



Full wwPDB EM Validation Report ⓘ

Apr 1, 2025 – 11:03 PM EDT

PDB ID : 8OES / pdb_00008oes
EMDB ID : EMD-16808
Title : MUC5B amino acids 26-1435 Three beads
Authors : Khmel'nitsky, L.; Fass, D.
Deposited on : 2023-03-12
Resolution : 3.00 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev117
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

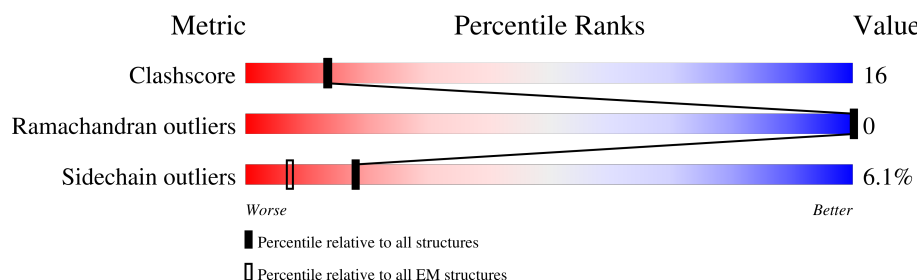
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1227	
1	B	1227	
1	C	1227	
1	D	1227	
1	E	1227	
1	F	1227	
1	G	1227	
1	H	1227	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	I	100	<div><div></div><div>12%</div><div>62%</div><div>34%</div><div></div></div>
2	J	100	<div><div></div><div>11%</div><div>60%</div><div>38%</div><div></div></div>
2	K	100	<div><div></div><div>43%</div><div>61%</div><div>35%</div><div></div></div>
2	L	100	<div><div></div><div>30%</div><div>62%</div><div>34%</div><div></div></div>
2	M	100	<div><div></div><div>95%</div><div>62%</div><div>35%</div><div></div></div>
2	N	100	<div><div></div><div>94%</div><div>63%</div><div>34%</div><div></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 57846 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 Mucin-5B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1168	Total	C	N	O	S	2	0
			8793	5438	1533	1700	122		
1	B	1168	Total	C	N	O	S	2	0
			8793	5438	1533	1700	122		
1	C	1168	Total	C	N	O	S	2	0
			8793	5438	1533	1700	122		
1	D	1168	Total	C	N	O	S	2	0
			8793	5438	1533	1700	122		
1	E	715	Total	C	N	O	S	2	0
			5383	3331	943	1041	68		
1	F	715	Total	C	N	O	S	2	0
			5383	3331	943	1041	68		
1	G	453	Total	C	N	O	S	0	0
			3410	2107	590	659	54		
1	H	453	Total	C	N	O	S	0	0
			3410	2107	590	659	54		

- Molecule 2 is a protein called Mucin-5B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	100	Total	C	N	O	S	0	0
			781	482	137	149	13		
2	J	100	Total	C	N	O	S	0	0
			781	482	137	149	13		
2	K	100	Total	C	N	O	S	0	0
			781	482	137	149	13		
2	L	100	Total	C	N	O	S	0	0
			781	482	137	149	13		
2	M	100	Total	C	N	O	S	0	0
			781	482	137	149	13		
2	N	100	Total	C	N	O	S	0	0
			781	482	137	149	13		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
3	A	3	Total 3	Ca 3	0
3	B	3	Total 3	Ca 3	0
3	C	3	Total 3	Ca 3	0
3	D	3	Total 3	Ca 3	0
3	E	2	Total 2	Ca 2	0
3	F	2	Total 2	Ca 2	0
3	G	1	Total 1	Ca 1	0
3	H	1	Total 1	Ca 1	0
3	I	1	Total 1	Ca 1	0
3	J	1	Total 1	Ca 1	0
3	K	1	Total 1	Ca 1	0
3	L	1	Total 1	Ca 1	0
3	M	1	Total 1	Ca 1	0
3	N	1	Total 1	Ca 1	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

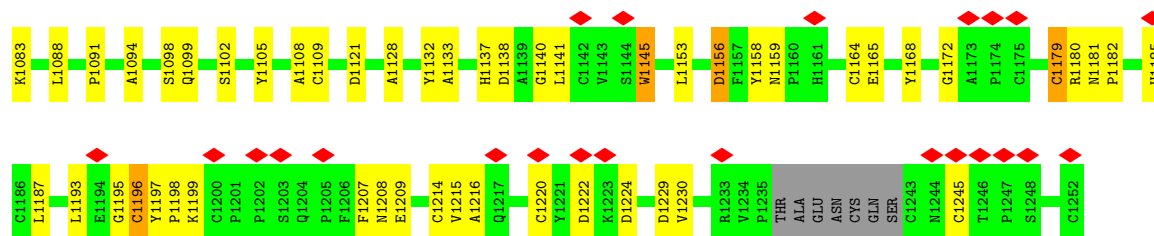


Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	

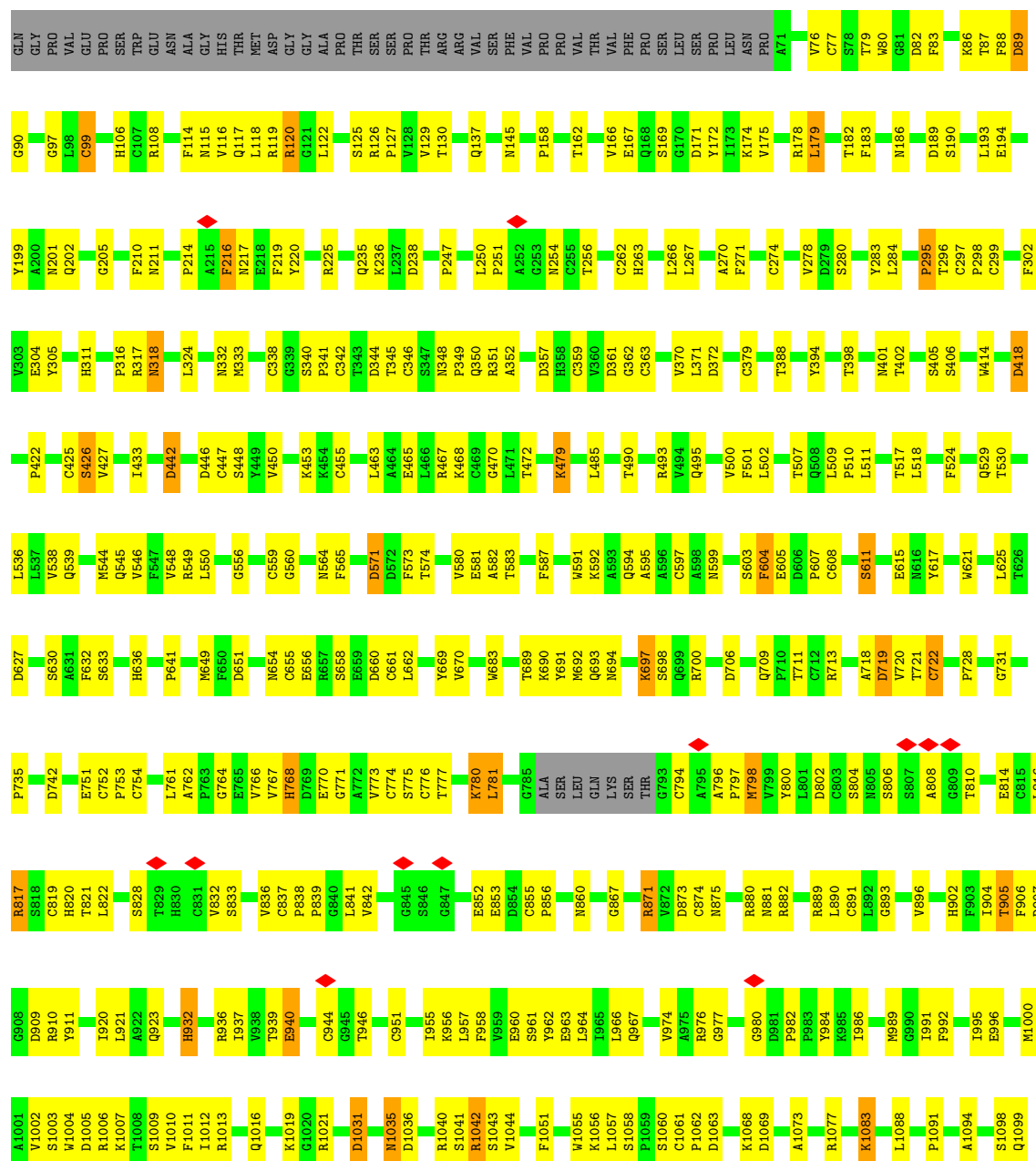
Continued on next page...

