:ARG:HB2	4:G:332:LYS:CD	2.44	0.47
1:A:279:TRP:O	1:A:283:ARG:HG3	2.14	0.47
2:C:268:ILE:HG22	2:C:346:ARG:HH21	1.79	0.47
2:C:278:TRP:CE2	2:C:346:ARG:HB2	2.49	0.47
2:D:45:GLY:O	2:D:157:THR:HA	2.15	0.47
2:D:65:GLU:OE2	2:D:65:GLU:HA	2.14	0.47
2:D:74:GLY:O	2:D:79:CYS:CB	2.62	0.47
2:D:112:GLN:CG	2:D:113:TYR:N	2.78	0.47
2:D:291:ARG:O	2:D:294:MET:HB2	2.14	0.47
3:E:27:LEU:HD11	3:E:162:HIS:HB3	1.96	0.47
3:E:236:LEU:HA	3:E:244:ARG:CB	2.45	0.47
4:G:13:PRO:HB3	4:G:55:ALA:CB	2.44	0.47
1:A:275:LYS:HE3	1:A:276:HIS:HE1	1.80	0.47
2:B:8:ARG:HD3	2:C:145:GLU:HB3	1.97	0.47
2:C:74:GLY:CA	2:C:83:GLU:OE1	2.63	0.47
2:C:282:LEU:HA	2:C:285:MET:CE	2.43	0.47
2:C:351:MET:HG2	2:D:329:TYR:CD1	2.49	0.47
2:D:64:CYS:SG	2:D:79:CYS:SG	3.10	0.47
2:D:114:ALA:HB2	4:G:366:LEU:CD2	2.42	0.47
2:D:125:ILE:H	2:D:125:ILE:HD12	1.79	0.47
3:E:71:GLY:C	3:E:73:HIS:H	2.17	0.47
3:E:73:HIS:O	3:E:76:TYR:HB3	2.14	0.47
4:F:251:ASN:OD1	4:F:341:THR:HA	2.13	0.47
4:F:358:ALA:O	4:F:359:TYR:CD1	2.68	0.47
4:G:91:GLN:HB2	4:G:100:ARG:HH12	1.80	0.47
4:G:125:GLU:OE2	4:G:191:HIS:CE1	2.68	0.47
1:A:18:ARG:CG	1:A:21:TYR:CE2	2.98	0.47
1:A:169:VAL:O	1:A:173:CYS:SG	2.73	0.47
1:A:225:LYS:CB	1:A:228:ARG:HB3	2.45	0.47
1:A:272:LEU:HD23	1:A:273:PHE:H	1.80	0.47
2:B:177:ALA:HA	2:B:212:GLY:HA2	1.96	0.47
2:B:339:LEU:HD13	2:B:345:ARG:HB3	1.96	0.47
2:C:362:ARG:CB	2:C:363:MET:SD	3.03	0.47
3:E:307:ASN:HB3	3:E:310:LEU:HB3	1.96	0.47
4:F:6:GLU:OE2	4:F:9:HIS:CD2	2.68	0.47
4:F:97:MET:HB2	4:F:110:THR:CG2	2.45	0.47
4:F:126:VAL:CG2	4:F:191:HIS:CE1	2.98	0.47
4:F:338:MET:O	4:F:339:MET:SD	2.73	0.47
4:G:8:GLU:OE1	4:G:85:GLY:HA2	2.15	0.47
1:A:61:TRP:CE3	1:A:61:TRP:HA	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:87:PHE:CZ	2:B:117:ARG:HB3	2.50	0.47
2:C:198:HIS:HA	2:C:232:VAL:HB	1.96	0.47
2:C:343:PRO:HB3	2:D:286:LEU:HB2	1.97	0.47
2:D:43:PHE:HB2	2:D:155:ALA:HA	1.97	0.47
2:D:63:ASN:HB3	2:D:78:ASN:HD22	1.80	0.47
2:D:188:GLU:CG	2:D:203:LEU:HD13	2.44	0.47
3:E:14:LEU:HB3	3:E:18:TYR:CZ	2.50	0.47
3:E:18:TYR:CA	3:E:140:TRP:CH2	2.98	0.47
4:F:331:LEU:HG	4:F:333:CYS:HB3	1.96	0.47
4:G:54:VAL:O	4:G:230:PHE:HA	2.15	0.47
4:G:256:LEU:HD22	4:G:310:TYR:CD1	2.50	0.47
4:G:283:LEU:HD12	4:G:318:GLY:HA2	1.96	0.47
4:G:350:GLU:HB2	4:G:355:GLN:OE1	2.14	0.47
2:B:73:CYS:HB2	2:B:79:CYS:SG	2.55	0.47
2:C:256:MET:O	2:C:360:HIS:CE1	2.68	0.47
3:E:1:MET:N	3:E:33:PRO:O	2.48	0.47
4:F:362:MET:HE3	4:F:363:PRO:HD2	1.97	0.47
4:G:350:GLU:HA	4:G:357:ALA:O	2.15	0.47
1:A:11:ALA:O	1:A:15:GLU:HG3	2.15	0.47
1:A:167:ASN:HD22	1:A:168:GLN:N	2.13	0.47
2:C:199:GLU:HG2	2:C:202:ALA:CB	2.45	0.47
2:D:14:THR:HA	2:D:57:LEU:HD21	1.96	0.47
2:D:123:TYR:HB2	2:D:151:LYS:O	2.15	0.47
2:D:210:ALA:CB	2:D:217:ALA:HB2	2.44	0.47
3:E:3:TRP:HA	3:E:7:LEU:CD1	2.43	0.47
3:E:32:LEU:H	3:E:32:LEU:HD12	1.79	0.47
3:E:49:LEU:CD1	3:E:76:TYR:HB2	2.44	0.47
3:E:245:LEU:CD1	3:E:300:LEU:HD12	2.45	0.47
4:F:3:PHE:CB	4:F:59:LEU:CD2	2.93	0.47
4:F:192:SER:O	4:F:238:ASP:OD1	2.33	0.47
4:F:206:MET:SD	4:F:232:PHE:HB3	2.55	0.47
4:G:163:GLU:OE1	4:G:168:ARG:HB3	2.15	0.47
2:B:48:GLY:HA3	2:B:215:ARG:H	1.79	0.46
2:B:282:LEU:HD21	2:B:349:VAL:HG22	1.97	0.46
2:C:238:SER:HB2	2:C:243:THR:O	2.16	0.46
2:C:292:ILE:HG23	2:C:317:ALA:CA	2.45	0.46
2:D:42:LEU:N	2:D:171:LEU:O	2.48	0.46
2:D:151:LYS:HB3	2:D:151:LYS:HE3	1.72	0.46
3:E:229:TRP:O	3:E:316:LEU:HD22	2.15	0.46
3:E:233:LEU:CD1	3:E:312:ILE:HB	2.46	0.46
4:F:137:ARG:HA	4:F:332:LYS:CE	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:310:TYR:CG	4:F:311:SER:N	2.82	0.46
4:G:7:ARG:CD	4:G:84:GLU:HA	2.45	0.46
2:C:191:LEU:O	2:C:195:HIS:HA	2.14	0.46
2:C:357:LEU:O	2:C:360:HIS:HB2	2.15	0.46
2:D:81:GLU:HA	2:D:84:GLN:OE1	2.15	0.46
2:D:148:GLU:O	2:D:149:HIS:CG	2.69	0.46
3:E:10:ASP:CB	3:E:162:HIS:CE1	2.98	0.46
4:F:115:ASP:O	4:F:116:PHE:HB2	2.15	0.46
4:G:53:MET:CE	4:G:206:MET:CE	2.93	0.46
4:G:310:TYR:CE1	4:G:312:GLY:O	2.68	0.46
2:B:62:LEU:O	2:B:119:ARG:HB2	2.15	0.46
2:B:344:ASP:OD2	2:B:346:ARG:HB3	2.15	0.46
2:D:2:SER:O	2:D:3:TYR:CB	2.63	0.46
2:D:14:THR:HA	2:D:57:LEU:CD2	2.45	0.46
2:D:21:GLN:O	2:D:24:VAL:HB	2.15	0.46
2:D:290:HIS:CE1	2:D:291:ARG:NE	2.83	0.46
3:E:15:VAL:HG13	3:E:47:TYR:CZ	2.49	0.46
3:E:30:GLN:CA	3:E:148:PRO:HD3	2.45	0.46
3:E:68:MET:HG2	3:E:76:TYR:CD1	2.50	0.46
3:E:303:VAL:HB	3:E:306:ILE:HB	1.96	0.46
4:F:161:GLU:O	4:F:167:LEU:HD12	2.15	0.46
4:F:212:ASN:O	4:F:214:LEU:CD2	2.63	0.46
4:G:365:ARG:C	4:G:366:LEU:HD22	2.36	0.46
1:A:78:GLN:H	1:A:107:ASP:CA	2.25	0.46
2:B:63:ASN:HD22	2:B:82:ILE:HD11	1.80	0.46
2:C:82:ILE:HG13	2:C:87:PHE:CG	2.50	0.46
3:E:204:LEU:HB3	3:E:210:TRP:CE3	2.50	0.46
4:F:22:GLY:C	4:F:24:ARG:H	2.18	0.46
4:F:144:PHE:CZ	4:F:176:ARG:HB2	2.50	0.46
4:F:264:LYS:HA	4:F:328:LEU:CD2	2.45	0.46
4:F:313:ALA:O	4:F:315:MET:HE3	2.16	0.46
4:G:3:PHE:HB3	4:G:63:HIS:ND1	2.31	0.46
4:G:20:PRO:CG	4:G:53:MET:HB2	2.46	0.46
4:G:53:MET:HG3	4:G:230:PHE:CD1	2.50	0.46
2:B:60:LYS:CA	2:B:82:ILE:HG21	2.45	0.46
2:C:244:LEU:CD2	2:C:274:ARG:HD3	2.45	0.46
2:C:357:LEU:HD23	2:C:360:HIS:CD2	2.50	0.46
2:D:220:LEU:HA	2:D:223:GLN:OE1	2.15	0.46
3:E:321:HIS:O	3:E:324:GLN:HB2	2.16	0.46
4:F:21:LEU:CD2	4:F:46:GLY:CA	2.94	0.46
4:F:24:ARG:HH12	4:F:72:ALA:HB3	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:55:ALA:HA	4:F:230:PHE:CD1	2.51	0.46
4:F:341:THR:H	4:F:347:VAL:HG12	1.80	0.46
1:A:47:PHE:CD2	1:A:77:ARG:CB	2.99	0.46
2:B:183:ILE:HD13	2:B:210:ALA:O	2.15	0.46
2:C:65:GLU:HG3	2:C:76:CYS:SG	2.56	0.46
2:D:21:GLN:CA	2:D:23:HIS:CE1	2.94	0.46
2:D:75:VAL:HG23	2:D:80:ARG:HG2	1.96	0.46
2:D:188:GLU:HG3	2:D:203:LEU:HD13	1.97	0.46
2:D:295:VAL:HG21	2:D:313:MET:HB3	1.97	0.46
3:E:17:SER:C	3:E:23:GLY:HA3	2.36	0.46
3:E:176:LEU:HD23	3:E:187:LEU:HB3	1.98	0.46
3:E:177:SER:CB	3:E:184:GLN:HE22	2.29	0.46
4:F:42:LEU:HB2	4:F:59:LEU:HD22	1.98	0.46
4:F:182:MET:HE3	4:F:355:GLN:HG3	1.98	0.46
4:F:193:VAL:HG23	4:F:238:ASP:HA	1.97	0.46
1:A:158:LEU:HD13	1:A:185:LEU:CD1	2.45	0.46
1:A:163:ASP:HB3	1:A:198:THR:HA	1.96	0.46
2:B:147:PRO:O	2:B:150:VAL:HG22	2.15	0.46
2:D:199:GLU:HG2	2:D:233:SER:C	2.36	0.46
2:D:292:ILE:HG23	2:D:317:ALA:CA	2.45	0.46
4:F:56:ARG:HB2	4:F:229:ASP:CG	2.36	0.46
4:F:140:GLU:OE1	4:F:332:LYS:HE2	2.16	0.46
4:G:159:LEU:HG	4:G:160:PHE:N	2.31	0.46
1:A:158:LEU:C	1:A:160:LEU:H	2.18	0.46
2:B:62:LEU:HB3	2:B:120:PHE:CD2	2.50	0.46
2:C:23:HIS:ND1	2:C:24:VAL:HG23	2.31	0.46
2:D:3:TYR:CZ	2:D:4:GLN:O	2.69	0.46
2:D:89:ASP:OD1	2:D:118:GLY:HA3	2.15	0.46
3:E:7:LEU:HB3	3:E:40:LEU:HB2	1.98	0.46
3:E:90:VAL:HA	3:E:124:ALA:CA	2.43	0.46
4:F:3:PHE:HB3	4:F:59:LEU:CD2	2.46	0.46
4:F:286:SER:HB2	4:F:288:ASN:OD1	2.15	0.46
4:G:181:SER:HB3	4:G:356:SER:HA	1.98	0.46
4:G:286:SER:HB2	4:G:289:GLN:HB2	1.97	0.46
1:A:217:TRP:HB2	1:A:232:ILE:CG2	2.45	0.46
1:A:297:GLN:OE1	1:A:333:HIS:CG	2.69	0.46
2:B:68:ILE:HD11	2:B:119:ARG:HB2	1.98	0.46
2:B:73:CYS:O	2:B:79:CYS:HB2	2.16	0.46
2:C:358:ALA:C	2:C:364:PRO:HB3	2.36	0.46
2:D:51:LYS:HA	2:D:175:LEU:HD11	1.97	0.46
2:D:75:VAL:CG2	2:D:80:ARG:HG2	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:51:GLN:OE1	3:E:109:ALA:N	2.48	0.46
3:E:140:TRP:CB	3:E:142:PHE:CZ	2.99	0.46
3:E:318:ARG:O	3:E:321:HIS:CB	2.64	0.46
4:F:223:ILE:HG21	4:F:236:LEU:HD21	1.98	0.46
4:G:207:LEU:CD2	4:G:214:LEU:HB2	2.35	0.46
1:A:50:HIS:CD2	1:A:50:HIS:O	2.69	0.46
2:B:188:GLU:O	2:B:192:ASN:HB2	2.16	0.46
2:B:295:VAL:HG11	2:B:314:ARG:HA	1.98	0.46
2:C:324:ASP:O	2:C:328:TYR:CD2	2.70	0.46
2:D:198:HIS:HD2	2:D:203:LEU:HD12	1.81	0.46
2:D:201:ARG:HG2	2:D:234:THR:CG2	2.38	0.46
3:E:154:THR:O	3:E:158:ARG:HD2	2.16	0.46
3:E:209:ASN:HA	3:E:247:TRP:CH2	2.51	0.46
4:F:156:ASN:O	4:F:197:ARG:HB2	2.15	0.46
4:G:7:ARG:CZ	4:G:80:ARG:HA	2.46	0.46
2:B:76:CYS:HB2	2:B:79:CYS:SG	2.55	0.45
2:B:177:ALA:CA	2:B:212:GLY:HA2	2.46	0.45
2:D:42:LEU:HB3	2:D:172:GLN:HA	1.98	0.45
2:D:246:ASP:HB3	2:D:248:GLN:OE1	2.15	0.45
2:D:295:VAL:HB	2:D:317:ALA:HB2	1.97	0.45
3:E:42:TYR:CD1	3:E:113:TRP:CZ2	3.03	0.45
4:F:4:THR:O	4:F:59:LEU:CD1	2.64	0.45
4:G:70:VAL:HG12	4:G:110:THR:HA	1.98	0.45
4:G:91:GLN:HB3	4:G:93:GLU:OE1	2.16	0.45
4:G:135:MET:CG	4:G:207:LEU:CD1	2.94	0.45
4:G:166:GLU:HG2	4:G:183:PRO:HA	1.97	0.45
4:G:257:GLU:OE1	4:G:352:ALA:CB	2.65	0.45
4:G:340:LEU:HB3	4:G:347:VAL:CG1	2.45	0.45
1:A:95:GLU:CD	1:A:95:GLU:N	2.70	0.45
2:B:115:PRO:HG3	2:B:121:LYS:N	2.32	0.45
2:C:53:SER:O	2:C:57:LEU:HG	2.16	0.45
2:C:110:ASN:HA	2:C:113:TYR:CD2	2.52	0.45
2:C:252:LEU:CD1	2:C:267:LEU:HB2	2.46	0.45
2:C:328:TYR:CE1	2:C:360:HIS:CD2	3.05	0.45
2:C:341:TYR:CG	2:D:337:LYS:HB2	2.51	0.45
2:D:60:LYS:HA	2:D:82:ILE:HD12	1.98	0.45
2:D:291:ARG:O	2:D:295:VAL:N	2.48	0.45
3:E:67:LEU:HB2	3:E:73:HIS:HD2	1.80	0.45
4:F:8:GLU:C	4:F:11:LEU:H	2.18	0.45
4:F:106:PHE:CE1	4:G:302:ALA:HB1	2.51	0.45
4:F:147:ALA:O	4:F:156:ASN:HA	2.15	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:165:GLU:HB3	4:F:185:GLY:HA2	1.98	0.45
4:G:44:LEU:HD12	4:G:44:LEU:HA	1.74	0.45
4:G:143:GLN:HA	4:G:158:MET:CE	2.46	0.45
1:A:70:ALA:HB2	4:F:364:MET:SD	2.55	0.45
2:B:43:PHE:HB2	2:B:155:ALA:HA	1.97	0.45
2:B:292:ILE:CG2	2:B:317:ALA:HA	2.41	0.45
2:C:15:PHE:HA	2:C:57:LEU:HD13	1.99	0.45
2:C:206:LEU:HD11	2:C:232:VAL:CG1	2.45	0.45
2:C:244:LEU:HD13	2:C:274:ARG:NH1	2.30	0.45
2:C:244:LEU:HD22	2:C:274:ARG:HD3	1.99	0.45
2:C:350:GLU:OE2	2:D:294:MET:HE1	2.16	0.45
2:D:74:GLY:O	2:D:79:CYS:HB3	2.16	0.45
2:D:159:PRO:HB2	2:D:167:LEU:HD21	1.97	0.45
3:E:208:ASP:O	3:E:212:ALA:CB	2.64	0.45
4:F:199:GLY:HA2	4:F:232:PHE:CZ	2.52	0.45
4:F:251:ASN:HB2	4:F:340:LEU:O	2.15	0.45
4:F:254:LYS:HA	4:F:312:GLY:HA3	1.99	0.45
4:F:340:LEU:HB3	4:F:341:THR:O	2.16	0.45
4:G:3:PHE:CA	4:G:63:HIS:HA	2.46	0.45
4:G:5:VAL:HG12	4:G:59:LEU:CD1	2.46	0.45
4:G:159:LEU:HB2	4:G:241:PHE:CG	2.51	0.45
4:G:251:ASN:O	4:G:341:THR:HG23	2.17	0.45
1:A:219:ASP:OD2	1:A:285:MET:HG3	2.17	0.45
2:B:88:VAL:HG11	2:B:116:ALA:HB3	1.99	0.45
2:B:296:GLN:HG3	2:B:317:ALA:HB1	1.98	0.45
2:C:6:LEU:O	2:C:10:TRP:CD1	2.69	0.45
2:C:60:LYS:HD3	2:C:83:GLU:OE1	2.16	0.45
2:D:259:ALA:O	2:D:357:LEU:HD11	2.17	0.45
2:D:339:LEU:N	2:D:340:PRO:CD	2.80	0.45
3:E:49:LEU:HD13	3:E:68:MET:HG2	1.98	0.45
3:E:318:ARG:O	3:E:321:HIS:HB3	2.17	0.45
4:F:6:GLU:HG3	4:F:87:GLU:OE2	2.16	0.45
4:F:8:GLU:OE2	4:F:11:LEU:HD22	2.17	0.45
4:F:122:TRP:CE3	4:F:122:TRP:N	2.85	0.45
4:F:148:HIS:CD2	4:F:148:HIS:H	2.35	0.45
4:F:317:ILE:HD12	4:F:343:SER:N	2.31	0.45
4:G:20:PRO:HG2	4:G:53:MET:HB2	1.98	0.45
4:G:71:PRO:HB2	4:G:74:LYS:HG3	1.98	0.45
4:G:193:VAL:HG22	4:G:223:ILE:CG2	2.46	0.45
4:G:254:LYS:HB2	4:G:340:LEU:CD1	2.46	0.45
1:A:27:ASP:OD2	1:A:29:LEU:HB3	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:ARG:CA	1:A:107:ASP:HA	2.44	0.45
2:B:55:ALA:HB1	2:B:124:LEU:HD13	1.98	0.45
2:C:355:ARG:O	2:C:359:PHE:CG	2.70	0.45
2:D:60:LYS:O	2:D:64:CYS:CA	2.65	0.45
2:D:64:CYS:SG	2:D:66:THR:OG1	2.73	0.45
3:E:12:GLU:CG	3:E:56:HIS:CD2	3.00	0.45
4:F:222:ASN:ND2	4:F:235:LYS:HG2	2.32	0.45
4:F:256:LEU:HD23	4:F:256:LEU:C	2.37	0.45
4:F:261:ASP:HA	4:F:264:LYS:CB	2.47	0.45
4:G:154:TYR:O	4:G:241:PHE:CE2	2.70	0.45
4:G:337:ARG:CZ	4:G:337:ARG:CB	2.95	0.45
2:C:343:PRO:HA	2:D:336:ARG:HH12	1.80	0.45
2:D:24:VAL:HG21	2:D:175:LEU:HA	1.97	0.45
3:E:32:LEU:HD13	3:E:197:SER:HB3	1.98	0.45
3:E:49:LEU:HD11	3:E:76:TYR:N	2.32	0.45
3:E:73:HIS:ND1	3:E:75:ASP:HB2	2.32	0.45
3:E:189:ALA:CB	3:E:269:ASP:OD2	2.64	0.45
3:E:245:LEU:HD13	3:E:297:ARG:HA	1.97	0.45
4:F:68:THR:HA	4:F:113:ALA:H	1.81	0.45
4:F:138:LEU:HG	4:F:182:MET:HG2	1.98	0.45
4:F:279:ARG:HB3	4:F:321:VAL:HG12	1.98	0.45
4:G:158:MET:HA	4:G:241:PHE:CZ	2.51	0.45
1:A:272:LEU:HG	1:A:273:PHE:CE1	2.51	0.45
2:C:261:GLY:HA2	2:C:264:VAL:HG22	1.99	0.45
2:D:23:HIS:HE1	2:D:176:LYS:HG2	1.82	0.45
2:D:122:VAL:HG22	2:D:151:LYS:CG	2.44	0.45
2:D:127:GLU:HB3	2:D:129:HIS:HE1	1.82	0.45
3:E:57:LYS:HB3	3:E:59:CYS:H	1.82	0.45
3:E:122:ASP:O	3:E:126:ASN:HB2	2.17	0.45
3:E:145:THR:HB	3:E:150:ARG:HB2	1.99	0.45
3:E:146:ARG:C	3:E:146:ARG:HD3	2.37	0.45
3:E:235:ALA:O	3:E:244:ARG:HD3	2.17	0.45
4:F:120:ASP:O	4:F:222:ASN:CB	2.65	0.45
4:F:195:VAL:HG12	4:F:236:LEU:CD2	2.46	0.45
4:F:206:MET:HA	4:F:208:ASP:OD1	2.16	0.45
4:F:264:LYS:HB2	4:F:328:LEU:HD23	1.99	0.45
4:F:337:ARG:CZ	4:F:350:GLU:HG3	2.47	0.45
4:G:57:VAL:HG12	4:G:59:LEU:HB3	1.99	0.45
4:G:215:ARG:HB2	4:G:226:HIS:HD2	1.82	0.45
1:A:150:TRP:CH2	1:A:154:ARG:HG2	2.52	0.45
2:B:76:CYS:CB	2:B:79:CYS:SG	3.05	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:250:LEU:HD23	2:C:312:ARG:HH21	1.82	0.45
2:C:265:MET:HB3	2:D:301:ALA:O	2.16	0.45
2:D:101:VAL:HG22	2:D:132:SER:OG	2.17	0.45
3:E:29:ILE:HD13	3:E:162:HIS:O	2.17	0.45
3:E:276:GLU:HA	3:E:279:ASN:HB3	1.99	0.45
4:F:13:PRO:CB	4:F:55:ALA:CB	2.95	0.45
4:F:161:GLU:HA	4:F:191:HIS:O	2.17	0.45
4:F:254:LYS:O	4:F:339:MET:HA	2.17	0.45
4:F:286:SER:HB2	4:F:289:GLN:HB2	1.99	0.45
1:A:270:ARG:N	1:A:272:LEU:CD2	2.80	0.45
1:A:273:PHE:CE2	1:A:283:ARG:O	2.70	0.45
2:C:251:SER:O	2:C:263:ARG:NH2	2.50	0.45
2:C:252:LEU:HD12	2:C:267:LEU:HB3	1.99	0.45
2:D:6:LEU:O	2:D:9:LYS:HB3	2.16	0.45
4:F:106:PHE:HE1	4:G:302:ALA:HB1	1.81	0.45
4:F:147:ALA:CB	4:F:150:ASP:OD2	2.65	0.45
4:F:222:ASN:HD21	4:F:235:LYS:HG2	1.82	0.45
4:F:285:VAL:HG22	4:F:310:TYR:CG	2.52	0.45
4:G:21:LEU:HD22	4:G:33:LEU:HD21	1.99	0.45
4:G:53:MET:SD	4:G:232:PHE:HB2	2.57	0.45
4:G:287:GLU:C	4:G:289:GLN:H	2.20	0.45
1:A:18:ARG:CA	1:A:133:ARG:O	2.64	0.45
2:B:10:TRP:O	2:B:18:VAL:HG22	2.17	0.45
2:C:357:LEU:C	2:C:359:PHE:H	2.21	0.45
2:D:33:SER:HB3	2:D:70:ALA:HB2	1.99	0.45
2:D:295:VAL:HG22	2:D:314:ARG:NH1	2.32	0.45
4:F:160:PHE:HB2	4:F:193:VAL:HG12	1.99	0.45
4:F:176:ARG:HD3	4:F:323:TYR:CD1	2.52	0.45
4:F:337:ARG:NH2	4:F:350:GLU:HG3	2.32	0.45
4:G:144:PHE:CD1	4:G:144:PHE:C	2.91	0.45
1:A:77:ARG:CZ	1:A:106:ASP:HA	2.47	0.44
1:A:142:PRO:HA	1:A:146:GLN:NE2	2.31	0.44
1:A:279:TRP:H	1:A:282:ARG:HH21	1.63	0.44
2:B:150:VAL:CG2	2:B:152:PHE:CE2	3.00	0.44
2:C:57:LEU:HD22	2:C:60:LYS:HZ1	1.82	0.44
2:D:184:ARG:CD	2:D:204:GLN:HG2	2.45	0.44
2:D:300:ALA:N	2:D:302:LEU:HD12	2.33	0.44
3:E:15:VAL:HG13	3:E:47:TYR:OH	2.16	0.44
3:E:169:GLU:HA	3:E:172:ALA:HB3	1.99	0.44
3:E:213:ARG:O	3:E:217:CYS:SG	2.75	0.44
4:F:203:LEU:O	4:F:207:LEU:N	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:257:GLU:HA	4:F:336:VAL:O	2.16	0.44
4:G:32:ASN:HB3	4:G:69:THR:HG22	1.98	0.44
1:A:308:THR:HA	1:A:323:GLU:OE1	2.17	0.44
2:D:64:CYS:SG	2:D:76:CYS:SG	3.13	0.44
2:D:179:ASP:H	2:D:182:GLN:NE2	2.14	0.44
3:E:49:LEU:HD21	3:E:73:HIS:ND1	2.32	0.44
4:F:21:LEU:HA	4:F:25:PRO:CD	2.48	0.44
4:F:27:LEU:HA	4:F:28:PRO:HD3	1.79	0.44