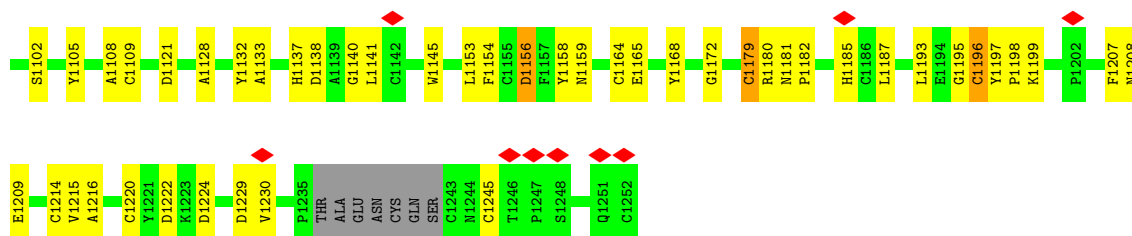
Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	D	1	Total	C	N	O	0
			14	8	1	5	
4	D	1	Total	C	N	O	0
			14	8	1	5	
4	D	1	Total	C	N	O	0
			14	8	1	5	
4	D	1	Total	C	N	O	0
			14	8	1	5	
4	E	1	Total	C	N	O	0
			14	8	1	5	
4	E	1	Total	C	N	O	0
			14	8	1	5	
4	E	1	Total	C	N	O	0
			14	8	1	5	
4	E	1	Total	C	N	O	0
			14	8	1	5	
4	F	1	Total	C	N	O	0
			14	8	1	5	
4	F	1	Total	C	N	O	0
			14	8	1	5	
4	F	1	Total	C	N	O	0
			14	8	1	5	
4	F	1	Total	C	N	O	0
			14	8	1	5	