4:F:138:LEU:CG	4:F:182:MET:HG2	2.48	0.44
4:F:202:GLU:HB3	4:F:232:PHE:CE2	2.52	0.44
4:F:251:ASN:OD1	4:F:254:LYS:NZ	2.51	0.44
4:G:168:ARG:CZ	4:G:181:SER:HB2	2.46	0.44
4:G:262:LEU:HB3	4:G:306:LEU:HD21	1.99	0.44
1:A:263:GLN:CA	1:A:266:HIS:CE1	2.95	0.44
2:B:225:ILE:HG23	2:B:230:GLY:HA2	1.99	0.44
2:C:279:GLU:CG	2:C:282:LEU:HD12	2.48	0.44
2:C:279:GLU:CG	2:C:339:LEU:HD22	2.47	0.44
2:D:292:ILE:HG23	2:D:317:ALA:N	2.32	0.44
3:E:31:ALA:CB	3:E:35:MET:SD	3.03	0.44
3:E:45:SER:HB2	3:E:113:TRP:CD1	2.52	0.44
3:E:223:SER:CB	3:E:228:ASP:O	2.65	0.44
3:E:224:VAL:HB	3:E:225:PRO:CD	2.47	0.44
3:E:281:LEU:HA	3:E:285:ARG:NE	2.29	0.44
4:F:252:PRO:O	4:F:339:MET:HB3	2.17	0.44
4:F:283:LEU:O	4:F:316:GLU:HA	2.18	0.44
4:G:82:LEU:HD22	4:G:101:SER:HB3	2.00	0.44
4:G:137:ARG:HH11	4:G:357:ALA:HB3	1.81	0.44
1:A:97:LEU:HB3	1:A:126:TRP:HB2	1.99	0.44
1:A:270:ARG:HH11	1:A:283:ARG:HE	1.64	0.44
1:A:274:ASP:CG	1:A:283:ARG:HD3	2.38	0.44
2:B:129:HIS:HB3	2:B:161:LYS:HB2	2.00	0.44
2:B:268:ILE:HG23	2:B:346:ARG:NH2	2.32	0.44
2:C:14:THR:HG22	2:C:73:CYS:HA	1.99	0.44
2:C:328:TYR:CE1	2:C:361:PRO:CD	3.01	0.44
2:D:291:ARG:CG	2:D:306:MET:SD	3.06	0.44
2:D:354:LEU:CD2	3:E:260:HIS:CD2	3.01	0.44
3:E:18:TYR:HB3	3:E:140:TRP:CZ3	2.52	0.44
3:E:18:TYR:CB	3:E:140:TRP:CH2	3.01	0.44
3:E:250:THR:HB	3:E:267:ASN:OD1	2.17	0.44
4:F:53:MET:HE1	4:F:206:MET:HB3	1.99	0.44
4:G:53:MET:SD	4:G:230:PHE:HB3	2.57	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:LEU:HD23	1:A:112:VAL:HB	2.00	0.44
1:A:260:LEU:O	1:A:264:SER:HB3	2.17	0.44
1:A:273:PHE:O	1:A:277:ARG:C	2.56	0.44
2:B:114:ALA:O	2:B:121:LYS:HE2	2.17	0.44
2:C:282:LEU:HB2	2:C:336:ARG:HD3	1.99	0.44
2:D:61:GLY:O	2:D:68:ILE:HA	2.18	0.44
2:D:189:HIS:ND1	2:D:190:ILE:HG13	2.32	0.44
2:D:191:LEU:CG	2:D:198:HIS:HA	2.48	0.44
2:D:291:ARG:HB3	2:D:313:MET:SD	2.58	0.44
3:E:146:ARG:HH11	3:E:147:GLU:HG2	1.82	0.44
3:E:187:LEU:HA	3:E:205:PHE:HZ	1.82	0.44
3:E:240:GLN:O	3:E:244:ARG:HG3	2.18	0.44
3:E:322:TYR:CE1	3:E:327:VAL:HG12	2.53	0.44
4:F:2:LYS:O	4:F:63:HIS:HA	2.17	0.44
4:F:6:GLU:OE2	4:F:9:HIS:CG	2.70	0.44
4:F:150:ASP:CB	4:F:155:LEU:HB2	2.47	0.44
4:G:156:ASN:HB2	4:G:197:ARG:HB3	1.98	0.44
4:G:279:ARG:O	4:G:321:VAL:HG12	2.18	0.44
1:A:18:ARG:HB2	1:A:21:TYR:CD2	2.52	0.44
1:A:274:ASP:OD1	1:A:278:VAL:O	2.35	0.44
2:B:19:VAL:HG22	2:B:186:GLN:HA	1.99	0.44
2:B:149:HIS:NE2	2:B:150:VAL:HG13	2.32	0.44
2:B:352:THR:HA	2:B:355:ARG:HH21	1.82	0.44
2:C:345:ARG:O	2:C:349:VAL:HG23	2.18	0.44
2:D:97:SER:OG	3:E:127:ALA:HA	2.18	0.44
2:D:120:PHE:HD1	2:D:120:PHE:HA	1.71	0.44
2:D:199:GLU:HG2	2:D:234:THR:N	2.31	0.44
4:F:122:TRP:CZ2	4:F:124:SER:HB2	2.53	0.44
4:F:151:VAL:C	4:F:153:TYR:H	2.21	0.44
4:F:182:MET:SD	4:F:355:GLN:HG2	2.58	0.44
4:F:193:VAL:HG13	4:F:195:VAL:HG12	2.00	0.44
4:F:285:VAL:O	4:F:314:GLU:CB	2.66	0.44
4:F:306:LEU:HA	4:G:103:ARG:HH11	1.82	0.44
4:G:37:VAL:O	4:G:63:HIS:CG	2.71	0.44
4:G:68:THR:OG1	4:G:110:THR:HG23	2.18	0.44
4:G:130:LEU:HD22	4:G:130:LEU:N	2.33	0.44
1:A:61:TRP:NE1	1:A:93:ILE:HA	2.32	0.44
2:B:121:LYS:CB	2:B:150:VAL:HA	2.48	0.44
2:B:338:GLU:O	2:B:342:ALA:N	2.51	0.44
2:D:257:VAL:HG13	2:D:360:HIS:CD2	2.52	0.44
2:D:290:HIS:HE1	2:D:291:ARG:CZ	2.29	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:51:GLN:HA	3:E:51:GLN:OE1	2.17	0.44
3:E:229:TRP:HB3	3:E:316:LEU:HD22	2.00	0.44
3:E:273:LEU:HA	3:E:276:GLU:OE2	2.17	0.44
4:F:174:GLY:C	4:F:175:HIS:CD2	2.91	0.44
4:G:179:VAL:O	4:G:358:ALA:O	2.35	0.44
1:A:55:ILE:HD12	1:A:55:ILE:HA	1.88	0.44
1:A:148:PRO:HA	1:A:171:CYS:SG	2.58	0.44
2:B:121:LYS:HB2	2:B:150:VAL:HA	2.00	0.44
2:C:355:ARG:HA	2:D:326:GLN:HG3	2.00	0.44
2:C:355:ARG:HH11	2:D:330:GLN:CG	2.31	0.44
2:D:195:HIS:CG	2:D:196:ILE:H	2.36	0.44
2:D:219:SER:HB3	3:E:157:SER:O	2.17	0.44
3:E:90:VAL:HB	3:E:123:ALA:C	2.38	0.44
3:E:186:ALA:HB1	3:E:210:TRP:NE1	2.33	0.44
4:G:41:THR:HA	4:G:57:VAL:O	2.17	0.44
4:G:51:MET:SD	4:G:198:LYS:HB2	2.57	0.44
1:A:270:ARG:HB2	1:A:283:ARG:HB3	1.99	0.44
1:A:277:ARG:NE	1:A:277:ARG:HA	2.33	0.44
2:B:278:TRP:HA	2:B:278:TRP:CE3	2.53	0.44
2:C:223:GLN:HE22	2:D:172:GLN:NE2	2.16	0.44
2:C:247:ASP:HA	2:C:312:ARG:NH2	2.32	0.44
2:C:358:ALA:O	2:D:323:THR:CG2	2.66	0.44
2:D:21:GLN:CD	2:D:21:GLN:N	2.71	0.44
2:D:63:ASN:O	2:D:78:ASN:CB	2.66	0.44
2:D:63:ASN:O	2:D:78:ASN:HB2	2.18	0.44
2:D:75:VAL:HA	2:D:80:ARG:HD3	2.00	0.44
2:D:292:ILE:HG13	2:D:313:MET:SD	2.58	0.44
3:E:10:ASP:HA	3:E:162:HIS:HE1	1.78	0.44
4:F:159:LEU:HD12	4:F:159:LEU:HA	1.77	0.44
4:F:270:ALA:HB2	4:F:292:ILE:HD12	1.99	0.44
4:G:333:CYS:SG	4:G:335:ASN:O	2.75	0.44
2:B:49:VAL:HG23	2:B:175:LEU:HD13	1.99	0.43
2:D:60:LYS:HA	2:D:82:ILE:CD1	2.47	0.43
2:D:86:ARG:O	2:D:87:PHE:HB2	2.18	0.43
2:D:96:ALA:C	3:E:126:ASN:HB3	2.38	0.43
2:D:295:VAL:HA	2:D:299:PRO:HA	1.99	0.43
2:D:296:GLN:HE22	2:D:322:PRO:N	2.16	0.43
3:E:278:ALA:HA	3:E:286:LEU:CD1	2.48	0.43
4:F:177:LEU:HD21	4:F:179:VAL:HG23	2.00	0.43
4:F:255:HIS:HA	4:F:339:MET:SD	2.57	0.43
4:F:256:LEU:HB2	4:F:310:TYR:HD1	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:317:ILE:HA	4:F:343:SER:CB	2.45	0.43
4:G:73:ARG:O	4:G:76:PHE:HB3	2.18	0.43
1:A:52:THR:HA	1:A:81:LEU:HB3	1.99	0.43
1:A:73:LEU:HD22	4:F:177:LEU:HD12	1.96	0.43
1:A:270:ARG:O	1:A:283:ARG:HD2	2.18	0.43
1:A:272:LEU:HD23	1:A:272:LEU:N	2.33	0.43
1:A:273:PHE:HD2	1:A:283:ARG:HA	1.71	0.43
2:B:64:CYS:HA	2:B:79:CYS:SG	2.58	0.43
2:C:82:ILE:HG13	2:C:87:PHE:HB2	2.00	0.43
2:C:360:HIS:ND1	2:C:362:ARG:HB2	2.33	0.43
2:D:15:PHE:HA	2:D:57:LEU:CD1	2.47	0.43
2:D:121:LYS:HG2	2:D:123:TYR:OH	2.18	0.43
3:E:46:ARG:HA	3:E:68:MET:HE1	2.00	0.43
3:E:194:SER:OG	3:E:201:ALA:HA	2.18	0.43
4:F:24:ARG:HD3	4:F:31:GLY:HA3	2.00	0.43
4:F:56:ARG:HB2	4:F:229:ASP:OD2	2.18	0.43
4:F:132:GLN:NE2	4:F:212:ASN:H	2.16	0.43
4:F:320:ASN:OD1	4:F:323:TYR:N	2.51	0.43
4:G:16:GLN:O	4:G:53:MET:HG2	2.18	0.43
1:A:47:PHE:HA	1:A:77:ARG:O	2.17	0.43
1:A:96:GLN:OE1	1:A:96:GLN:HA	2.18	0.43
2:B:223:GLN:HB3	2:B:240:MET:SD	2.58	0.43
2:B:339:LEU:O	2:B:342:ALA:HB3	2.18	0.43
2:B:357:LEU:HA	2:B:360:HIS:O	2.18	0.43
2:C:255:ALA:HB2	2:C:263:ARG:HE	1.81	0.43
2:C:338:GLU:HB3	2:D:333:LEU:CD2	2.48	0.43
2:D:188:GLU:HA	2:D:203:LEU:HD13	2.00	0.43
2:D:259:ALA:C	2:D:357:LEU:HD11	2.38	0.43
3:E:300:LEU:HD13	3:E:308:ARG:NH1	2.33	0.43
4:F:3:PHE:CG	4:F:42:LEU:HD22	2.53	0.43
4:G:6:GLU:CB	4:G:9:HIS:HB2	2.47	0.43
4:G:20:PRO:HG3	4:G:53:MET:HE2	1.99	0.43
4:G:175:HIS:HB2	4:G:323:TYR:CE2	2.53	0.43
1:A:12:GLN:CB	1:A:135:VAL:HG21	2.48	0.43
1:A:12:GLN:HA	1:A:15:GLU:HG3	1.99	0.43
1:A:158:LEU:HD12	1:A:158:LEU:N	2.33	0.43
2:B:60:LYS:HD3	2:B:79:CYS:HB3	2.00	0.43
2:C:84:GLN:HB3	2:C:86:ARG:HG2	2.00	0.43
2:C:149:HIS:CD2	2:C:149:HIS:C	2.92	0.43
2:C:358:ALA:HA	2:C:365:LEU:HD22	2.00	0.43
2:D:32:LEU:HG	2:D:58:LEU:CD1	2.47	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:298:SER:HB2	2:D:301:ALA:N	2.32	0.43
3:E:211:GLN:H	3:E:211:GLN:HG3	1.66	0.43
4:F:8:GLU:HG2	4:F:85:GLY:HA2	2.00	0.43
4:F:55:ALA:HB1	4:F:230:PHE:CE1	2.51	0.43
4:F:279:ARG:HD3	4:F:279:ARG:HA	1.87	0.43
4:F:286:SER:HA	4:F:314:GLU:CD	2.39	0.43
4:G:139:ILE:HG22	4:G:204:MET:SD	2.59	0.43
4:G:336:VAL:HG23	4:G:350:GLU:O	2.18	0.43
2:C:292:ILE:HG23	2:C:317:ALA:N	2.33	0.43
3:E:19:GLN:HG3	3:E:52:GLN:NE2	2.33	0.43
3:E:149:GLU:HB2	3:E:150:ARG:NH1	2.34	0.43
3:E:245:LEU:HD11	3:E:300:LEU:HD12	2.01	0.43
3:E:254:ASP:HB3	3:E:265:VAL:CG1	2.46	0.43
4:F:217:GLN:OE1	4:F:226:HIS:CE1	2.72	0.43
4:G:315:MET:HB2	4:G:340:LEU:HD22	1.99	0.43
1:A:50:HIS:O	1:A:50:HIS:CG	2.71	0.43
1:A:223:MET:SD	1:A:225:LYS:HD3	2.58	0.43
2:B:129:HIS:HB2	2:B:161:LYS:HB2	1.99	0.43
2:C:137:ASN:HA	2:C:140:LEU:HG	2.00	0.43
2:C:279:GLU:HG2	2:C:339:LEU:HD22	1.99	0.43
2:C:360:HIS:HB3	2:C:363:MET:N	2.33	0.43
2:D:48:GLY:HA2	2:D:52:THR:OG1	2.19	0.43
2:D:332:LEU:HD21	2:D:356:ALA:CB	2.49	0.43
3:E:32:LEU:HG	3:E:146:ARG:CD	2.48	0.43
3:E:49:LEU:HD23	3:E:50:CYS:HA	2.00	0.43
3:E:180:VAL:HG23	3:E:187:LEU:HD21	2.01	0.43
3:E:224:VAL:HG22	3:E:229:TRP:CH2	2.53	0.43
4:F:3:PHE:HB3	4:F:59:LEU:HD21	1.99	0.43
4:F:27:LEU:O	4:F:30:LEU:HB2	2.19	0.43
4:F:255:HIS:HB2	4:F:339:MET:CE	2.49	0.43
4:G:256:LEU:CD2	4:G:310:TYR:CD1	3.02	0.43
1:A:9:LEU:HD21	1:A:38:VAL:HG23	1.99	0.43
1:A:196:LYS:HD3	1:A:196:LYS:HA	1.82	0.43
2:D:292:ILE:CG2	2:D:317:ALA:HA	2.48	0.43
3:E:18:TYR:HA	3:E:140:TRP:CH2	2.53	0.43
4:F:20:PRO:C	4:F:21:LEU:HD12	2.39	0.43
4:F:343:SER:O	4:F:363:PRO:HG2	2.18	0.43
4:G:8:GLU:HG3	4:G:85:GLY:H	1.82	0.43
4:G:44:LEU:O	4:G:54:VAL:HA	2.19	0.43
4:G:132:GLN:H	4:G:132:GLN:CD	2.21	0.43
4:G:137:ARG:HE	4:G:332:LYS:CG	2.31	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:145:SER:OG	4:G:176:ARG:HD2	2.18	0.43
4:G:259:GLY:O	4:G:263:LEU:HB2	2.18	0.43
2:B:78:ASN:HA	2:B:81:GLU:OE1	2.19	0.43
2:C:250:LEU:HG	2:C:312:ARG:CZ	2.49	0.43
2:C:341:TYR:CD1	2:D:337:LYS:HB2	2.54	0.43
2:D:154:LEU:CD1	2:D:170:CYS:SG	3.07	0.43
2:D:322:PRO:O	2:D:326:GLN:HG2	2.19	0.43
3:E:31:ALA:HB2	3:E:164:LEU:O	2.19	0.43
4:F:61:GLN:H	4:F:61:GLN:HG3	1.61	0.43
4:F:95:GLU:OE1	4:F:112:PRO:HD3	2.19	0.43
4:F:254:LYS:HG2	4:F:312:GLY:HA3	2.00	0.43
4:G:132:GLN:HA	4:G:135:MET:HB3	2.00	0.43
4:G:132:GLN:CG	4:G:209:GLY:H	2.32	0.43
4:G:228:GLY:C	4:G:230:PHE:H	2.21	0.43
4:G:295:ASN:OD1	4:G:301:GLU:HB3	2.19	0.43
4:G:337:ARG:HB3	4:G:350:GLU:OE1	2.18	0.43
1:A:68:CYS:SG	1:A:70:ALA:HB2	2.59	0.43
1:A:278:VAL:O	1:A:283:ARG:HG2	2.19	0.43
2:D:111:VAL:HB	2:D:150:VAL:HG21	1.99	0.43
3:E:31:ALA:CA	3:E:164:LEU:O	2.67	0.43
4:F:148:HIS:HA	4:F:197:ARG:NH1	2.34	0.43
4:G:135:MET:HG3	4:G:207:LEU:CD1	2.49	0.43
4:G:154:TYR:CE1	4:G:237:VAL:HG21	2.53	0.43
4:G:218:ILE:HA	4:G:223:ILE:HG22	2.01	0.43
1:A:5:TYR:HB3	1:A:8:GLN:OE1	2.19	0.43
1:A:270:ARG:HB3	1:A:283:ARG:HB3	1.99	0.43
2:C:174:HIS:CD2	2:C:176:LYS:HG2	2.54	0.43
2:C:360:HIS:HB3	2:C:363:MET:H	1.84	0.43
2:D:4:GLN:HG3	2:D:5:VAL:O	2.19	0.43
2:D:65:GLU:HG3	2:D:78:ASN:OD1	2.19	0.43
3:E:68:MET:HG2	3:E:76:TYR:HB2	2.00	0.43
4:F:13:PRO:CA	4:F:55:ALA:CB	2.96	0.43
4:F:132:GLN:HE22	4:F:209:GLY:C	2.21	0.43
4:F:200:VAL:O	4:F:203:LEU:HB3	2.19	0.43
4:F:223:ILE:HG22	4:F:236:LEU:HG	2.00	0.43
4:F:256:LEU:HD21	4:F:258:ALA:HB2	2.01	0.43
4:G:82:LEU:HA	4:G:82:LEU:HD23	1.76	0.43
1:A:73:LEU:HD12	4:F:175:HIS:H	1.79	0.42
1:A:78:GLN:N	1:A:107:ASP:HA	2.28	0.42
1:A:116:LYS:HD3	1:A:116:LYS:HA	1.85	0.42
1:A:192:TRP:HB3	1:A:193:PRO:HD2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:HIS:CD2	1:A:213:THR:CA	3.02	0.42
1:A:220:ALA:O	1:A:225:LYS:HB2	2.19	0.42
1:A:228:ARG:HE	1:A:232:ILE:CG1	2.31	0.42
1:A:273:PHE:CZ	1:A:287:GLY:HA2	2.54	0.42
2:B:62:LEU:O	2:B:119:ARG:CD	2.67	0.42
2:B:62:LEU:HD13	2:B:120:PHE:CB	2.49	0.42
2:B:149:HIS:CD2	2:B:150:VAL:CG1	3.01	0.42
2:C:63:ASN:CB	2:C:119:ARG:H	2.32	0.42
2:C:75:VAL:O	2:C:76:CYS:SG	2.73	0.42
2:C:111:VAL:HG22	2:C:152:PHE:CE2	2.54	0.42
2:C:184:ARG:NH2	2:C:185:HIS:HA	2.34	0.42
2:C:278:TRP:CD1	2:C:345:ARG:CB	3.02	0.42
2:C:347:MET:SD	2:D:287:GLY:CA	2.99	0.42
2:D:235:GLN:HA	2:D:238:SER:OG	2.19	0.42
3:E:28:LEU:HD22	3:E:151:LEU:HD12	2.00	0.42
3:E:75:ASP:HB3	3:E:110:LYS:CA	2.45	0.42
3:E:236:LEU:HA	3:E:244:ARG:HB3	2.01	0.42
3:E:300:LEU:HD22	3:E:308:ARG:HG3	2.01	0.42
4:F:21:LEU:CD2	4:F:30:LEU:O	2.67	0.42
4:F:68:THR:CA	4:F:113:ALA:H	2.32	0.42
4:F:206:MET:SD	4:F:232:PHE:HB2	2.59	0.42
4:G:2:LYS:HB2	4:G:64:GLU:CD	2.39	0.42
4:G:159:LEU:HB2	4:G:241:PHE:HB2	1.99	0.42
1:A:219:ASP:CG	1:A:285:MET:HG3	2.39	0.42
1:A:231:HIS:CE1	1:A:235:GLN:HG2	2.54	0.42
2:C:80:ARG:O	2:C:83:GLU:HG2	2.19	0.42
2:C:89:ASP:HB3	2:C:122:VAL:H	1.83	0.42
2:C:121:LYS:HG2	2:C:123:TYR:CE1	2.54	0.42
2:C:138:ALA:HA	2:C:141:LYS:HE3	2.02	0.42
2:C:237:VAL:O	2:C:241:LEU:HG	2.19	0.42
3:E:31:ALA:HB2	3:E:164:LEU:HG	2.01	0.42
3:E:46:ARG:CB	3:E:58:SER:O	2.67	0.42
3:E:63:ARG:HA	3:E:66:GLN:CG	2.49	0.42
4:F:202:GLU:CG	4:F:232:PHE:CD2	3.02	0.42
4:F:337:ARG:CZ	4:F:337:ARG:HB3	2.49	0.42
4:G:275:ASN:HA	4:G:297:PRO:CD	2.48	0.42
1:A:39:ARG:HH22	1:A:81:LEU:HB2	1.84	0.42
2:B:50:GLY:CA	2:B:53:SER:OG	2.68	0.42
2:C:140:LEU:HA	2:C:166:ILE:HG21	2.01	0.42
2:C:267:LEU:HA	2:C:270:GLU:HB3	1.99	0.42
2:C:278:TRP:CZ2	2:C:346:ARG:HB2	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:199:GLU:HB3	2:D:232:VAL:HG12	2.00	0.42
2:D:344:ASP:O	2:D:347:MET:HB3	2.19	0.42
3:E:228:ASP:HA	3:E:320:GLU:OE1	2.19	0.42
4:F:365:ARG:N	4:F:365:ARG:CD	2.82	0.42
4:G:132:GLN:HB3	4:G:207:LEU:CD2	2.41	0.42
4:G:146:MET:HA	4:G:156:ASN:HA	2.01	0.42
4:G:255:HIS:HA	4:G:338:MET:O	2.18	0.42
1:A:90:ASN:H	1:A:93:ILE:HD12	1.85	0.42
1:A:273:PHE:CD1	1:A:286:MET:HG3	2.54	0.42
1:A:333:HIS:O	1:A:337:ALA:C	2.58	0.42
2:B:48:GLY:HA2	2:B:215:ARG:HB2	2.02	0.42
2:B:63:ASN:HA	2:B:119:ARG:N	2.34	0.42
2:B:181:GLU:HG3	2:B:182:GLN:N	2.34	0.42
2:D:258:GLU:HB2	2:D:260:ASN:CB	2.49	0.42
4:F:2:LYS:HB3	4:F:64:GLU:HB3	2.01	0.42
4:F:287:GLU:OE1	4:F:310:TYR:CD2	2.72	0.42
4:F:331:LEU:CD2	4:F:333:CYS:SG	3.07	0.42
4:G:37:VAL:HG12	4:G:39:ASP:N	2.33	0.42
4:G:53:MET:SD	4:G:230:PHE:CB	3.08	0.42
4:G:256:LEU:HD21	4:G:310:TYR:CE1	2.54	0.42
1:A:274:ASP:OD1	1:A:277:ARG:NH2	2.52	0.42
1:A:281:ASN:ND2	1:A:282:ARG:HG3	2.35	0.42
2:B:39:HIS:CE1	2:B:150:VAL:HG23	2.54	0.42
2:B:178:LEU:H	2:B:212:GLY:CA	2.32	0.42
2:D:281:LEU:O	2:D:285:MET:SD	2.78	0.42
3:E:64:GLY:O	3:E:68:MET:HG3	2.20	0.42
3:E:230:TYR:HE1	3:E:313:THR:HG23	1.84	0.42
3:E:294:CYS:O	3:E:297:ARG:N	2.53	0.42
4:F:318:GLY:HA3	4:F:365:ARG:HA	2.01	0.42
4:G:175:HIS:C	4:G:362:MET:HE2	2.40	0.42
1:A:4:LEU:CD2	1:A:9:LEU:HA	2.49	0.42
1:A:117:LEU:HB2	1:A:122:GLU:HG3	2.01	0.42
1:A:261:LYS:HE3	1:A:294:SER:HA	2.01	0.42
2:B:49:VAL:HG23	2:B:51:LYS:HA	2.00	0.42
2:C:111:VAL:HG12	2:C:147:PRO:HG2	2.00	0.42
2:C:347:MET:O	2:C:351:MET:HB2	2.19	0.42
2:D:5:VAL:HA	2:D:222:ASP:OD2	2.19	0.42
3:E:47:TYR:CD2	3:E:52:GLN:HA	2.54	0.42
3:E:49:LEU:HD22	3:E:68:MET:SD	2.58	0.42
3:E:100:LEU:HD23	3:E:105:ARG:HH12	1.85	0.42
3:E:229:TRP:CE2	3:E:319:ILE:HG21	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:281:VAL:HG13	4:G:283:LEU:HD11	2.01	0.42
1:A:5:TYR:CG	1:A:6:PRO:HD2	2.54	0.42
1:A:74:PHE:HD2	4:F:174:GLY:HA2	1.85	0.42
1:A:165:ALA:HA	1:A:168:GLN:NE2	2.34	0.42
1:A:273:PHE:HB3	1:A:278:VAL:CB	2.48	0.42
2:B:61:GLY:HA2	2:B:64:CYS:SG	2.60	0.42
2:B:111:VAL:HG22	2:B:150:VAL:HG11	2.02	0.42
2:C:358:ALA:O	2:D:323:THR:HG22	2.20	0.42
2:D:180:VAL:HG13	2:D:181:GLU:H	1.85	0.42
3:E:41:ILE:HG22	3:E:113:TRP:CE3	2.54	0.42
3:E:49:LEU:HA	3:E:109:ALA:O	2.20	0.42
3:E:118:ALA:HB1	3:E:150:ARG:CB	2.44	0.42
3:E:220:LEU:CD1	3:E:224:VAL:HG23	2.50	0.42
4:F:265:GLN:OE1	4:F:265:GLN:O	2.38	0.42