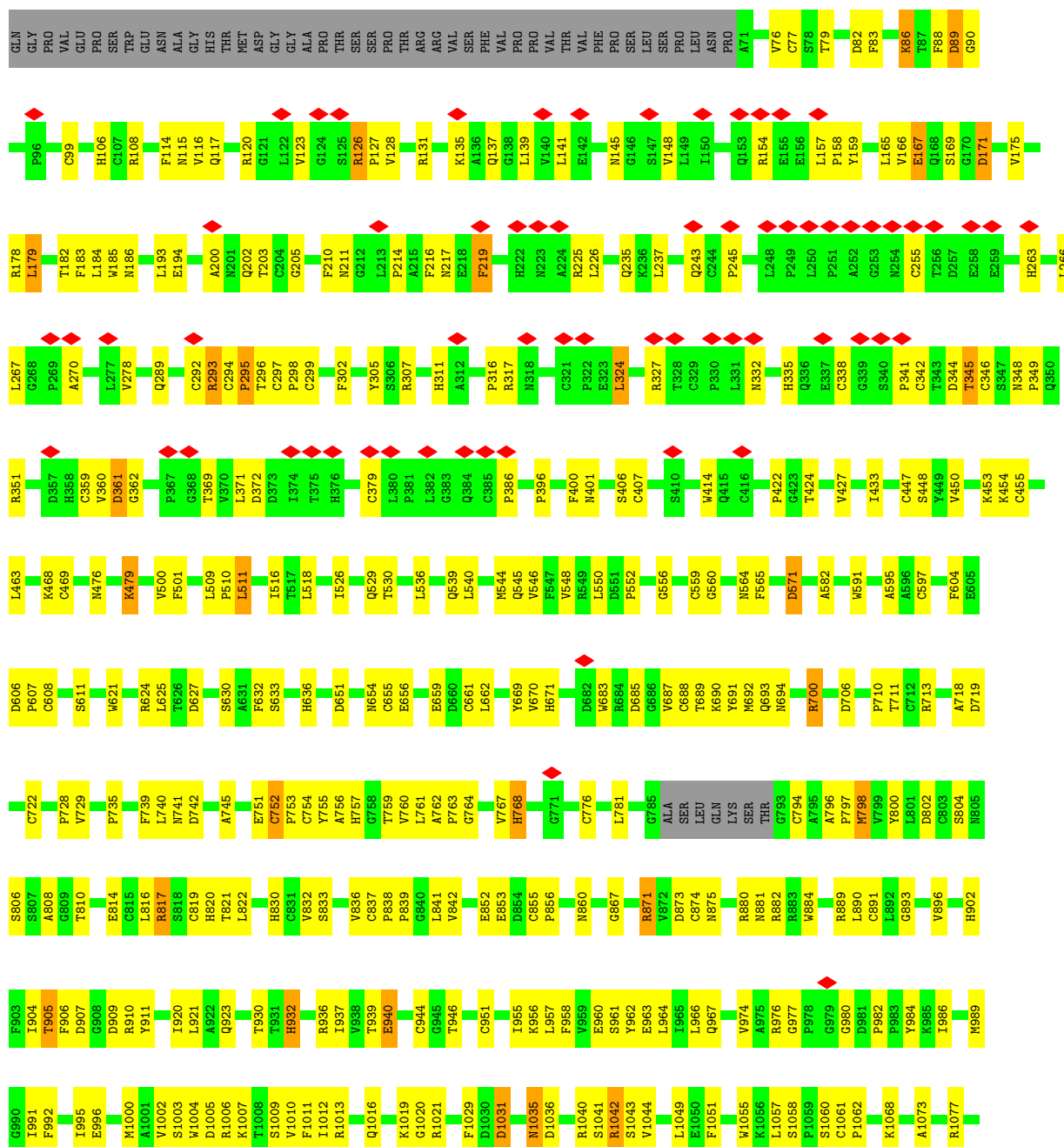


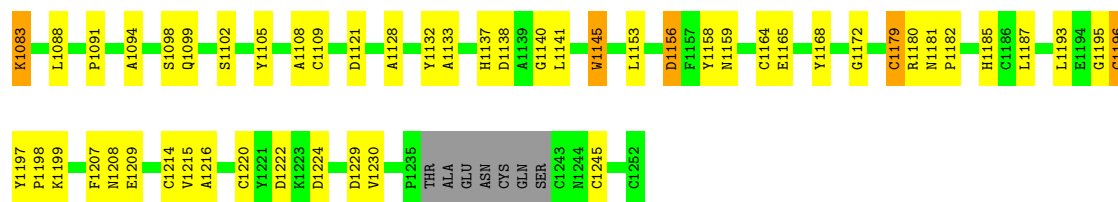
• Molecule 1: Mucin-5B





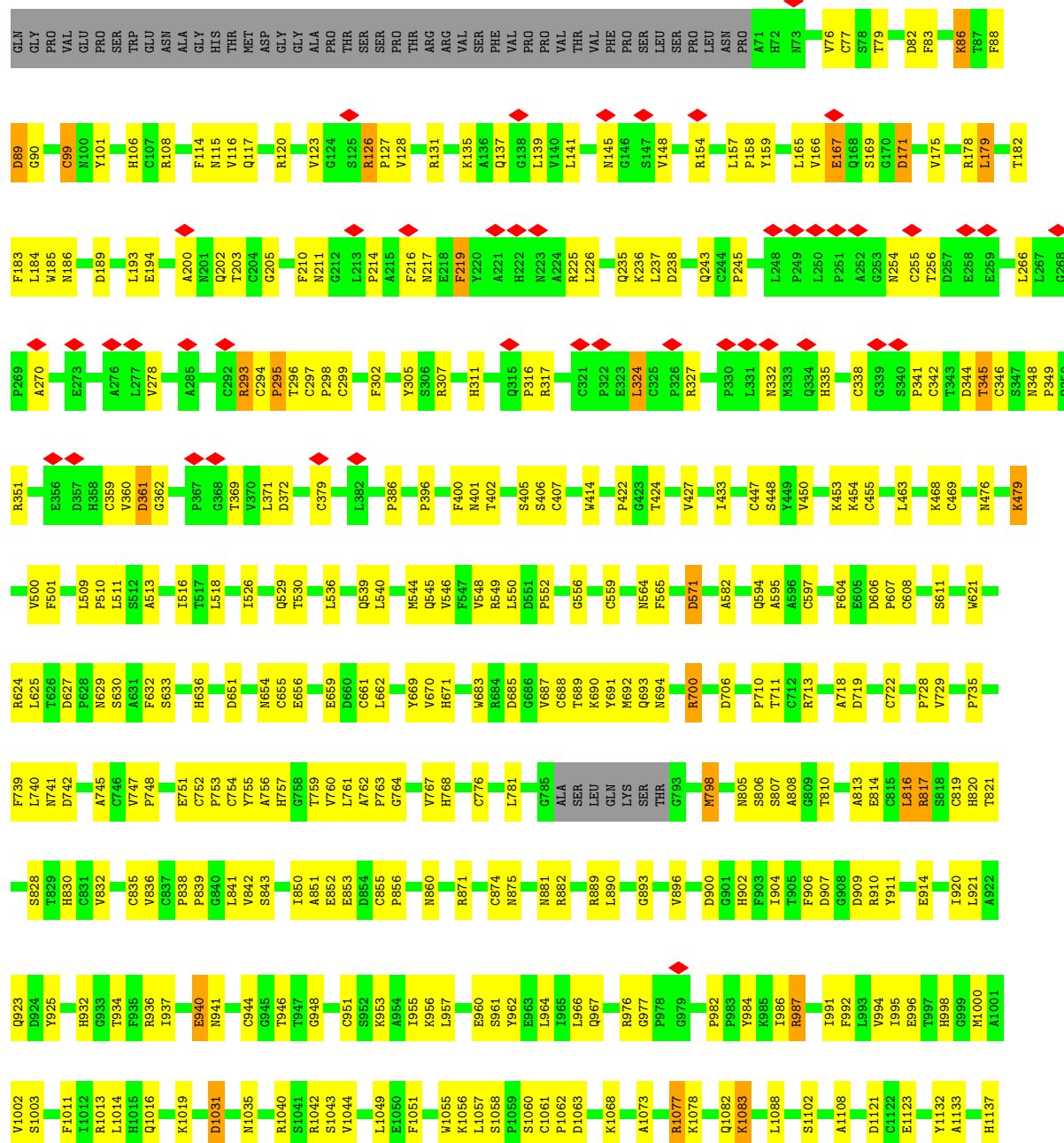
• Molecule 1: Mucin-5B





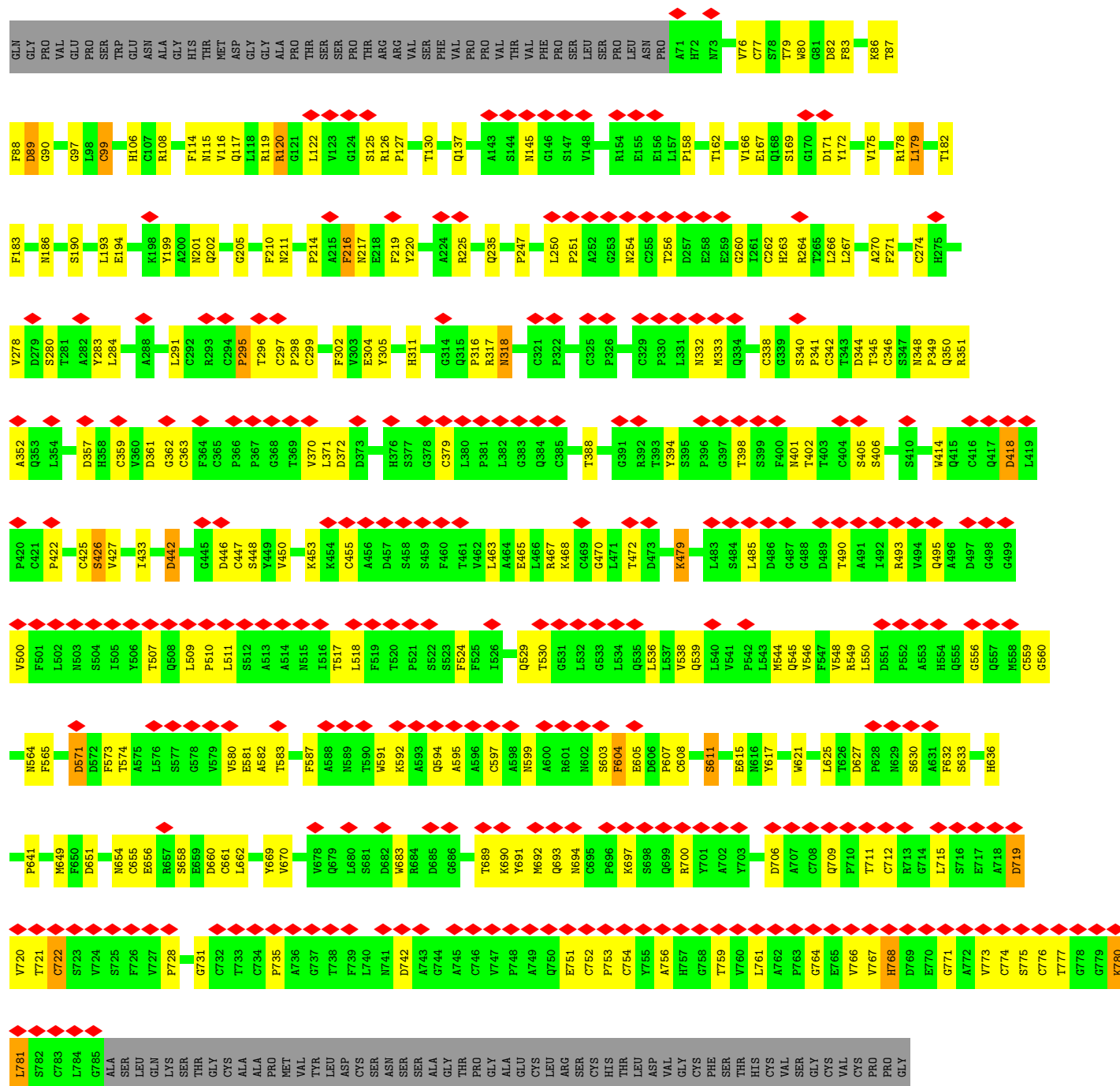
• Molecule 1: Mucin-5B

Chain D: 63% 30% 5%



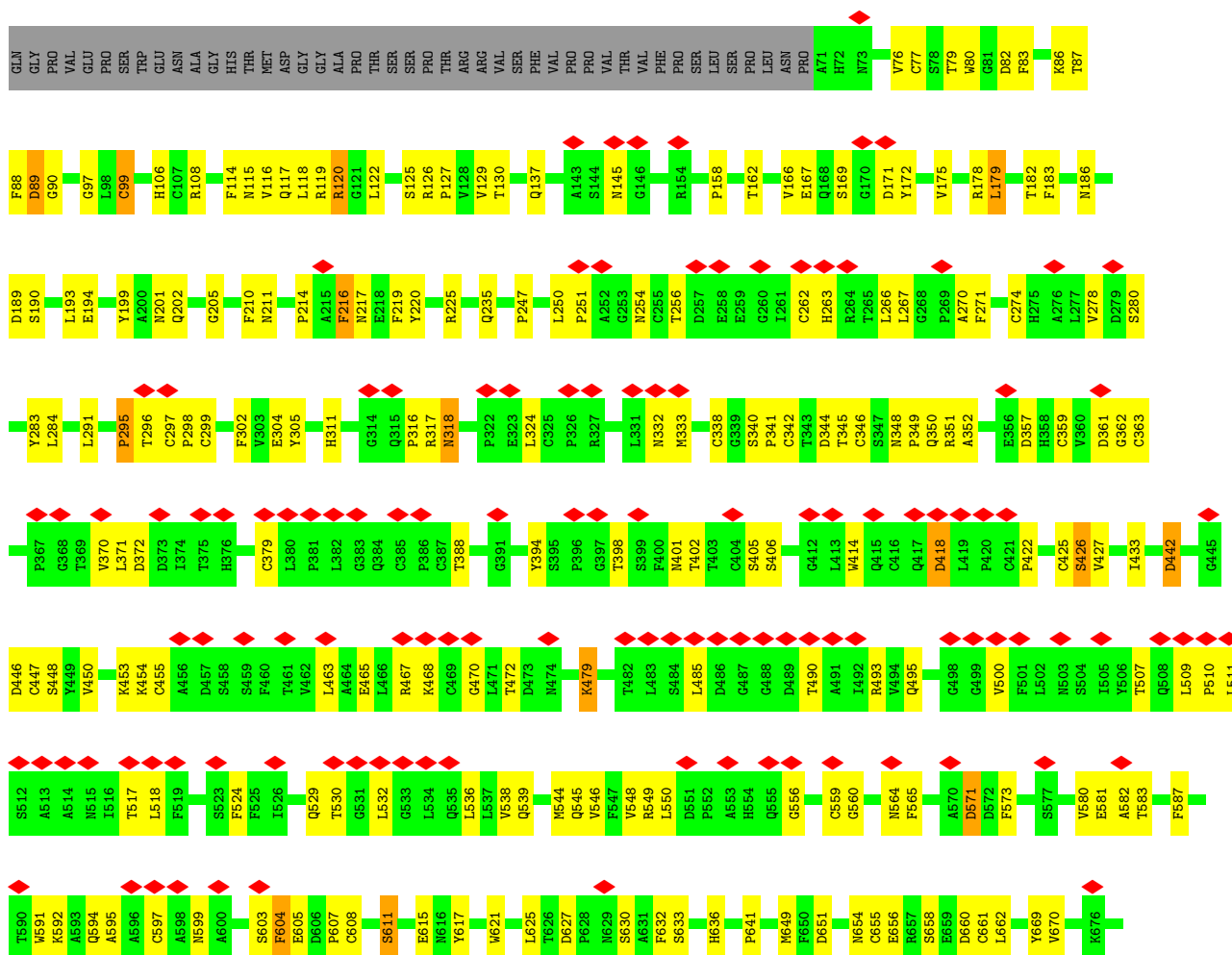


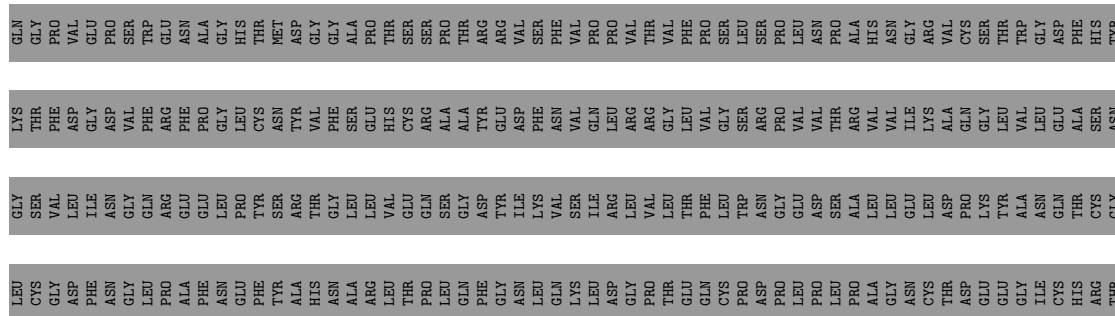
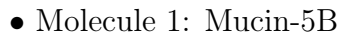
• Molecule 1: Mucin-5B

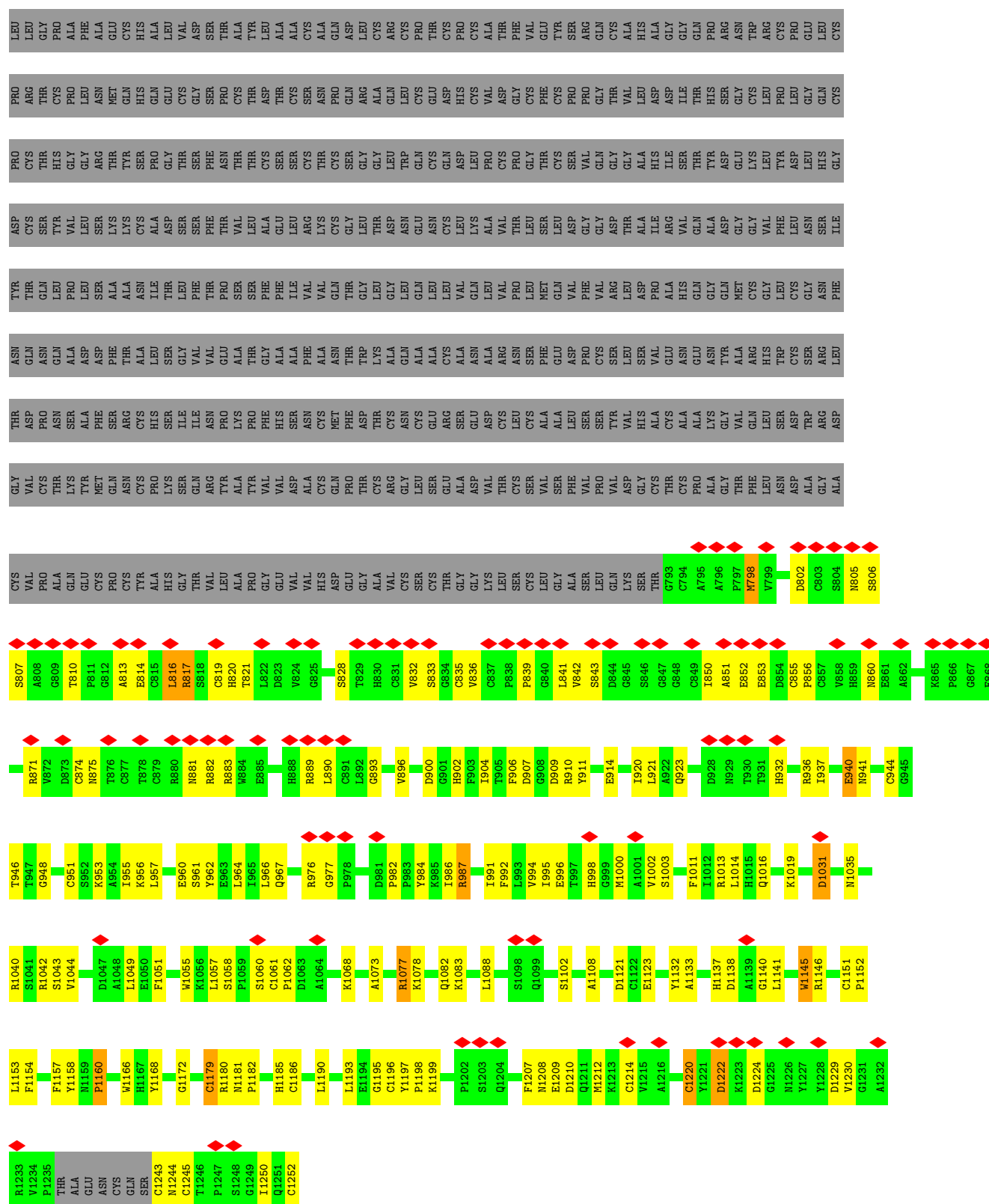


PRO	LEU	ALA	ARG	SER	GLY	LEU
PRO	CYS	GLN	VAL	TYR	HIS	VAL
SER	VAL	GLN	CYS	GLU	PHE	SER
GLN	SER	GLN	GLY	LEU	ILE	ASP
PRO	TRP	CYS	LEU	ILE	THR	GLY
PHE	ARG	SER	CYS	LEU	PHE	SER
PHE	THR	ILE	GLY	GLN	ASP	GLY
ASN	PRO	LEU	ASN	GLU	GLY	CYS
ASP	THR	GLY	PHE	THR	ARG	ILE
GLN	CYS	PRO	ASP	PHE	TYR	ALA
MET	PRO	THR	ASN	LYS	SER	GLU
LYS	LEU	PHE	ALA	ALA	PHE	GLU
CYS	PHE	ALA	ILE	VAL	GLU	ASP
VAL	CYS	ALA	ASN	ALA	GLY	CYS
ALA	ASP	CYS	ASP	ARG	SER	PRO
ALA	PHE	ARG	PHE	GLY	CYS	CYS
GLN	THR	SER	ALA	PRO	VAL	VAL
CYS	ASN	GLN	THR	GLY	TYR	HIS
CYS	PRO	VAL	ARG	GLY	ILE	ASN
TYR	HIS	TYR	SER	ASP	LEU	GLU
ASP	GLY	SER	ARG	PRO	ALA	ALA
LYS	GLY	THR	SER	PRO	GLN	THR
ASP	CYS	LYS	VAL	TYR	ASP	THR
GLY	GLU	TYR	VAL	LYS	THR	LYS
ASN	TRP	GLY	GLY	ILE	CYS	PRO
TYR	HIS	TYR	ASP	ARG	GLY	GLY
ASP	THR	ALA	TYR	ALA	ASP	GLU
VAL	GLN	CYS	LEU	MET	ASN	THR
PRO	PRO	VAL	GLU	GLY	THR	ILE
GLY	CYS	ASN	PHE	ILE	THR	ARG
ALA	GLY	ASP	GLY	PHE	HIS	VAL
ALA	ARG	ALA	ASN	VAL	GLY	ASP
VAL	PRO	CYS	SER	VAL	THR	CYS
PRO	CYS	ALA	TRP	ILE	PHE	ASN
THR	LEU	CYS	LYS	GLU	ARG	THR
ALA	LYS	ASP	LEU	THR	ILE	CYS
GLU	THR	SER	SER	HIS	VAL	THR
ASN	CYS	GLY	PRO	GLY	THR	CYS
CYS	ASN	GLY	SER	MET	GLU	ASN
GLN	ASN	ASP	CYS	ASN	ASN	ARG
SER	PRO	CYS	PRO	VAL	ILE	ARG
CYS	SER	GLU	ASP	SER	PRO	ARG
ASN	GLY	CYS	ALA	TRP	CYS	TRP
THR	HIS	PHE	LEU	ASP	GLY	GLU
CYS	HIS	PHE	ASP	ARG	THR	CYS
THR	THR	THR	ALA	ARG	THR	SER
PRO	LEU	THR	PRO	LYS	THR	HIS
SER	VAL	ALA	LYS	THR	GLY	ARG
GLY	ASP	VAL	ASP	SER	THR	THR
ILE	LEU	ALA	PRO	PHE	THR	LEU
GLN	PRO	ALA	CYS	VAL	CYS	CYS
CYS	LEU	TYR	THR	ILE	SER	LEU
	GLY	ALA	ALA	ARG	LYS	GLY
	GLU	GLN	ASN	LEU	ALA	THR
	GLY	ALA	PRO	LEU	ILE	CYS
	CYS	CYS	PHE	GLN	LYS	VAL
	CYS	CYS	THR	ASN	ILE	THR
	TYR	HIS	ARG	SER	GLY	ASP
	THR	ASP	LYS	TYR	PHE	VAL
	PRO	ASP	THR	THR	GLY	THR
	LYS	ALA	TER	GLY	THR	ASN

- Molecule 1: Mucin-5B



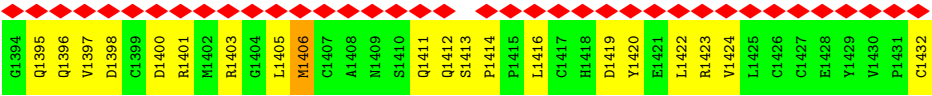




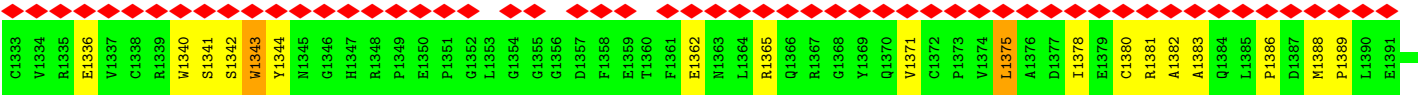
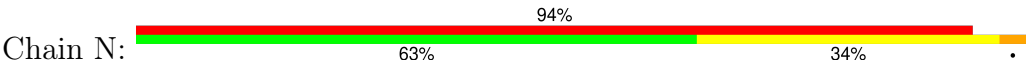
• Molecule 2: Mucin-5B







● Molecule 2: Mucin-5B



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	88708	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.710	Depositor
Minimum map value	-0.488	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.056	Depositor
Map size (Å)	578.48, 578.48, 578.48	wwPDB
Map dimensions	700, 700, 700	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8264, 0.8264, 0.8264	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.38	0/9014	0.58	1/12269 (0.0%)
1	B	0.46	4/9014 (0.0%)	0.61	6/12269 (0.0%)
1	C	0.38	0/9014	0.58	1/12269 (0.0%)
1	D	0.38	0/9014	0.57	2/12269 (0.0%)
1	E	0.49	4/5514 (0.1%)	0.64	6/7511 (0.1%)
1	F	0.49	4/5514 (0.1%)	0.64	6/7511 (0.1%)
1	G	0.40	0/3500	0.55	1/4758 (0.0%)
1	H	0.40	0/3500	0.55	1/4758 (0.0%)
2	I	0.28	0/800	0.62	0/1087
2	J	0.30	0/800	0.60	1/1087 (0.1%)
2	K	0.28	0/800	0.62	0/1087
2	L	0.28	0/800	0.62	0/1087
2	M	0.30	0/800	0.60	1/1087 (0.1%)
2	N	0.30	0/800	0.60	1/1087 (0.1%)
All	All	0.41	12/58884 (0.0%)	0.59	27/80136 (0.0%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	295	PRO	CG-CD	-17.80	0.92	1.50
1	B	295	PRO	CG-CD	-17.79	0.92	1.50
1	F	295	PRO	CG-CD	-17.79	0.92	1.50
1	E	295	PRO	N-CD	10.94	1.63	1.47
1	F	295	PRO	N-CD	10.94	1.63	1.47
1	B	295	PRO	N-CD	10.93	1.63	1.47
1	F	295	PRO	CB-CG	7.96	1.89	1.50
1	B	295	PRO	CB-CG	7.95	1.89	1.50
1	E	295	PRO	CB-CG	7.95	1.89	1.50
1	B	295	PRO	N-CA	-5.65	1.37	1.47
1	E	295	PRO	N-CA	-5.65	1.37	1.47
1	F	295	PRO	N-CA	-5.64	1.37	1.47