4:F:358:ALA:C	4:F:359:TYR:CG	2.92	0.42
4:G:148:HIS:CE1	4:G:156:ASN:HB3	2.55	0.42
4:G:200:VAL:HA	4:G:203:LEU:HD12	2.02	0.42
4:G:351:ASP:OD1	4:G:351:ASP:N	2.52	0.42
1:A:25:GLY:HA3	1:A:139:CYS:HB2	2.02	0.42
2:B:312:ARG:HA	2:B:312:ARG:HE	1.85	0.42
2:C:252:LEU:CA	2:C:267:LEU:CD1	2.97	0.42
2:D:50:GLY:HA2	2:D:53:SER:HB2	2.02	0.42
2:D:148:GLU:O	2:D:150:VAL:HG23	2.19	0.42
2:D:219:SER:CB	3:E:157:SER:O	2.67	0.42
2:D:335:GLY:O	2:D:339:LEU:N	2.53	0.42
4:G:3:PHE:CD1	4:G:37:VAL:HG23	2.54	0.42
4:G:197:ARG:HG2	4:G:198:LYS:N	2.35	0.42
1:A:60:ASP:O	1:A:61:TRP:HB2	2.20	0.42
1:A:164:ASP:OD1	1:A:167:ASN:HB3	2.19	0.42
1:A:217:TRP:CD1	1:A:217:TRP:C	2.91	0.42
1:A:228:ARG:HG2	1:A:228:ARG:HH11	1.84	0.42
1:A:273:PHE:CE2	1:A:287:GLY:CA	3.03	0.42
2:B:32:LEU:HA	2:B:37:ILE:CG2	2.50	0.42
2:B:63:ASN:ND2	2:B:89:ASP:HB2	2.35	0.42
2:B:126:ASP:CB	2:B:155:ALA:HB3	2.50	0.42
2:B:220:LEU:HB3	2:B:240:MET:HE1	2.02	0.42
2:C:358:ALA:O	2:C:364:PRO:CB	2.68	0.42
2:D:2:SER:CB	3:E:25:HIS:HB3	2.50	0.42
2:D:64:CYS:SG	2:D:72:PRO:O	2.77	0.42
2:D:312:ARG:HA	2:D:315:GLU:OE2	2.20	0.42
2:D:320:ILE:HG22	2:D:324:ASP:HB2	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:46:ARG:N	3:E:68:MET:HE1	2.35	0.42
3:E:177:SER:HB3	3:E:187:LEU:CD1	2.50	0.42
3:E:216:LEU:HD13	3:E:235:ALA:CB	2.49	0.42
4:F:11:LEU:O	4:F:14:LEU:HB2	2.20	0.42
4:F:192:SER:CB	4:F:240:ARG:HB3	2.50	0.42
4:F:255:HIS:HB3	4:F:311:SER:HB3	2.02	0.42
1:A:282:ARG:O	1:A:286:MET:HB2	2.20	0.42
2:B:18:VAL:CG1	2:B:214:LEU:CD2	2.98	0.42
2:B:344:ASP:O	2:B:348:GLY:N	2.50	0.42
2:C:115:PRO:HB3	2:C:120:PHE:C	2.40	0.42
2:D:26:THR:O	2:D:30:ASN:CG	2.58	0.42
2:D:191:LEU:HG	2:D:198:HIS:HB3	2.01	0.42
3:E:30:GLN:O	3:E:147:GLU:HA	2.19	0.42
3:E:177:SER:HA	3:E:187:LEU:CD1	2.50	0.42
4:F:21:LEU:HD23	4:F:30:LEU:O	2.20	0.42
4:F:194:ILE:O	4:F:237:VAL:O	2.38	0.42
4:F:310:TYR:HE1	4:F:340:LEU:HD13	1.84	0.42
4:F:340:LEU:N	4:F:340:LEU:CD1	2.83	0.42
4:G:192:SER:O	4:G:236:LEU:HD13	2.20	0.42
1:A:77:ARG:HA	1:A:107:ASP:OD1	2.20	0.41
1:A:222:LEU:HB2	1:A:285:MET:HB3	2.01	0.41
1:A:231:HIS:CE1	1:A:235:GLN:NE2	2.81	0.41
1:A:278:VAL:HG12	1:A:283:ARG:HG2	2.02	0.41
2:C:125:ILE:HG22	2:C:126:ASP:N	2.35	0.41
2:C:359:PHE:CE1	2:D:323:THR:CA	3.02	0.41
2:D:60:LYS:HB3	2:D:72:PRO:HB2	2.02	0.41
3:E:29:ILE:HB	3:E:37:ASP:OD1	2.19	0.41
3:E:59:CYS:HB3	3:E:65:CYS:HB3	2.02	0.41
3:E:73:HIS:HB3	3:E:76:TYR:HB3	2.01	0.41
3:E:300:LEU:HD23	3:E:300:LEU:HA	1.88	0.41
4:F:202:GLU:HG2	4:F:232:PHE:CD2	2.54	0.41
4:F:236:LEU:HA	4:F:236:LEU:HD23	1.75	0.41
4:G:125:GLU:OE1	4:G:219:GLY:CA	2.68	0.41
1:A:273:PHE:CD2	1:A:286:MET:HB3	2.54	0.41
1:A:293:LEU:HD22	1:A:331:LEU:O	2.20	0.41
2:B:60:LYS:N	2:B:82:ILE:HG21	2.36	0.41
2:B:120:PHE:O	2:B:122:VAL:HG23	2.19	0.41
3:E:30:GLN:CB	3:E:148:PRO:HD3	2.51	0.41
3:E:220:LEU:C	3:E:222:TYR:H	2.23	0.41
3:E:224:VAL:HG12	3:E:280:HIS:ND1	2.35	0.41
3:E:303:VAL:HG11	3:E:306:ILE:HD13	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:10:LEU:HA	4:F:10:LEU:HD12	1.74	0.41
4:F:328:LEU:CB	4:F:329:ASN:OD1	2.68	0.41
4:G:90:VAL:O	4:G:90:VAL:HG23	2.20	0.41
1:A:51:HIS:CE1	1:A:78:GLN:CB	3.02	0.41
2:C:192:ASN:O	2:C:195:HIS:CD2	2.73	0.41
2:C:250:LEU:HG	2:C:312:ARG:NE	2.35	0.41
2:C:260:ASN:CB	2:C:263:ARG:HB2	2.50	0.41
2:C:327:LEU:O	2:C:330:GLN:HB3	2.20	0.41
2:C:358:ALA:C	2:C:364:PRO:CB	2.88	0.41
2:D:352:THR:HA	2:D:355:ARG:HH21	1.85	0.41
3:E:171:TYR:CZ	3:E:175:TRP:HB2	2.55	0.41
4:F:160:PHE:O	4:F:192:SER:HA	2.20	0.41
4:F:184:ILE:CG2	4:F:186:GLN:HG3	2.51	0.41
4:G:256:LEU:HB3	4:G:308:VAL:HG11	2.02	0.41
4:G:256:LEU:HB2	4:G:338:MET:HB2	2.02	0.41
1:A:26:ASN:HA	1:A:31:LEU:HD11	2.02	0.41
1:A:279:TRP:CB	1:A:281:ASN:OD1	2.68	0.41
2:B:65:GLU:HG3	2:B:78:ASN:HB2	2.02	0.41
2:B:125:ILE:O	2:B:154:LEU:HA	2.20	0.41
2:B:128:VAL:O	2:B:162:LEU:HD11	2.20	0.41
2:B:177:ALA:HB1	2:B:212:GLY:HA2	2.01	0.41
2:D:23:HIS:CE1	2:D:176:LYS:HG2	2.55	0.41
3:E:32:LEU:CD2	3:E:200:ALA:HB2	2.51	0.41
3:E:33:PRO:CD	3:E:34:GLY:H	2.32	0.41
3:E:90:VAL:HG13	3:E:91:ASP:CG	2.41	0.41
3:E:219:ALA:O	3:E:222:TYR:HB3	2.21	0.41
4:F:136:LYS:HA	4:F:139:ILE:HB	2.02	0.41
4:F:138:LEU:HG	4:F:182:MET:CG	2.50	0.41
4:F:222:ASN:HA	4:F:234:SER:O	2.20	0.41
4:G:16:GLN:HG3	4:G:230:PHE:CZ	2.56	0.41
4:G:71:PRO:HB3	4:G:73:ARG:HH21	1.85	0.41
4:G:254:LYS:HZ3	4:G:312:GLY:CA	2.34	0.41
4:G:254:LYS:O	4:G:339:MET:HA	2.20	0.41
4:G:275:ASN:OD1	4:G:277:LYS:HE2	2.19	0.41
4:G:296:ASN:ND2	4:G:298:GLU:HB3	2.28	0.41
4:G:310:TYR:OH	4:G:342:ASP:HB3	2.21	0.41
1:A:51:HIS:CE1	1:A:78:GLN:HB2	2.52	0.41
1:A:279:TRP:O	1:A:283:ARG:CG	2.68	0.41
1:A:299:ARG:NH1	3:E:320:GLU:HB3	2.35	0.41
2:B:297:LEU:O	2:B:298:SER:HB3	2.21	0.41
2:C:166:ILE:HG22	2:C:169:ARG:HH12	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:278:TRP:CD2	2:C:346:ARG:HA	2.56	0.41
2:C:286:LEU:CD2	2:C:329:TYR:O	2.69	0.41
3:E:9:PRO:HA	3:E:12:GLU:OE2	2.20	0.41
3:E:166:PRO:HB3	3:E:197:SER:HA	2.02	0.41
3:E:244:ARG:CD	3:E:247:TRP:CZ3	3.03	0.41
4:F:340:LEU:HA	4:F:347:VAL:HG12	2.01	0.41
4:G:73:ARG:O	4:G:77:ASP:CG	2.58	0.41
4:G:206:MET:HB2	4:G:227:VAL:HG21	2.01	0.41
2:B:314:ARG:O	2:B:318:ARG:HG3	2.21	0.41
2:C:78:ASN:O	2:C:82:ILE:HG13	2.21	0.41
2:D:3:TYR:CD1	2:D:4:GLN:N	2.88	0.41
2:D:75:VAL:HA	2:D:80:ARG:HG2	2.03	0.41
2:D:188:GLU:O	2:D:192:ASN:CG	2.59	0.41
2:D:255:ALA:O	2:D:260:ASN:HB3	2.21	0.41
2:D:321:PRO:HA	2:D:322:PRO:HD3	1.86	0.41
3:E:176:LEU:O	3:E:180:VAL:HG22	2.20	0.41
4:F:130:LEU:HD23	4:F:131:PRO:HD2	2.03	0.41
4:G:6:GLU:HA	4:G:87:GLU:OE1	2.21	0.41
1:A:55:ILE:HG22	1:A:85:PRO:HD3	2.03	0.41
1:A:158:LEU:HD12	1:A:158:LEU:H	1.86	0.41
2:B:269:ASN:HA	2:B:346:ARG:NH2	2.35	0.41
2:C:129:HIS:HB2	2:C:161:LYS:HE2	2.01	0.41
2:C:227:SER:HA	2:D:27:ALA:CA	2.50	0.41
2:D:23:HIS:O	2:D:27:ALA:CB	2.67	0.41
2:D:198:HIS:HD2	2:D:203:LEU:HD11	1.84	0.41
2:D:339:LEU:HG	2:D:340:PRO:N	2.35	0.41
3:E:18:TYR:O	3:E:140:TRP:CH2	2.74	0.41
3:E:50:CYS:HB2	3:E:53:PRO:HD3	2.02	0.41
3:E:82:GLU:OE2	3:E:89:GLY:C	2.59	0.41
3:E:229:TRP:HE1	3:E:323:LEU:HD11	1.86	0.41
4:F:5:VAL:HG21	4:F:10:LEU:HD13	2.01	0.41
4:F:84:GLU:C	4:F:86:ALA:H	2.23	0.41
4:F:223:ILE:HG22	4:F:234:SER:O	2.21	0.41
4:G:193:VAL:CG2	4:G:223:ILE:CG2	2.99	0.41
4:G:331:LEU:HD12	4:G:331:LEU:HA	1.78	0.41
1:A:170:LEU:HD22	1:A:174:TYR:HE2	1.85	0.41
1:A:220:ALA:O	1:A:223:MET:HB2	2.21	0.41
1:A:234:GLN:HG2	2:B:304:ASN:CG	2.41	0.41
1:A:272:LEU:HD23	1:A:272:LEU:H	1.86	0.41
1:A:273:PHE:HB3	1:A:278:VAL:CG1	2.51	0.41
2:B:277:GLU:O	2:B:281:LEU:HB2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:180:VAL:O	2:C:184:ARG:HB2	2.21	0.41
2:D:6:LEU:O	2:D:10:TRP:CD1	2.74	0.41
2:D:293:ALA:O	2:D:296:GLN:HB2	2.20	0.41
2:D:298:SER:C	2:D:300:ALA:H	2.24	0.41
3:E:30:GLN:HG3	3:E:147:GLU:OE2	2.21	0.41
3:E:32:LEU:HD12	3:E:147:GLU:OE1	2.21	0.41
3:E:121:THR:O	3:E:124:ALA:HB3	2.20	0.41
3:E:169:GLU:H	3:E:169:GLU:CD	2.24	0.41
3:E:242:PRO:HG3	3:E:301:MET:SD	2.61	0.41
3:E:250:THR:O	3:E:254:ASP:CG	2.59	0.41
4:F:59:LEU:HD11	4:F:61:GLN:O	2.21	0.41
4:F:122:TRP:HE1	4:F:219:GLY:HA3	1.82	0.41
4:F:137:ARG:HG2	4:F:182:MET:HE2	2.03	0.41
4:F:152:ARG:HB2	4:F:155:LEU:CD1	2.50	0.41
4:G:176:ARG:O	4:G:176:ARG:HG3	2.21	0.41
4:G:206:MET:HG3	4:G:227:VAL:CG2	2.50	0.41
4:G:325:LEU:O	4:G:329:ASN:CG	2.59	0.41
4:G:355:GLN:HE21	4:G:358:ALA:HB2	1.86	0.41
1:A:9:LEU:HD13	1:A:137:VAL:CG2	2.51	0.41
1:A:55:ILE:HG12	1:A:93:ILE:CG2	2.50	0.41
1:A:73:LEU:HD12	4:F:175:HIS:C	2.40	0.41
1:A:160:LEU:H	1:A:160:LEU:HG	1.71	0.41
1:A:270:ARG:HA	1:A:273:PHE:HB2	2.02	0.41
1:A:309:GLU:HG2	3:E:310:LEU:CD2	2.51	0.41
2:B:60:LYS:O	2:B:64:CYS:N	2.54	0.41
2:B:65:GLU:C	2:B:76:CYS:SG	2.99	0.41
2:C:64:CYS:SG	2:C:79:CYS:SG	3.16	0.41
2:C:65:GLU:HB2	2:C:76:CYS:HB2	2.03	0.41
2:C:265:MET:CB	2:D:301:ALA:HB1	2.51	0.41
2:C:293:ALA:HA	2:C:296:GLN:OE1	2.21	0.41
2:C:295:VAL:HG11	2:C:314:ARG:HA	2.02	0.41
2:C:341:TYR:CD2	2:C:341:TYR:N	2.88	0.41
2:C:365:LEU:HD13	2:C:365:LEU:HA	1.77	0.41
2:D:23:HIS:H	2:D:23:HIS:HD1	1.69	0.41
2:D:41:TYR:CE1	2:D:171:LEU:HD12	2.56	0.41
2:D:69:THR:CB	2:D:73:CYS:SG	3.09	0.41
2:D:293:ALA:HB2	2:D:325:ILE:CG2	2.51	0.41
2:D:299:PRO:O	2:D:314:ARG:NH2	2.54	0.41
3:E:7:LEU:HA	3:E:10:ASP:OD2	2.20	0.41
3:E:10:ASP:HA	3:E:162:HIS:NE2	2.36	0.41
3:E:14:LEU:O	3:E:18:TYR:CD2	2.73	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:14:LEU:HD11	3:E:162:HIS:CG	2.55	0.41
3:E:29:ILE:HA	3:E:162:HIS:O	2.21	0.41
3:E:31:ALA:N	3:E:164:LEU:O	2.54	0.41
3:E:42:TYR:HB2	3:E:113:TRP:CH2	2.55	0.41
3:E:46:ARG:HA	3:E:68:MET:SD	2.61	0.41
3:E:62:CYS:HB2	3:E:65:CYS:H	1.85	0.41
3:E:67:LEU:O	3:E:73:HIS:HB2	2.21	0.41
3:E:118:ALA:CA	3:E:150:ARG:HB3	2.51	0.41
3:E:118:ALA:HA	3:E:150:ARG:HB3	2.03	0.41
3:E:318:ARG:HG2	3:E:322:TYR:CE2	2.55	0.41
4:F:12:LYS:HB3	4:F:13:PRO:HD3	2.02	0.41
4:F:16:GLN:HB3	4:F:53:MET:HE3	2.01	0.41
4:F:193:VAL:CG2	4:F:238:ASP:HA	2.51	0.41
4:F:206:MET:O	4:F:227:VAL:HG21	2.21	0.41
4:F:250:LYS:H	4:F:345:SER:HB3	1.86	0.41
4:F:257:GLU:CG	4:F:337:ARG:HA	2.51	0.41
4:F:264:LYS:HG3	4:F:325:LEU:HD12	2.02	0.41
4:F:282:ARG:HH21	4:F:318:GLY:H	1.68	0.41
4:F:323:TYR:HA	4:F:326:ASP:OD2	2.20	0.41
4:G:141:ALA:O	4:G:144:PHE:CE2	2.74	0.41
4:G:158:MET:CA	4:G:241:PHE:CE2	3.04	0.41
4:G:162:THR:HB	4:G:164:GLY:O	2.20	0.41
4:G:180:CYS:HA	4:G:356:SER:O	2.20	0.41
4:G:193:VAL:CG1	4:G:223:ILE:HG21	2.51	0.41
4:G:254:LYS:HB2	4:G:340:LEU:HG	2.03	0.41
4:G:318:GLY:O	4:G:363:PRO:HA	2.20	0.41
1:A:160:LEU:C	1:A:160:LEU:HD12	2.42	0.41
1:A:192:TRP:HB3	1:A:193:PRO:CD	2.51	0.41
1:A:211:HIS:CD2	1:A:213:THR:N	2.89	0.41
2:B:48:GLY:O	2:B:214:LEU:HB3	2.21	0.41
2:B:119:ARG:N	2:B:119:ARG:HD2	2.36	0.41
2:B:249:ALA:HB2	2:B:284:GLU:CD	2.42	0.41
2:C:84:GLN:HB2	2:C:86:ARG:HG2	2.03	0.41
2:C:111:VAL:HG12	2:C:147:PRO:CG	2.51	0.41
2:C:279:GLU:OE2	2:C:339:LEU:HB2	2.20	0.41
2:C:315:GLU:C	2:C:315:GLU:CD	2.80	0.41
2:C:324:ASP:HB3	2:C:328:TYR:CE2	2.56	0.41
2:D:57:LEU:HA	2:D:57:LEU:HD23	1.88	0.41
2:D:123:TYR:CD2	2:D:150:VAL:HG13	2.56	0.41
3:E:30:GLN:HA	3:E:148:PRO:HD3	2.03	0.41
3:E:41:ILE:CG2	3:E:113:TRP:CE3	3.04	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:207:GLY:C	3:E:209:ASN:N	2.73	0.41
3:E:316:LEU:O	3:E:320:GLU:CG	2.69	0.41
4:F:41:THR:HG22	4:F:42:LEU:N	2.36	0.41
4:F:140:GLU:OE1	4:F:332:LYS:CE	2.69	0.41
4:F:192:SER:HB2	4:F:240:ARG:HB3	2.02	0.41
4:F:328:LEU:HA	4:F:328:LEU:HD12	1.84	0.41
4:G:137:ARG:HA	4:G:140:GLU:CD	2.41	0.41
4:G:143:GLN:O	4:G:146:MET:HG2	2.21	0.41
4:G:250:LYS:O	4:G:341:THR:CG2	2.69	0.41
1:A:20:ALA:CB	1:A:130:LEU:HD22	2.52	0.40
1:A:87:ASN:O	1:A:117:LEU:HA	2.21	0.40
2:B:120:PHE:CE1	2:B:148:GLU:OE2	2.74	0.40
2:C:79:CYS:HA	2:C:82:ILE:HD12	2.03	0.40
2:D:99:THR:HA	2:D:131:LEU:HA	2.02	0.40
3:E:46:ARG:HB3	3:E:58:SER:O	2.20	0.40
3:E:49:LEU:HD23	3:E:49:LEU:C	2.41	0.40
3:E:257:LYS:HB3	3:E:262:ALA:HB3	2.03	0.40
3:E:320:GLU:O	3:E:324:GLN:NE2	2.47	0.40
4:G:61:GLN:CD	4:G:87:GLU:OE2	2.60	0.40
4:G:249:PRO:HD2	4:G:252:PRO:HB3	2.02	0.40
4:G:288:ASN:HA	4:G:308:VAL:O	2.21	0.40
1:A:84:LEU:HD22	1:A:89:PRO:HG3	2.02	0.40
2:C:265:MET:SD	2:D:302:LEU:HA	2.61	0.40
2:C:281:LEU:O	2:C:285:MET:HG3	2.20	0.40
2:C:351:MET:HG2	2:D:329:TYR:CE1	2.56	0.40
2:D:69:THR:HB	2:D:71:THR:O	2.21	0.40
2:D:99:THR:CG2	2:D:130:MET:HE2	2.51	0.40
2:D:258:GLU:HB2	2:D:260:ASN:HB3	2.04	0.40
2:D:290:HIS:NE2	2:D:294:MET:HG3	2.36	0.40
3:E:32:LEU:HB2	3:E:35:MET:H	1.87	0.40
3:E:177:SER:HA	3:E:187:LEU:HD11	2.02	0.40
3:E:275:ALA:O	3:E:279:ASN:HB2	2.21	0.40
4:F:4:THR:O	4:F:61:GLN:HB2	2.21	0.40
4:F:51:MET:CE	4:F:202:GLU:HG2	2.51	0.40
4:F:103:ARG:HB2	4:G:305:ILE:HB	2.03	0.40
4:F:220:SER:O	4:F:236:LEU:HB2	2.21	0.40
4:F:285:VAL:O	4:F:285:VAL:HG22	2.21	0.40
4:F:333:CYS:SG	4:F:336:VAL:HB	2.62	0.40
4:G:219:GLY:O	4:G:236:LEU:HD11	2.21	0.40
4:G:333:CYS:SG	4:G:351:ASP:CB	3.09	0.40
4:G:344:VAL:H	4:G:344:VAL:HG23	1.63	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:GLN:O	1:A:47:PHE:CD1	2.74	0.40
2:C:43:PHE:CD1	2:C:173:PHE:HB2	2.56	0.40
2:D:198:HIS:CD2	2:D:203:LEU:HD11	2.56	0.40
2:D:332:LEU:HD21	2:D:356:ALA:HB2	2.04	0.40
4:F:53:MET:CE	4:F:206:MET:SD	3.08	0.40
4:F:135:MET:O	4:F:139:ILE:HG12	2.21	0.40
4:F:202:GLU:CB	4:F:205:ARG:HH21	2.31	0.40
4:F:255:HIS:NE2	4:F:257:GLU:N	2.70	0.40
4:F:286:SER:C	4:F:288:ASN:H	2.25	0.40
4:G:57:VAL:CG1	4:G:59:LEU:HB3	2.52	0.40
4:G:137:ARG:HA	4:G:140:GLU:OE1	2.21	0.40
4:G:139:ILE:HD12	4:G:207:LEU:HD12	2.02	0.40
1:A:219:ASP:OD1	1:A:222:LEU:HD12	2.22	0.40
2:B:115:PRO:HG3	2:B:121:LYS:H	1.86	0.40
2:B:159:PRO:HA	2:B:162:LEU:HD13	2.04	0.40
2:B:310:GLU:O	2:B:314:ARG:HB2	2.21	0.40
2:C:238:SER:O	2:C:242:GLY:N	2.54	0.40
2:C:354:LEU:O	2:C:358:ALA:HB2	2.21	0.40
2:C:358:ALA:HB1	2:D:322:PRO:C	2.42	0.40
2:D:121:LYS:HG3	2:D:123:TYR:CE2	2.56	0.40
3:E:14:LEU:HD22	3:E:18:TYR:OH	2.22	0.40
4:F:127:GLU:HG2	4:F:217:GLN:HA	2.01	0.40
4:F:220:SER:N	4:F:236:LEU:HD12	2.36	0.40
4:F:254:LYS:HA	4:F:311:SER:O	2.21	0.40
4:G:8:GLU:O	4:G:11:LEU:HB3	2.22	0.40
4:G:139:ILE:HD12	4:G:204:MET:HA	2.03	0.40
4:G:267:PHE:CB	4:G:325:LEU:HD21	2.52	0.40
4:G:319:PHE:HA	4:G:364:MET:SD	2.61	0.40
1:A:228:ARG:HE	1:A:232:ILE:HG12	1.86	0.40
2:B:64:CYS:O	2:B:119:ARG:CZ	2.69	0.40
2:B:322:PRO:O	2:B:325:ILE:HB	2.21	0.40
2:C:106:ASP:HA	2:C:109:ASP:OD2	2.22	0.40
2:D:29:ALA:O	2:D:70:ALA:HA	2.22	0.40
2:D:39:HIS:O	2:D:152:PHE:N	2.55	0.40
2:D:202:ALA:HA	2:D:205:LEU:CG	2.51	0.40
2:D:291:ARG:HD3	2:D:291:ARG:HA	1.72	0.40
2:D:292:ILE:O	2:D:295:VAL:HB	2.21	0.40
2:D:306:MET:HB2	2:D:313:MET:SD	2.62	0.40
3:E:50:CYS:O	3:E:51:GLN:CB	2.70	0.40
3:E:59:CYS:HB3	3:E:65:CYS:CB	2.51	0.40
3:E:171:TYR:HE1	3:E:178:ARG:HH12	1.67	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:250:THR:CB	3:E:267:ASN:OD1	2.70	0.40
3:E:295:HIS:O	3:E:298:GLU:HB2	2.21	0.40
4:F:12:LYS:O	4:F:15:GLN:CG	2.70	0.40
4:F:24:ARG:NH1	4:F:72:ALA:H	2.19	0.40
4:F:132:GLN:HA	4:F:214:LEU:HD11	2.04	0.40
4:F:137:ARG:NE	4:F:332:LYS:HE3	2.29	0.40
4:F:225:ALA:O	4:F:231:ILE:HG23	2.21	0.40
4:G:136:LYS:CD	4:G:208:ASP:HA	2.51	0.40
4:G:331:LEU:CG	4:G:333:CYS:HB3	2.52	0.40
4:G:348:GLN:CG	4:G:349:ILE:N	2.85	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	341/343 (99%)	295 (86%)	26 (8%)	20 (6%)	1	17
2	B	358/376 (95%)	323 (90%)	24 (7%)	11 (3%)	4	27
2	C	363/376 (96%)	331 (91%)	24 (7%)	8 (2%)	6	35
2	D	357/376 (95%)	313 (88%)	34 (10%)	10 (3%)	5	30
3	E	332/337 (98%)	291 (88%)	26 (8%)	15 (4%)	2	22
4	F	364/369 (99%)	308 (85%)	41 (11%)	15 (4%)	3	23
4	G	364/369 (99%)	297 (82%)	53 (15%)	14 (4%)	3	24
All	All	2479/2546 (97%)	2158 (87%)	228 (9%)	93 (4%)	5	24

All (93) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	72	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	76	SER
1	A	213	THR
1	A	265	ALA
1	A	270	ARG
1	A	278	VAL
1	A	338	ASP
2	B	112	GLN
2	B	129	HIS
2	C	129	HIS
2	D	3	TYR
2	D	87	PHE
3	E	51	GLN
3	E	62	CYS
3	E	182	MET
3	E	183	SER
3	E	270	VAL
4	F	49	LEU
4	F	51	MET
4	F	116	PHE
4	F	153	TYR
4	F	248	LEU
4	F	343	SER
4	G	39	ASP
4	G	126	VAL
4	G	208	ASP
4	G	243	ASP
4	G	343	SER
4	G	344	VAL
1	A	68	CYS
1	A	128	THR
1	A	162	LEU
1	A	333	HIS
2	B	21	GLN
2	C	33	SER
2	C	91	ILE
2	C	96	ALA
2	C	344	ASP
2	D	74	GLY
2	D	86	ARG
2	D	120	PHE
2	D	149	HIS
3	E	333	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	F	103	ARG
4	G	2	LYS
4	G	196	PRO
1	A	266	HIS
2	B	117	ARG
2	D	50	GLY
2	D	117	ARG
3	E	31	ALA
3	E	72	THR
3	E	106	LEU
3	E	164	LEU
4	F	23	GLY
4	F	150	ASP
4	F	211	ASP
4	F	242	PRO
4	G	28	PRO
4	G	118	ASN
4	G	253	ASP
1	A	67	LEU
2	B	17	ASP
2	B	95	ALA
2	B	115	PRO
2	B	275	GLY
2	C	5	VAL
2	C	149	HIS
2	D	231	GLN
3	E	52	GLN
3	E	56	HIS
3	E	261	GLY
4	F	187	SER
4	G	365	ARG
1	A	19	ALA
1	A	60	ASP
1	A	86	GLU
1	A	193	PRO
2	B	36	ARG
2	B	298	SER
2	D	47	ARG
4	F	278	PHE
4	G	65	PRO
1	A	61	TRP
1	A	163	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	86	ARG
2	C	141	LYS
3	E	79	LEU
4	F	183	PRO
4	G	176	ARG
3	E	225	PRO
4	F	19	GLY
1	A	334	LYS