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	295	PRO	CA-N-CD	-13.67	92.36	111.50
1	B	295	PRO	CA-N-CD	-13.66	92.38	111.50
1	F	295	PRO	CA-N-CD	-13.65	92.38	111.50
1	F	295	PRO	N-CD-CG	-13.30	83.25	103.20
1	E	295	PRO	N-CD-CG	-13.29	83.26	103.20
1	B	295	PRO	N-CD-CG	-13.29	83.27	103.20
1	C	295	PRO	CA-N-CD	-12.66	93.78	111.50
1	D	295	PRO	CA-N-CD	-12.64	93.80	111.50
1	A	295	PRO	CA-N-CD	-12.64	93.81	111.50
1	B	295	PRO	CA-CB-CG	-9.49	85.96	104.00
1	E	295	PRO	CA-CB-CG	-9.49	85.96	104.00
1	F	295	PRO	CA-CB-CG	-9.49	85.97	104.00
1	D	1160	PRO	CA-N-CD	-6.86	101.89	111.50
1	H	1160	PRO	CA-N-CD	-6.85	101.90	111.50
1	G	1160	PRO	CA-N-CD	-6.84	101.93	111.50
1	E	179	LEU	CA-CB-CG	6.12	129.38	115.30
2	N	1389	PRO	CA-N-CD	-6.12	102.93	111.50
1	B	179	LEU	CA-CB-CG	6.12	129.37	115.30
1	F	179	LEU	CA-CB-CG	6.11	129.35	115.30
2	J	1389	PRO	CA-N-CD	-6.10	102.96	111.50
2	M	1389	PRO	CA-N-CD	-6.06	103.01	111.50
1	E	722	CYS	CA-CB-SG	5.48	123.86	114.00
1	F	722	CYS	CA-CB-SG	5.46	123.84	114.00
1	B	722	CYS	CA-CB-SG	5.46	123.83	114.00
1	F	295	PRO	N-CA-CB	-5.18	96.91	102.60
1	B	295	PRO	N-CA-CB	-5.16	96.93	102.60
1	E	295	PRO	N-CA-CB	-5.12	96.97	102.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8793	0	8176	277	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	8793	0	8176	297	0
1	C	8793	0	8176	281	0
1	D	8793	0	8177	289	0
1	E	5383	0	5055	168	0
1	F	5383	0	5055	172	0
1	G	3410	0	3122	106	0
1	H	3410	0	3122	108	0
2	I	781	0	712	30	0
2	J	781	0	712	47	0
2	K	781	0	712	34	0
2	L	781	0	712	33	0
2	M	781	0	712	32	0
2	N	781	0	712	30	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
4	A	70	0	65	0	0
4	B	70	0	65	1	0
4	C	70	0	65	0	0
4	D	56	0	52	0	0
4	E	56	0	52	1	0
4	F	56	0	52	1	0
All	All	57846	0	53682	1760	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 16.