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	291/291 (100%)	272 (94%)	19 (6%)	17 42
2	B	296/312 (95%)	279 (94%)	17 (6%)	20 45
2	C	301/312 (96%)	286 (95%)	15 (5%)	24 49
2	D	294/312 (94%)	266 (90%)	28 (10%)	8 27
3	E	270/272 (99%)	251 (93%)	19 (7%)	15 40
4	F	313/315 (99%)	277 (88%)	36 (12%)	5 21
4	G	313/315 (99%)	270 (86%)	43 (14%)	3 17
All	All	2078/2129 (98%)	1901 (92%)	177 (8%)	14 33

All (177) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	50	HIS
1	A	58	ASN
1	A	86	GLU
1	A	95	GLU
1	A	128	THR
1	A	136	GLN
1	A	141	THR
1	A	148	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	167	ASN
1	A	216	HIS
1	A	217	TRP
1	A	228	ARG
1	A	272	LEU
1	A	315	ASP
1	A	331	LEU
1	A	332	CYS
1	A	338	ASP
1	A	341	ILE
2	B	1	MET
2	B	14	THR
2	B	57	LEU
2	B	64	CYS
2	B	66	THR
2	B	71	THR
2	B	110	ASN
2	B	126	ASP
2	B	129	HIS
2	B	130	MET
2	B	140	LEU
2	B	181	GLU
2	B	208	ARG
2	B	246	ASP
2	B	269	ASN
2	B	304	ASN
2	B	344	ASP
2	C	51	LYS
2	C	54	ILE
2	C	66	THR
2	C	94	ASP
2	C	100	LYS
2	C	124	LEU
2	C	179	ASP
2	C	208	ARG
2	C	243	THR
2	C	253	VAL
2	C	270	GLU
2	C	276	ILE
2	C	344	ASP
2	C	360	HIS
2	C	363	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	33	SER
2	D	39	HIS
2	D	44	SER
2	D	46	THR
2	D	47	ARG
2	D	69	THR
2	D	75	VAL
2	D	86	ARG
2	D	94	ASP
2	D	104	THR
2	D	109	ASP
2	D	117	ARG
2	D	119	ARG
2	D	180	VAL
2	D	185	HIS
2	D	188	GLU
2	D	189	HIS
2	D	195	HIS
2	D	196	ILE
2	D	206	LEU
2	D	213	SER
2	D	223	GLN
2	D	309	ILE
2	D	310	GLU
2	D	318	ARG
2	D	339	LEU
2	D	341	TYR
2	D	353	LEU
3	E	2	ARG
3	E	11	PHE
3	E	13	LYS
3	E	41	ILE
3	E	49	LEU
3	E	51	GLN
3	E	65	CYS
3	E	105	ARG
3	E	110	LYS
3	E	126	ASN
3	E	158	ARG
3	E	160	ARG
3	E	210	TRP
3	E	213	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	E	218	GLN
3	E	222	TYR
3	E	298	GLU
3	E	304	THR
3	E	317	LEU
4	F	5	VAL
4	F	9	HIS
4	F	53	MET
4	F	61	GLN
4	F	62	PRO
4	F	64	GLU
4	F	69	THR
4	F	71	PRO
4	F	76	PHE
4	F	123	GLN
4	F	130	LEU
4	F	134	THR
4	F	144	PHE
4	F	150	ASP
4	F	162	THR
4	F	189	PRO
4	F	193	VAL
4	F	207	LEU
4	F	232	PHE
4	F	244	TYR
4	F	255	HIS
4	F	283	LEU
4	F	286	SER
4	F	307	ASP
4	F	309	THR
4	F	315	MET
4	F	322	SER
4	F	329	ASN
4	F	333	CYS
4	F	334	GLU
4	F	340	LEU
4	F	342	ASP
4	F	349	ILE
4	F	354	SER
4	F	356	SER
4	F	366	LEU
4	G	7	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	G	13	PRO
4	G	24	ARG
4	G	27	LEU
4	G	34	LEU
4	G	48	ASP
4	G	51	MET
4	G	59	LEU
4	G	69	THR
4	G	87	GLU
4	G	93	GLU
4	G	120	ASP
4	G	122	TRP
4	G	125	GLU
4	G	130	LEU
4	G	132	GLN
4	G	138	LEU
4	G	143	GLN
4	G	165	GLU
4	G	176	ARG
4	G	179	VAL
4	G	182	MET
4	G	202	GLU
4	G	208	ASP
4	G	215	ARG
4	G	221	ASN
4	G	227	VAL
4	G	245	ARG
4	G	253	ASP
4	G	256	LEU
4	G	260	CYS
4	G	261	ASP
4	G	262	LEU
4	G	300	GLU
4	G	309	THR
4	G	319	PHE
4	G	321	VAL
4	G	326	ASP
4	G	327	VAL
4	G	340	LEU
4	G	341	THR
4	G	342	ASP
4	G	351	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	45	GLN
1	A	50	HIS
1	A	51	HIS
1	A	69	GLN
1	A	105	HIS
1	A	144	GLN
1	A	146	GLN
1	A	157	GLN
1	A	167	ASN
1	A	168	GLN
1	A	231	HIS
1	A	266	HIS
1	A	300	GLN
1	A	333	HIS
2	B	13	GLN
2	B	23	HIS
2	B	38	HIS
2	B	137	ASN
2	B	248	GLN
2	C	21	GLN
2	C	129	HIS
2	C	149	HIS
2	C	182	GLN
2	C	223	GLN
2	C	269	ASN
2	D	4	GLN
2	D	78	ASN
2	D	182	GLN
2	D	186	GLN
2	D	195	HIS
2	D	198	HIS
2	D	204	GLN
2	D	235	GLN
2	D	360	HIS
3	E	61	HIS
3	E	162	HIS
3	E	218	GLN
3	E	240	GLN
3	E	295	HIS
4	F	132	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	F	148	HIS
4	F	226	HIS
4	F	265	GLN
4	F	335	ASN
4	F	348	GLN
4	G	9	HIS
4	G	16	GLN
4	G	191	HIS
4	G	222	ASN
4	G	265	GLN
4	G	275	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