All (1760) 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:B:295:PRO:CB	1:B:295:PRO:CG	1.89	1.49
1:E:295:PRO:CG	1:E:295:PRO:CB	1.89	1.49
1:F:295:PRO:CB	1:F:295:PRO:CG	1.89	1.46
1:B:295:PRO:CG	1:B:295:PRO:N	1.77	1.44
1:F:295:PRO:CG	1:F:295:PRO:N	1.77	1.40
1:E:295:PRO:CG	1:E:295:PRO:N	1.77	1.40
1:D:763:PRO:HD2	2:J:1384:GLN:OE1	1.46	1.12
1:F:295:PRO:CG	1:F:295:PRO:HD3	1.60	1.11
1:D:763:PRO:HD2	2:J:1384:GLN:CD	1.70	1.11
1:B:295:PRO:CG	1:B:295:PRO:HD3	1.60	1.09
1:F:295:PRO:CG	1:F:295:PRO:HD2	1.60	1.09
1:A:713:ARG:NH2	1:C:501:PHE:HE2	1.49	1.08
1:B:295:PRO:CG	1:B:295:PRO:HD2	1.60	1.08
1:E:295:PRO:CG	1:E:295:PRO:HD3	1.60	1.07
1:B:295:PRO:CG	1:B:295:PRO:CA	2.33	1.07
1:E:295:PRO:CD	1:E:295:PRO:HG2	1.57	1.06
1:E:295:PRO:CG	1:E:295:PRO:CA	2.33	1.06
1:F:295:PRO:CD	1:F:295:PRO:HG3	1.57	1.06
1:B:295:PRO:CD	1:B:295:PRO:HG3	1.57	1.05
1:F:295:PRO:CD	1:F:295:PRO:HG2	1.57	1.05
1:F:295:PRO:CG	1:F:295:PRO:CA	2.33	1.05
1:E:295:PRO:CG	1:E:295:PRO:HD2	1.60	1.04
1:E:295:PRO:CD	1:E:295:PRO:HG3	1.57	1.04
1:B:295:PRO:CD	1:B:295:PRO:HG2	1.57	1.03
1:C:757:HIS:HE1	1:C:830:HIS:NE2	1.60	1.00
1:D:762:ALA:HB1	2:J:1384:GLN:OE1	1.61	0.99
1:A:501:PHE:HE2	1:C:713:ARG:HH22	1.00	0.95
1:B:713:ARG:HH22	1:D:501:PHE:HE2	1.15	0.95
1:C:757:HIS:CE1	1:C:830:HIS:NE2	2.34	0.95
1:A:770:GLU:OE2	1:C:597:CYS:SG	2.26	0.93
1:F:295:PRO:CG	1:F:295:PRO:CD	0.92	0.92
1:B:295:PRO:CG	1:B:295:PRO:CD	0.91	0.91
1:E:295:PRO:CG	1:E:295:PRO:CD	0.91	0.91
1:F:345:THR:HG22	1:F:371:LEU:HB3	1.54	0.89
1:D:757:HIS:HE1	1:D:830:HIS:NE2	1.70	0.89
1:B:345:THR:HG22	1:B:371:LEU:HB3	1.54	0.89
1:D:757:HIS:CE1	1:D:830:HIS:CD2	2.61	0.88
1:B:767:VAL:HG12	2:L:1416:LEU:HD13	1.56	0.87
1:D:763:PRO:CD	2:J:1384:GLN:OE1	2.22	0.87
1:E:345:THR:HG22	1:E:371:LEU:HB3	1.54	0.87
1:B:295:PRO:N	1:B:295:PRO:HG3	1.71	0.86
1:F:295:PRO:N	1:F:295:PRO:HG3	1.71	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:718:ALA:HB2	1:A:808:ALA:HB3	1.57	0.84
1:C:757:HIS:CE1	1:C:830:HIS:CD2	2.66	0.83
1:C:763:PRO:O	2:I:1384:GLN:NE2	2.11	0.83
1:A:501:PHE:HE2	1:C:713:ARG:NH2	1.76	0.82
1:D:757:HIS:CE1	1:D:830:HIS:NE2	2.47	0.82
1:H:987:ARG:NH1	1:H:1186:CYS:SG	2.53	0.81
1:D:762:ALA:HB1	2:J:1384:GLN:CD	2.00	0.81
1:G:987:ARG:NH1	1:G:1186:CYS:SG	2.54	0.81
1:D:987:ARG:NH1	1:D:1186:CYS:SG	2.53	0.81
1:H:871:ARG:HH11	1:H:1140:GLY:HA2	1.45	0.81
1:C:651:ASP:HB3	1:C:661:CYS:HB3	1.64	0.80
1:G:871:ARG:HH11	1:G:1140:GLY:HA2	1.45	0.80
1:D:871:ARG:HH11	1:D:1140:GLY:HA2	1.45	0.79
1:A:651:ASP:HB3	1:A:661:CYS:HB3	1.64	0.78
2:L:1381:ARG:NH1	2:L:1421:GLU:OE1	2.17	0.78
1:A:338:CYS:HA	1:A:359:CYS:HB3	1.66	0.77
1:D:651:ASP:HB3	1:D:661:CYS:HB3	1.64	0.77
1:D:763:PRO:O	2:J:1384:GLN:NE2	2.16	0.77
1:D:890:LEU:HB3	1:D:1016:GLN:HG3	1.66	0.77
1:G:890:LEU:HB3	1:G:1016:GLN:HG3	1.67	0.77
1:C:338:CYS:HA	1:C:359:CYS:HB3	1.66	0.77
1:D:338:CYS:HA	1:D:359:CYS:HB3	1.66	0.76
1:H:890:LEU:HB3	1:H:1016:GLN:HG3	1.66	0.76
2:I:1381:ARG:NH1	2:I:1421:GLU:OE1	2.17	0.76
1:C:178:ARG:HD2	1:C:179:LEU:HD23	1.68	0.76
2:K:1381:ARG:NH1	2:K:1421:GLU:OE1	2.17	0.76
2:M:1381:ARG:NH1	2:M:1382:ALA:O	2.20	0.75
1:B:890:LEU:HB3	1:B:1016:GLN:HG3	1.69	0.75
1:C:763:PRO:HD3	2:I:1385:LEU:HD21	1.69	0.75
2:N:1381:ARG:NH1	2:N:1382:ALA:O	2.20	0.75
1:A:178:ARG:HD2	1:A:179:LEU:HD23	1.68	0.75
1:C:890:LEU:HB3	1:C:1016:GLN:HG3	1.69	0.75
1:D:178:ARG:HD2	1:D:179:LEU:HD23	1.68	0.75
2:J:1381:ARG:NH1	2:J:1382:ALA:O	2.20	0.75
1:D:427:VAL:HG22	1:D:433:ILE:HG12	1.70	0.74
1:A:427:VAL:HG22	1:A:433:ILE:HG12	1.70	0.74
1:A:757:HIS:HE1	1:A:830:HIS:NE2	1.85	0.74
1:A:890:LEU:HB3	1:A:1016:GLN:HG3	1.69	0.73
1:E:295:PRO:N	1:E:295:PRO:HG3	1.71	0.73
1:C:760:VAL:HG11	2:I:1388:MET:SD	2.28	0.73
1:B:875:ASN:ND2	1:B:889:ARG:O	2.21	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:332:ASN:ND2	1:C:379:CYS:O	2.22	0.73
1:A:875:ASN:ND2	1:A:889:ARG:O	2.21	0.73
1:C:427:VAL:HG22	1:C:433:ILE:HG12	1.69	0.73
1:D:299:CYS:HA	1:D:302:PHE:HD2	1.54	0.72
1:D:332:ASN:ND2	1:D:379:CYS:O	2.22	0.72
1:A:332:ASN:ND2	1:A:379:CYS:O	2.22	0.72
1:C:243:GLN:OE1	1:C:243:GLN:N	2.23	0.72
1:A:299:CYS:HA	1:A:302:PHE:HD2	1.54	0.72
1:C:875:ASN:ND2	1:C:889:ARG:O	2.21	0.72
1:A:243:GLN:OE1	1:A:243:GLN:N	2.23	0.72
1:C:299:CYS:HA	1:C:302:PHE:HD2	1.54	0.72
1:E:651:ASP:HB3	1:E:661:CYS:HB3	1.72	0.71
1:F:651:ASP:HB3	1:F:661:CYS:HB3	1.72	0.71
1:D:243:GLN:OE1	1:D:243:GLN:N	2.23	0.71
1:E:299:CYS:HA	1:E:302:PHE:HD2	1.56	0.71
1:B:120:ARG:HB3	1:B:120:ARG:HH11	1.56	0.70
1:B:651:ASP:HB3	1:B:661:CYS:HB3	1.72	0.70
1:E:120:ARG:HB3	1:E:120:ARG:HH11	1.56	0.70
1:A:768:HIS:O	2:K:1414:PRO:HB3	1.90	0.70
1:B:299:CYS:HA	1:B:302:PHE:HD2	1.56	0.70
1:H:911:TYR:HH	1:H:1051:PHE:HE2	1.37	0.70
1:F:299:CYS:HA	1:F:302:PHE:HD2	1.56	0.70
1:A:1181:ASN:ND2	1:A:1185:HIS:O	2.23	0.70
1:C:1181:ASN:ND2	1:C:1185:HIS:O	2.23	0.70
1:B:1181:ASN:ND2	1:B:1185:HIS:O	2.23	0.70
1:G:875:ASN:ND2	1:G:889:ARG:O	2.23	0.70
1:F:655:CYS:HB3	1:F:658:SER:HA	1.75	0.69
2:K:1381:ARG:HH21	2:K:1386:PRO:HB3	1.57	0.69
1:A:904:ILE:HG12	1:A:910:ARG:HG2	1.74	0.69
1:B:718:ALA:HB2	1:B:808:ALA:HB3	1.74	0.69
1:C:904:ILE:HG12	1:C:910:ARG:HG2	1.74	0.69
1:D:875:ASN:ND2	1:D:889:ARG:O	2.23	0.69
1:H:875:ASN:ND2	1:H:889:ARG:O	2.23	0.69
1:F:120:ARG:HB3	1:F:120:ARG:HH11	1.56	0.69
1:A:245:PRO:HD3	2:J:1403:ARG:HH12	1.58	0.68
1:C:718:ALA:HB2	1:C:808:ALA:HB3	1.73	0.68
1:B:332:ASN:ND2	1:B:379:CYS:O	2.26	0.68
1:F:332:ASN:ND2	1:F:379:CYS:O	2.26	0.68
1:B:655:CYS:HB3	1:B:658:SER:HA	1.75	0.68
1:B:761:LEU:HD12	1:B:776:CYS:HB2	1.75	0.68
2:L:1381:ARG:HH21	2:L:1386:PRO:HB3	1.57	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:767:VAL:HG12	2:I:1416:LEU:HD22	1.74	0.68
1:E:332:ASN:ND2	1:E:379:CYS:O	2.26	0.68
1:B:904:ILE:HG12	1:B:910:ARG:HG2	1.74	0.68
1:D:656:GLU:OE2	1:D:656:GLU:N	2.18	0.68
1:G:904:ILE:HG12	1:G:910:ARG:HG2	1.76	0.68
1:H:904:ILE:HG12	1:H:910:ARG:HG2	1.76	0.68
1:E:761:LEU:HD12	1:E:776:CYS:HB2	1.75	0.68
1:E:655:CYS:HB3	1:E:658:SER:HA	1.75	0.68
1:D:346:CYS:HA	1:D:349:PRO:HB3	1.77	0.67
1:D:904:ILE:HG12	1:D:910:ARG:HG2	1.76	0.67
1:F:761:LEU:HD12	1:F:776:CYS:HB2	1.75	0.67
1:A:757:HIS:CE1	1:A:830:HIS:NE2	2.61	0.67
1:E:82:ASP:HA	1:E:127:PRO:HG3	1.76	0.67
1:E:333:MET:HE3	1:E:363:CYS:HB3	1.76	0.67
2:I:1376:ALA:O	2:I:1401:ARG:NH2	2.19	0.67
2:I:1381:ARG:HH21	2:I:1386:PRO:HB3	1.57	0.67
2:K:1376:ALA:O	2:K:1401:ARG:NH2	2.19	0.67
1:B:764:GLY:N	1:B:776:CYS:O	2.24	0.67
1:D:245:PRO:HD3	2:N:1403:ARG:HH12	1.58	0.67
1:F:333:MET:HE3	1:F:363:CYS:HB3	1.76	0.67
1:C:245:PRO:HD3	2:M:1403:ARG:HH12	1.58	0.67
1:B:82:ASP:HA	1:B:127:PRO:HG3	1.76	0.66
1:B:871:ARG:NH1	1:B:873:ASP:O	2.28	0.66
1:A:346:CYS:HA	1:A:349:PRO:HB3	1.77	0.66
1:A:745:ALA:HB3	2:K:1387:ASP:OD2	1.95	0.66
1:C:529:GLN:NE2	1:C:530:THR:O	2.28	0.66
1:C:871:ARG:NH1	1:C:873:ASP:O	2.28	0.66
1:A:871:ARG:NH1	1:A:873:ASP:O	2.28	0.66
1:C:346:CYS:HA	1:C:349:PRO:HB3	1.77	0.66
1:F:158:PRO:HG2	1:H:1062:PRO:HG3	1.77	0.66
1:D:529:GLN:NE2	1:D:530:THR:O	2.28	0.66
1:H:1123:GLU:OE2	1:H:1123:GLU:N	2.27	0.66
1:F:82:ASP:HA	1:F:127:PRO:HG3	1.76	0.66
1:F:338:CYS:HA	1:F:359:CYS:HB3	1.78	0.66
1:A:529:GLN:NE2	1:A:530:THR:O	2.28	0.66
1:B:158:PRO:HG2	1:D:1062:PRO:HG3	1.77	0.66
1:E:764:GLY:N	1:E:776:CYS:O	2.24	0.66
1:D:453:LYS:HE2	1:D:455:CYS:HA	1.78	0.66
1:F:764:GLY:N	1:F:776:CYS:O	2.24	0.66
1:A:453:LYS:HE2	1:A:455:CYS:HA	1.78	0.65
1:A:967:GLN:HG3	1:C:179:LEU:HD11	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:ARG:NE	1:D:940:GLU:OE2	2.30	0.65
1:B:338:CYS:HA	1:B:359:CYS:HB3	1.78	0.65
1:E:178:ARG:NE	1:G:940:GLU:OE2	2.29	0.65
1:A:158:PRO:HG2	1:C:1062:PRO:HG3	1.79	0.65
1:B:967:GLN:HG3	1:D:179:LEU:HD11	1.78	0.65
1:E:280:SER:HA	1:E:283:TYR:HD2	1.61	0.65
1:B:627:ASP:HB3	1:B:630:SER:HB3	1.79	0.65
1:B:905:THR:OG1	1:B:906:PHE:N	2.29	0.65
1:B:493:ARG:HH22	1:B:495:GLN:HE21	1.45	0.65
1:A:179:LEU:HD11	1:C:967:GLN:HG3	1.78	0.65
1:A:1062:PRO:HG3	1:C:158:PRO:HG2	1.79	0.65
1:F:280:SER:HA	1:F:283:TYR:HD2	1.61	0.65
1:B:1062:PRO:HG3	1:D:158:PRO:HG2	1.79	0.65
1:F:178:ARG:NE	1:H:940:GLU:OE2	2.29	0.65
1:F:605:GLU:OE2	1:F:605:GLU:N	2.26	0.65
1:A:414:TRP:O	1:C:1042:ARG:NH2	2.30	0.65
1:E:158:PRO:HG2	1:G:1062:PRO:HG3	1.77	0.65
1:D:1222:ASP:OD1	1:D:1224:ASP:N	2.30	0.65
1:E:338:CYS:HA	1:E:359:CYS:HB3	1.78	0.64
1:E:493:ARG:HH22	1:E:495:GLN:HE21	1.45	0.64
1:D:539:GLN:OE1	1:D:545:GLN:NE2	2.31	0.64
1:G:1181:ASN:ND2	1:G:1185:HIS:O	2.30	0.64
1:H:1181:ASN:ND2	1:H:1185:HIS:O	2.30	0.64
1:B:280:SER:HA	1:B:283:TYR:HD2	1.61	0.64
1:A:905:THR:OG1	1:A:906:PHE:N	2.29	0.64
1:B:333:MET:HE3	1:B:363:CYS:HB3	1.77	0.64
1:A:1042:ARG:NH2	1:C:414:TRP:O	2.30	0.64
1:B:605:GLU:OE2	1:B:605:GLU:N	2.26	0.64
1:D:1181:ASN:ND2	1:D:1185:HIS:O	2.30	0.64
1:H:1222:ASP:OD1	1:H:1224:ASP:N	2.30	0.64
1:B:1042:ARG:NH2	1:D:414:TRP:O	2.30	0.64
1:C:453:LYS:HE2	1:C:455:CYS:HA	1.78	0.64
1:F:627:ASP:HB3	1:F:630:SER:HB3	1.79	0.64
1:A:767:VAL:HG12	2:K:1416:LEU:HD22	1.80	0.64
1:F:350:GLN:N	1:F:350:GLN:OE1	2.31	0.64
1:B:442:ASP:OD1	1:B:442:ASP:N	2.23	0.64
1:A:689:THR:HA	1:A:692:MET:HG2	1.80	0.63
1:C:539:GLN:OE1	1:C:545:GLN:NE2	2.31	0.63
1:D:689:THR:HA	1:D:692:MET:HG2	1.80	0.63
1:E:627:ASP:HB3	1:E:630:SER:HB3	1.79	0.63
1:F:493:ARG:HH22	1:F:495:GLN:HE21	1.45	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:GLN:OE1	1:A:545:GLN:NE2	2.31	0.63
1:D:1056:LYS:NZ	1:D:1063:ASP:OD1	2.24	0.63
1:A:115:ASN:OD1	1:A:117:GLN:NE2	2.30	0.63
1:E:605:GLU:OE2	1:E:605:GLU:N	2.26	0.63
1:C:656:GLU:OE2	1:C:656:GLU:N	2.18	0.63
1:D:115:ASN:OD1	1:D:117:GLN:NE2	2.30	0.63
1:F:179:LEU:HD11	1:H:967:GLN:HG3	1.81	0.63
1:B:1133:ALA:O	1:B:1137:HIS:ND1	2.24	0.62
1:C:182:THR:HB	1:C:194:GLU:HB2	1.82	0.62
1:H:992:PHE:HD2	1:H:1193:LEU:HD13	1.64	0.62
1:B:179:LEU:HD11	1:D:967:GLN:HG3	1.81	0.62
1:E:179:LEU:HD11	1:G:967:GLN:HG3	1.81	0.62
1:C:115:ASN:OD1	1:C:117:GLN:NE2	2.30	0.62
1:A:763:PRO:HD3	2:K:1385:LEU:HD21	1.82	0.62
1:D:992:PHE:HD2	1:D:1193:LEU:HD13	1.64	0.62
1:C:342:CYS:HB2	1:C:351:ARG:HG3	1.82	0.62
1:A:342:CYS:HB2	1:A:351:ARG:HG3	1.82	0.62
1:C:689:THR:HA	1:C:692:MET:HG2	1.80	0.62
1:D:1123:GLU:N	1:D:1123:GLU:OE2	2.27	0.62
1:B:762:ALA:HB1	2:L:1384:GLN:OE1	2.00	0.62
1:A:670:VAL:HG11	1:A:683:TRP:CH2	2.35	0.61
1:A:986:ILE:HG12	1:A:995:ILE:HG12	1.82	0.61
1:B:501:PHE:HE2	1:D:713:ARG:HH22	1.48	0.61
1:C:986:ILE:HG12	1:C:995:ILE:HG12	1.82	0.61
1:B:986:ILE:HG12	1:B:995:ILE:HG12	1.82	0.61
1:B:350:GLN:OE1	1:B:350:GLN:N	2.31	0.61
1:D:670:VAL:HG11	1:D:683:TRP:CH2	2.35	0.61
1:E:120:ARG:HB3	1:E:120:ARG:NH1	2.16	0.61
1:E:754:CYS:N	1:E:776:CYS:SG	2.72	0.61
1:D:342:CYS:HB2	1:D:351:ARG:HG3	1.82	0.61
1:G:1123:GLU:N	1:G:1123:GLU:OE2	2.27	0.61
1:D:718:ALA:HB2	1:D:808:ALA:HB3	1.82	0.61
1:A:182:THR:HB	1:A:194:GLU:HB2	1.82	0.61
1:A:713:ARG:NH1	1:A:742:ASP:OD2	2.34	0.61
1:C:713:ARG:NH1	1:C:742:ASP:OD2	2.34	0.61
1:F:691:TYR:HA	1:F:694:ASN:ND2	2.16	0.61
1:G:1222:ASP:OD1	1:G:1224:ASP:N	2.30	0.61
1:A:940:GLU:OE2	1:C:178:ARG:NE	2.34	0.61
1:B:713:ARG:NH2	1:D:501:PHE:HE2	1.92	0.61
1:C:1077:ARG:NH2	1:C:1121:ASP:OD2	2.28	0.61
1:F:182:THR:HB	1:F:194:GLU:HB2	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:905:THR:OG1	1:C:906:PHE:N	2.29	0.61
1:D:182:THR:HB	1:D:194:GLU:HB2	1.82	0.61
1:E:182:THR:HB	1:E:194:GLU:HB2	1.83	0.61
1:F:754:CYS:N	1:F:776:CYS:SG	2.72	0.61
1:G:1088:LEU:HD22	1:G:1132:TYR:HD2	1.66	0.61
1:H:923:GLN:HB3	1:H:936:ARG:HG2	1.82	0.61
1:D:713:ARG:NH1	1:D:742:ASP:OD2	2.34	0.60
1:G:1077:ARG:NH2	1:G:1121:ASP:OD2	2.32	0.60
1:B:345:THR:O	1:B:348:ASN:N	2.34	0.60
1:C:670:VAL:HG11	1:C:683:TRP:CH2	2.35	0.60
1:G:923:GLN:HB3	1:G:936:ARG:HG2	1.82	0.60
1:A:178:ARG:NE	1:C:940:GLU:OE2	2.34	0.60
1:C:691:TYR:HA	1:C:694:ASN:ND2	2.17	0.60
2:L:1376:ALA:O	2:L:1401:ARG:NH2	2.19	0.60
1:A:345:THR:O	1:A:348:ASN:N	2.35	0.60
1:B:278:VAL:HB	1:B:305:TYR:HE1	1.67	0.60
1:B:529:GLN:NE2	1:B:530:THR:O	2.35	0.60
1:F:278:VAL:HB	1:F:305:TYR:HE1	1.67	0.60