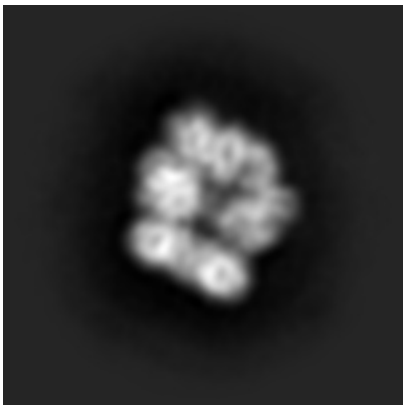
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-43096. These allow visual inspection of the internal detail of the map and identification of artifacts.

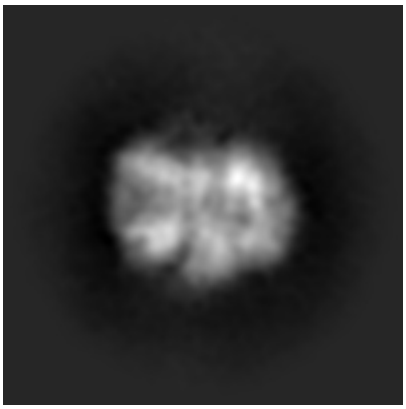
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

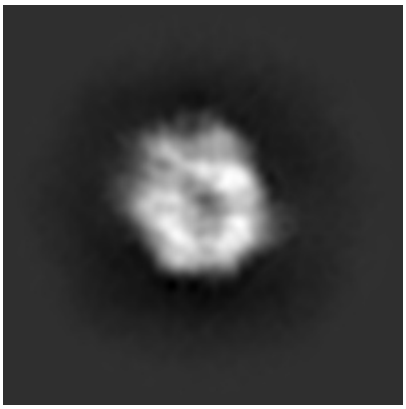
6.1.1 Primary map



X

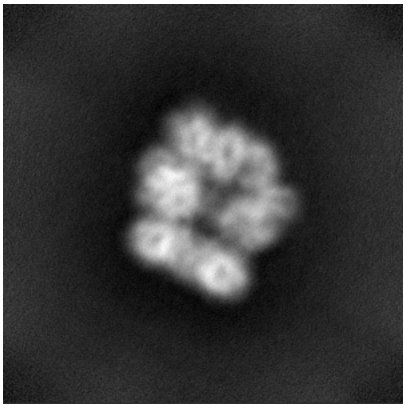


Y

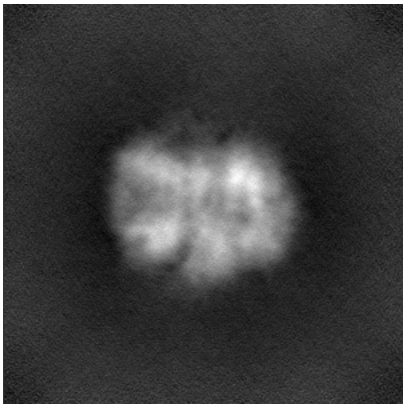


Z

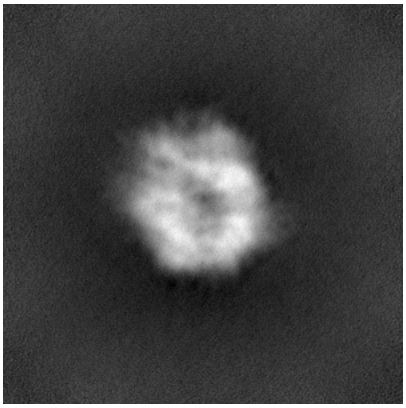
6.1.2 Raw map



X



Y

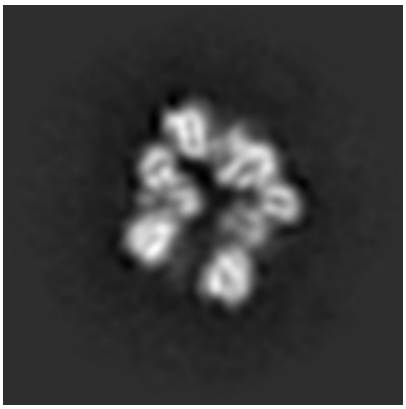


Z

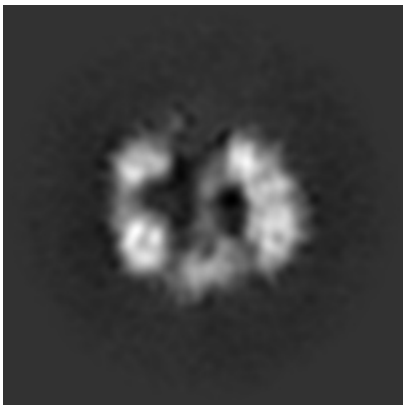
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



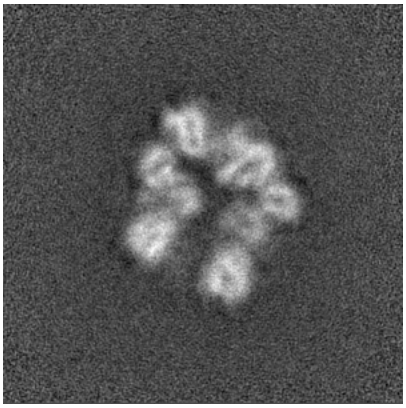
X Index: 150



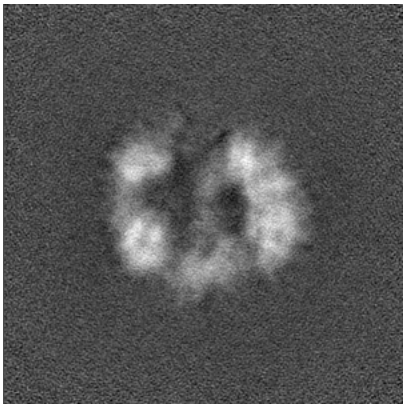
Y Index: 150

Z Index: 150

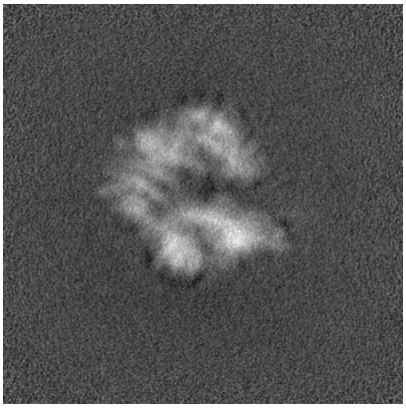
6.2.2 Raw map



X Index: 150



Y Index: 150

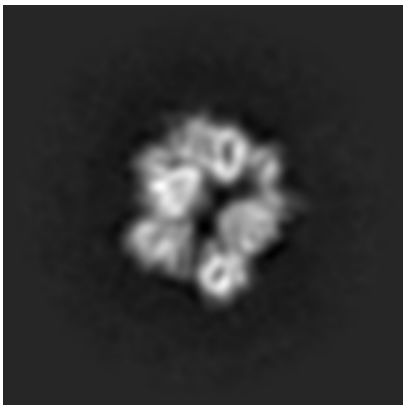


Z Index: 150

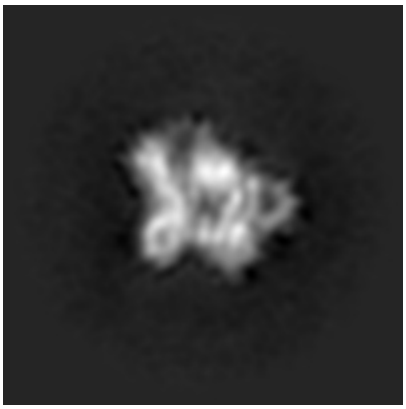
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

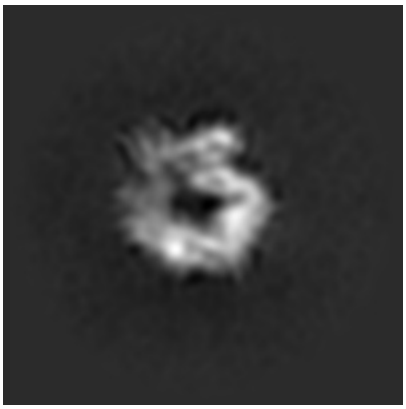
6.3.1 Primary map



X Index: 170

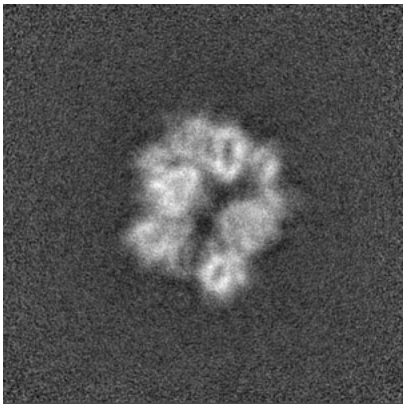


Y Index: 122

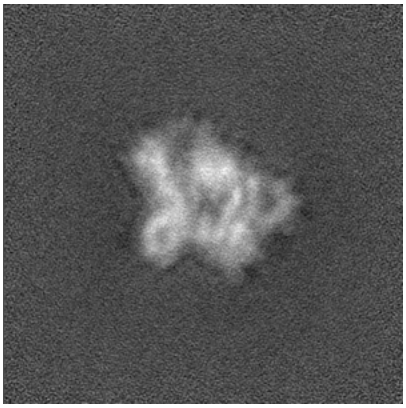


Z Index: 173

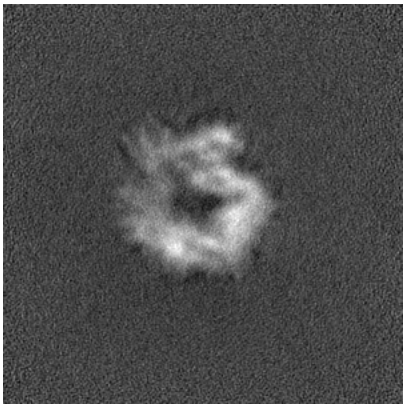
6.3.2 Raw map



X Index: 169



Y Index: 122

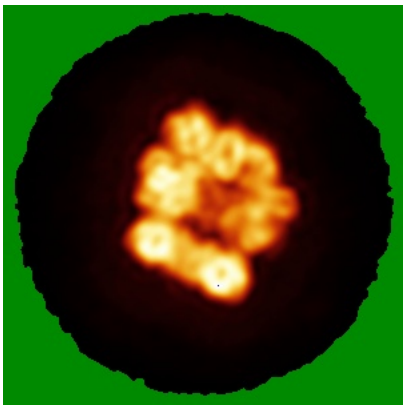


Z Index: 173

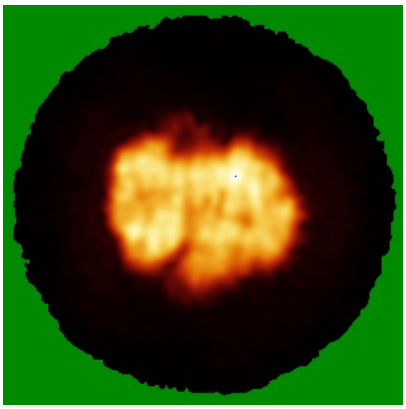
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

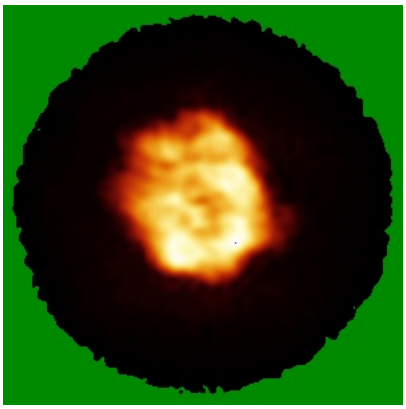
6.4.1 Primary map



X

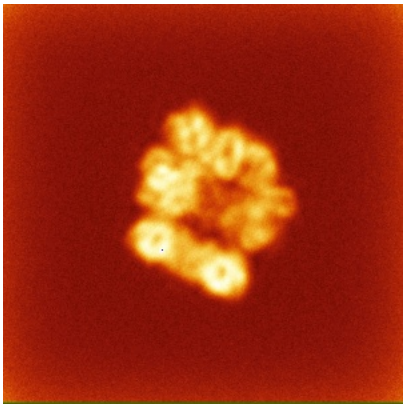


Y

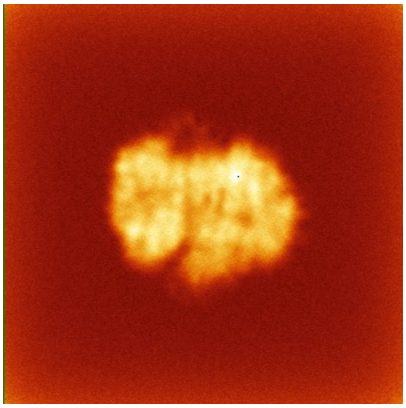


Z

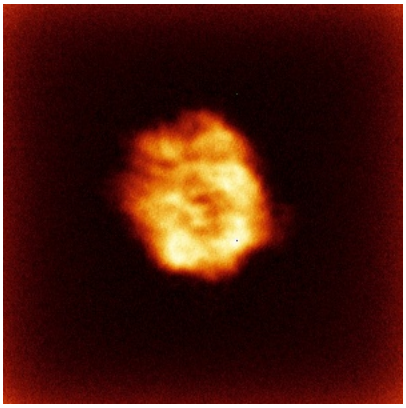
6.4.2 Raw map



X



Y

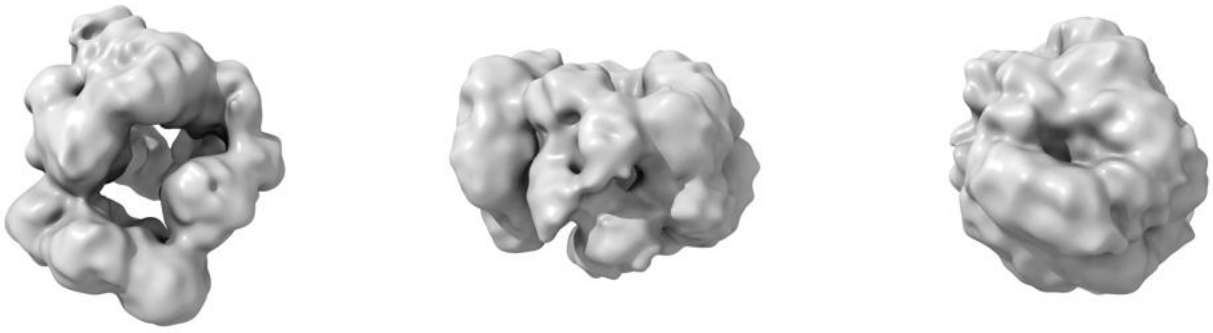


Z

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)

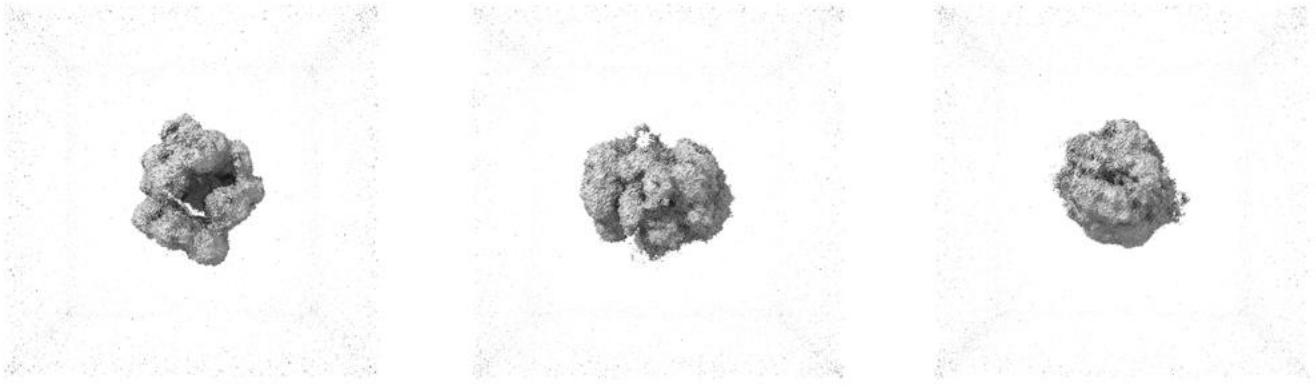
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.33. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

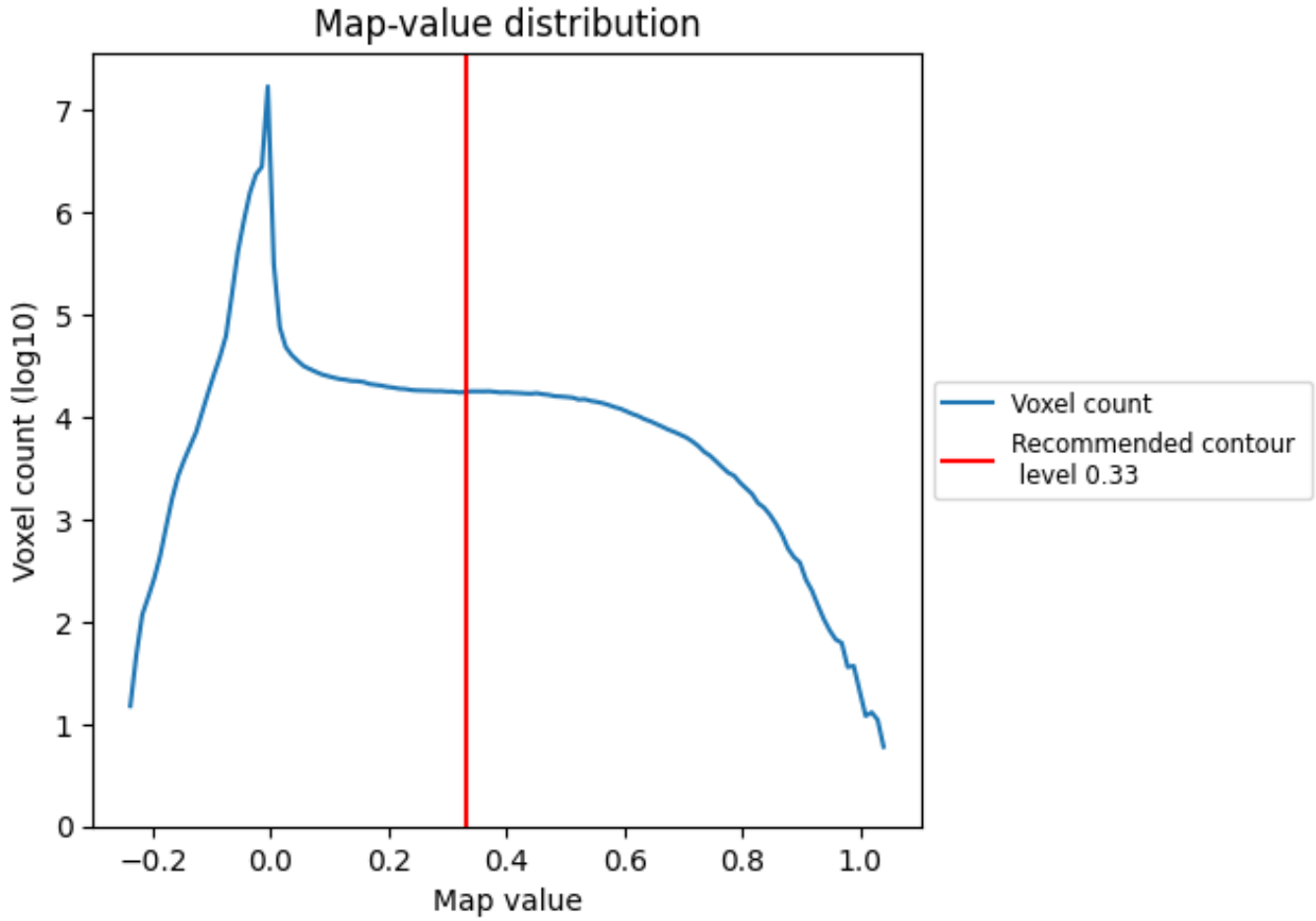
6.6 Mask visualisation (i)

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

7 Map analysis

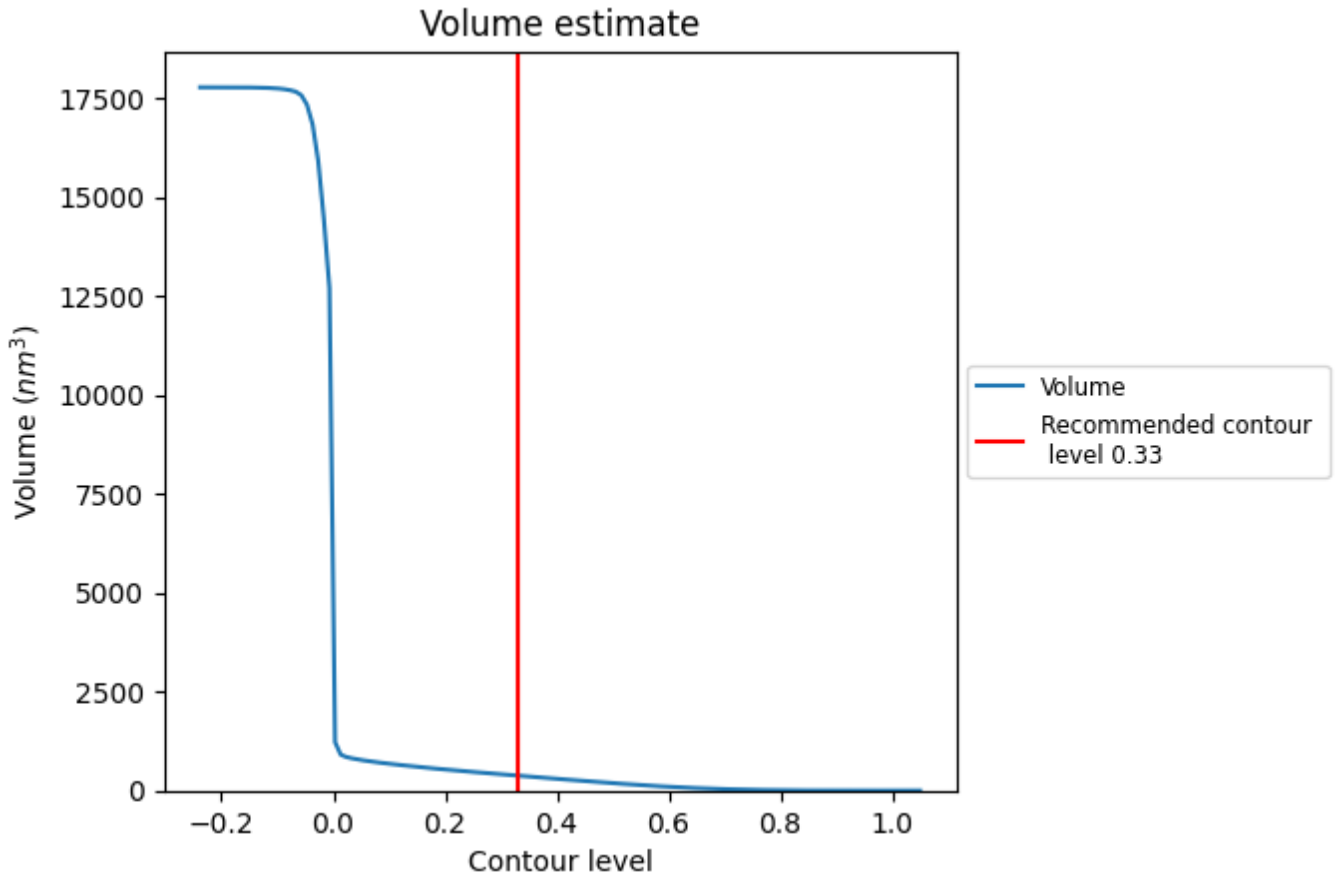
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

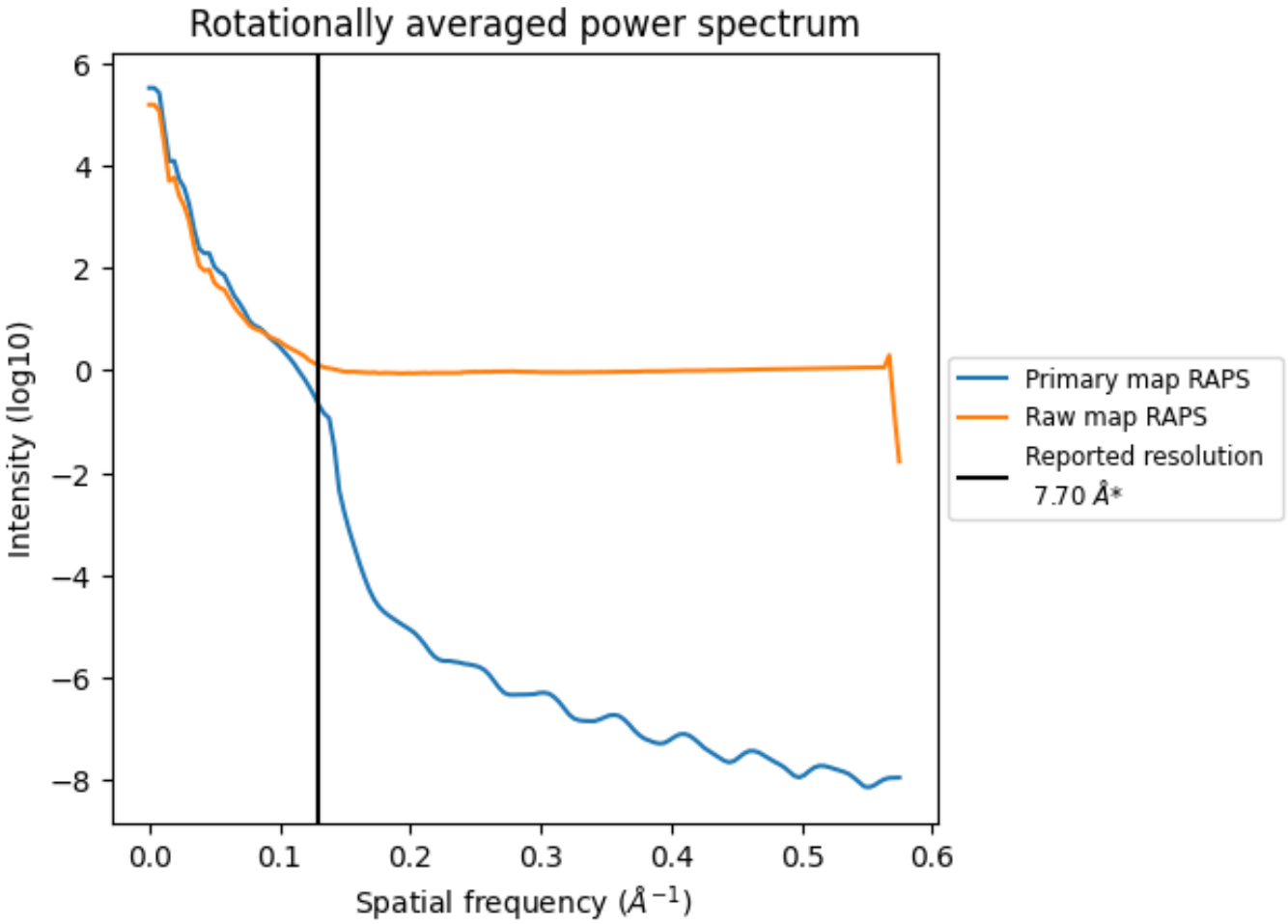
7.2 Volume estimate



The volume at the recommended contour level is 378 nm^3; this corresponds to an approximate mass of 341 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 (i)

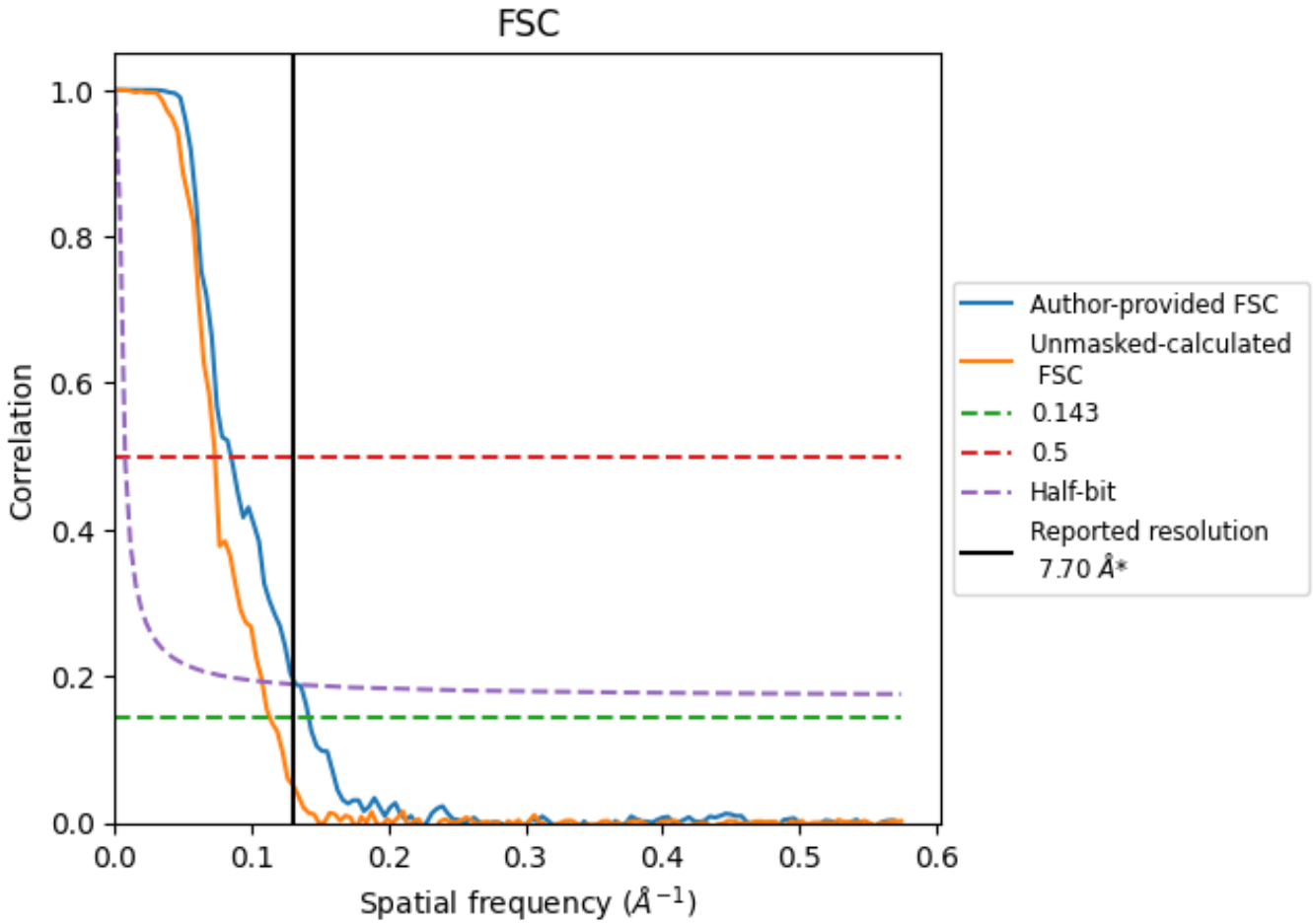


*Reported resolution corresponds to spatial frequency of 0.130 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.130 Å^{-1}

8.2 Resolution estimates (i)

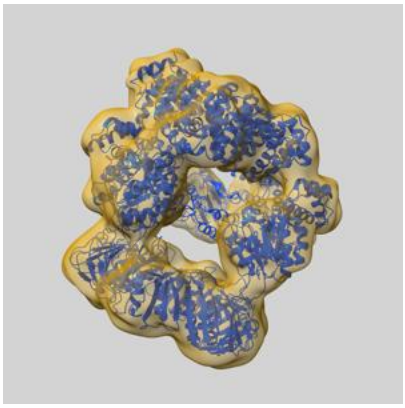
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.70	-	-
Author-provided FSC curve	7.05	11.78	7.56
Unmasked-calculated*	8.81	13.66	9.29

*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 8.81 differs from the reported value 7.7 by more than 10 %

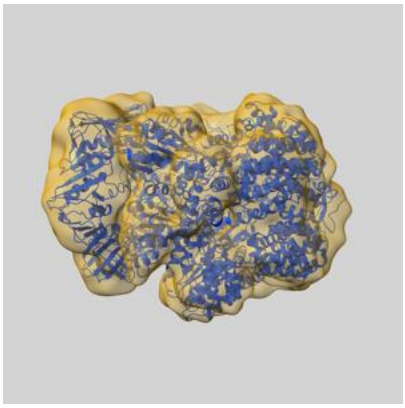
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-43096 and PDB model 8VAN. Per-residue inclusion information can be found in section 3 on page 5.

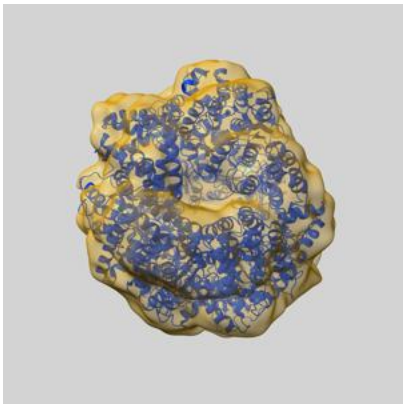
9.1 Map-model overlay



X



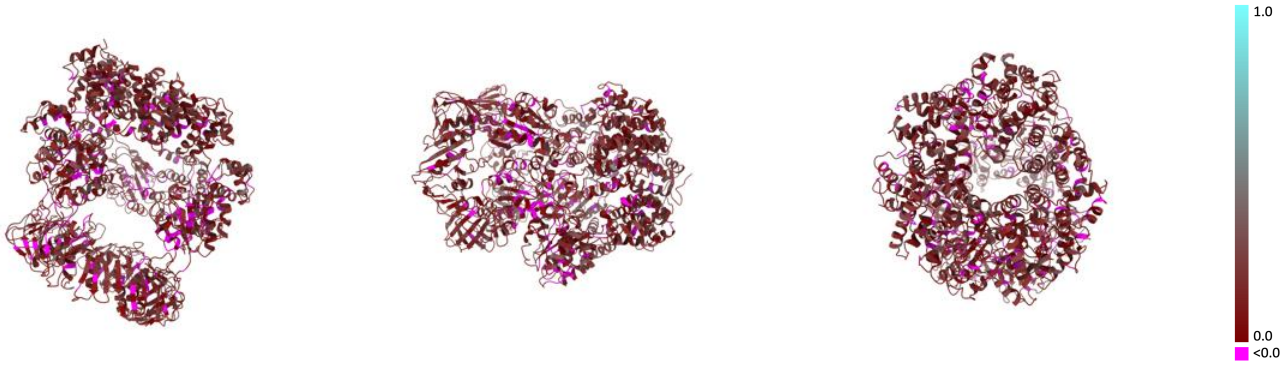
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.33 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

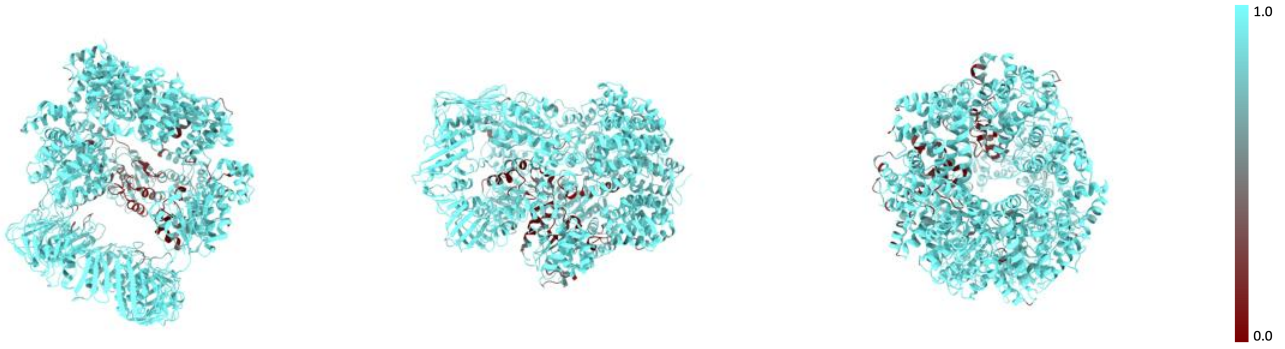
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

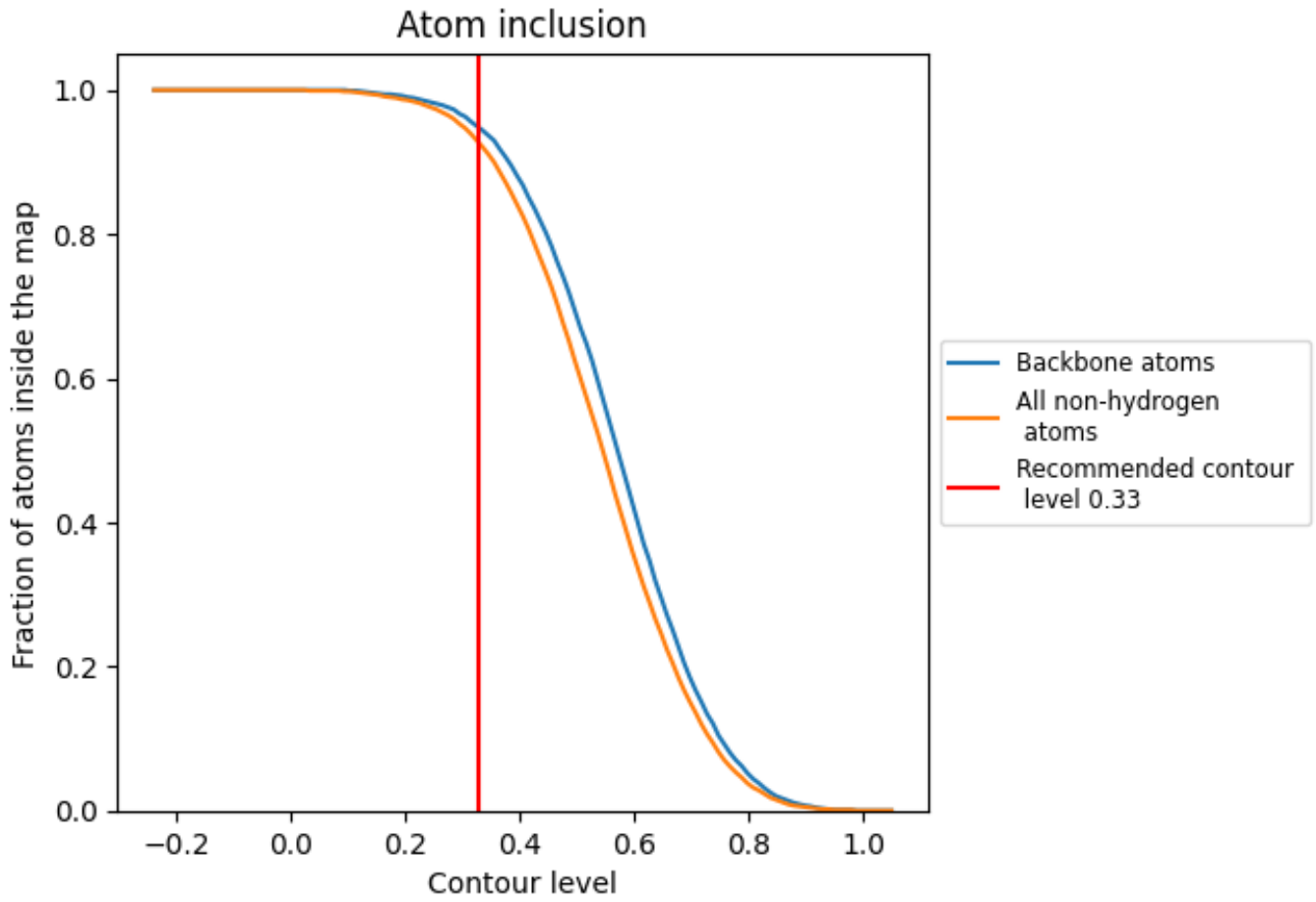
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.33).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 93% 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 (0.33) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9260	0.1420
A	0.9320	0.1460
B	0.8370	0.1280
C	0.8030	0.1320
D	0.9720	0.1470
E	0.9780	0.1450
F	0.9860	0.1540
G	0.9730	0.1460