1:G:992:PHE:HD2	1:G:1193:LEU:HD13	1.64	0.60
1:C:1153:LEU:H	1:D:1154:PHE:HD2	1.50	0.60
1:D:691:TYR:HA	1:D:694:ASN:ND2	2.17	0.60
1:E:691:TYR:HA	1:E:694:ASN:ND2	2.16	0.60
1:B:453:LYS:HE2	1:B:455:CYS:HA	1.84	0.60
1:D:923:GLN:HB3	1:D:936:ARG:HG2	1.82	0.60
1:A:656:GLU:OE2	1:A:656:GLU:N	2.18	0.60
1:B:120:ARG:HB3	1:B:120:ARG:NH1	2.16	0.60
1:B:418:ASP:OD1	1:B:418:ASP:N	2.34	0.60
1:B:754:CYS:N	1:B:776:CYS:SG	2.72	0.60
1:A:691:TYR:HA	1:A:694:ASN:ND2	2.16	0.60
1:D:762:ALA:HB1	2:J:1384:GLN:NE2	2.17	0.60
1:E:278:VAL:HB	1:E:305:TYR:HE1	1.67	0.60
1:F:120:ARG:HB3	1:F:120:ARG:NH1	2.16	0.60
1:B:86:LYS:HE2	1:B:90:GLY:HA2	1.84	0.59
1:B:182:THR:HB	1:B:194:GLU:HB2	1.83	0.59
1:D:1088:LEU:HD22	1:D:1132:TYR:HD2	1.66	0.59
1:A:1077:ARG:NH2	1:A:1121:ASP:OD2	2.28	0.59
1:E:350:GLN:OE1	1:E:350:GLN:N	2.31	0.59
1:E:529:GLN:NE2	1:E:530:THR:O	2.35	0.59
1:B:1077:ARG:NH2	1:B:1121:ASP:OD2	2.28	0.59
1:D:345:THR:O	1:D:348:ASN:N	2.35	0.59
1:D:1077:ARG:NH2	1:D:1121:ASP:OD2	2.32	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:115:ASN:OD1	1:E:117:GLN:NE2	2.34	0.59
1:E:345:THR:O	1:E:348:ASN:N	2.34	0.59
1:F:529:GLN:NE2	1:F:530:THR:O	2.35	0.59
1:H:1077:ARG:NH2	1:H:1121:ASP:OD2	2.32	0.59
1:G:955:ILE:HB	1:G:966:LEU:HB2	1.84	0.59
1:H:955:ILE:HB	1:H:966:LEU:HB2	1.84	0.59
1:B:940:GLU:OE2	1:D:178:ARG:NE	2.34	0.59
1:D:1198:PRO:HB2	1:D:1214:CYS:SG	2.43	0.59
1:F:453:LYS:HE2	1:F:455:CYS:HA	1.84	0.59
2:K:1376:ALA:HB3	2:K:1425:LEU:HD23	1.84	0.59
1:B:690:LYS:HA	1:B:693:GLN:HG3	1.85	0.59
1:C:450:VAL:HA	1:C:463:LEU:HD23	1.84	0.59
1:E:453:LYS:HE2	1:E:455:CYS:HA	1.84	0.59
1:H:1198:PRO:HB2	1:H:1214:CYS:SG	2.43	0.59
1:G:991:ILE:HG21	1:G:1153:LEU:HD21	1.85	0.59
1:C:345:THR:O	1:C:348:ASN:N	2.35	0.59
1:D:450:VAL:HA	1:D:463:LEU:HD23	1.84	0.59
1:D:955:ILE:HB	1:D:966:LEU:HB2	1.84	0.59
1:E:418:ASP:OD1	1:E:418:ASP:N	2.34	0.59
1:B:691:TYR:HA	1:B:694:ASN:ND2	2.16	0.59
1:C:768:HIS:O	2:I:1414:PRO:HB3	2.03	0.59
1:D:960:GLU:OE2	1:D:960:GLU:N	2.36	0.59
1:G:994:VAL:HA	1:G:1002:VAL:O	2.03	0.59
1:B:115:ASN:OD1	1:B:117:GLN:NE2	2.34	0.59
1:B:768:HIS:O	2:L:1414:PRO:HB3	2.02	0.59
1:D:991:ILE:HG21	1:D:1153:LEU:HD21	1.85	0.59
1:D:994:VAL:HA	1:D:1002:VAL:O	2.03	0.59
1:F:86:LYS:HE2	1:F:90:GLY:HA2	1.84	0.59
1:F:690:LYS:HA	1:F:693:GLN:HG3	1.85	0.58
1:G:1198:PRO:HB2	1:G:1214:CYS:SG	2.43	0.58
1:D:763:PRO:CD	2:J:1384:GLN:CD	2.61	0.58
1:F:427:VAL:HG22	1:F:433:ILE:HG12	1.85	0.58
1:H:994:VAL:HA	1:H:1002:VAL:O	2.03	0.58
1:H:1088:LEU:HD22	1:H:1132:TYR:HD2	1.66	0.58
1:A:1002:VAL:HG22	1:A:1012:ILE:HG12	1.85	0.58
1:E:427:VAL:HG22	1:E:433:ILE:HG12	1.85	0.58
1:E:690:LYS:HA	1:E:693:GLN:HG3	1.85	0.58
1:F:414:TRP:CD1	1:H:1043:SER:HB3	2.38	0.58
1:H:960:GLU:N	1:H:960:GLU:OE2	2.36	0.58
1:A:1133:ALA:O	1:A:1137:HIS:ND1	2.24	0.58
1:B:162:THR:OG1	1:D:948:GLY:O	2.17	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:86:LYS:HE2	1:E:90:GLY:HA2	1.84	0.58
1:F:468:LYS:NZ	1:F:470:GLY:O	2.25	0.58
1:G:960:GLU:N	1:G:960:GLU:OE2	2.36	0.58
2:L:1376:ALA:HB3	2:L:1425:LEU:HD23	1.84	0.58
1:A:361:ASP:OD1	1:A:362:GLY:N	2.37	0.58
1:B:502:LEU:HD21	1:D:513:ALA:HB2	1.86	0.58
1:F:115:ASN:OD1	1:F:117:GLN:NE2	2.34	0.58
1:G:986:ILE:HG12	1:G:995:ILE:HG12	1.86	0.58
1:A:516:ILE:HG23	1:A:530:THR:HG22	1.86	0.58
1:B:126:ARG:HH21	1:B:297:CYS:HB3	1.68	0.58
1:C:361:ASP:OD1	1:C:362:GLY:N	2.37	0.58
1:E:414:TRP:CD1	1:G:1043:SER:HB3	2.38	0.58
2:I:1376:ALA:HB3	2:I:1425:LEU:HD23	1.84	0.58
2:L:1402:MET:N	2:L:1402:MET:SD	2.77	0.58
1:B:414:TRP:CD1	1:D:1043:SER:HB3	2.38	0.58
1:H:986:ILE:HG12	1:H:995:ILE:HG12	1.86	0.58
1:H:992:PHE:CD2	1:H:1193:LEU:HD13	2.39	0.58
2:I:1402:MET:N	2:I:1402:MET:SD	2.77	0.58
1:A:450:VAL:HA	1:A:463:LEU:HD23	1.84	0.58
1:A:414:TRP:CD1	1:C:1043:SER:HB3	2.39	0.58
1:D:205:GLY:HA2	1:D:235:GLN:HG2	1.86	0.58
1:D:427:VAL:HB	1:D:546:VAL:HG12	1.86	0.58
1:D:516:ILE:HG23	1:D:530:THR:HG22	1.86	0.58
1:F:126:ARG:HH21	1:F:297:CYS:HB3	1.68	0.58
2:K:1402:MET:N	2:K:1402:MET:SD	2.77	0.58
1:A:1043:SER:HB3	1:C:414:TRP:CD1	2.39	0.57
1:B:1153:LEU:H	1:H:1154:PHE:HD2	1.50	0.57
1:B:1043:SER:HB3	1:D:414:TRP:CD1	2.39	0.57
1:G:992:PHE:CD2	1:G:1193:LEU:HD13	2.39	0.57
1:H:991:ILE:HG21	1:H:1153:LEU:HD21	1.85	0.57
2:K:1381:ARG:HE	2:K:1386:PRO:HA	1.69	0.57
1:A:1153:LEU:H	1:G:1154:PHE:HD2	1.50	0.57
1:C:761:LEU:HD21	1:C:767:VAL:HG11	1.87	0.57
1:D:755:TYR:HE1	1:D:760:VAL:HG22	1.70	0.57
1:E:126:ARG:HH21	1:E:297:CYS:HB3	1.68	0.57
2:I:1381:ARG:HE	2:I:1386:PRO:HA	1.70	0.57
1:C:516:ILE:HG23	1:C:530:THR:HG22	1.86	0.57
1:C:1002:VAL:HG22	1:C:1012:ILE:HG12	1.85	0.57
1:B:992:PHE:CD2	1:B:1193:LEU:HD13	2.39	0.57
1:B:1002:VAL:HG22	1:B:1012:ILE:HG12	1.85	0.57
1:C:992:PHE:CD2	1:C:1193:LEU:HD13	2.40	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:992:PHE:HD2	1:C:1193:LEU:HD13	1.70	0.57
2:L:1398:ASP:OD1	2:L:1406:MET:HB3	2.05	0.57
1:B:923:GLN:HB3	1:B:936:ARG:HG2	1.87	0.57
1:C:991:ILE:HG21	1:C:1153:LEU:HD21	1.87	0.57
1:C:1179:CYS:HB2	1:C:1208:ASN:HA	1.87	0.57
1:D:361:ASP:OD1	1:D:362:GLY:N	2.37	0.57
1:A:295:PRO:HD2	1:A:296:THR:N	2.18	0.57
2:L:1381:ARG:HE	2:L:1386:PRO:HA	1.70	0.57
1:A:761:LEU:HD21	1:A:767:VAL:HG11	1.87	0.57
1:A:991:ILE:HG21	1:A:1153:LEU:HD21	1.87	0.57
1:A:1179:CYS:HB2	1:A:1208:ASN:HA	1.87	0.57
1:B:770:GLU:OE2	1:D:597:CYS:SG	2.62	0.57
1:B:955:ILE:HB	1:B:966:LEU:HB2	1.87	0.57
1:C:205:GLY:HA2	1:C:235:GLN:HG2	1.86	0.57
1:C:427:VAL:HB	1:C:546:VAL:HG12	1.86	0.57
1:C:755:TYR:HE1	1:C:760:VAL:HG22	1.70	0.57
1:C:955:ILE:HB	1:C:966:LEU:HB2	1.87	0.57
1:C:961:SER:HB3	1:C:977:GLY:HA3	1.87	0.57
1:E:573:PHE:HB2	1:E:580:VAL:HG13	1.87	0.57
1:G:816:LEU:HD23	1:G:836:VAL:HG13	1.87	0.57
2:K:1398:ASP:OD1	2:K:1406:MET:HB3	2.05	0.57
1:A:500:VAL:HG11	1:A:518:LEU:HD23	1.87	0.57
1:B:767:VAL:HG12	2:L:1416:LEU:HD22	1.86	0.57
1:C:923:GLN:HB3	1:C:936:ARG:HG2	1.87	0.57
1:F:780:LYS:H	1:F:780:LYS:HD2	1.70	0.57
1:G:1229:ASP:OD1	1:G:1230:VAL:N	2.38	0.57
2:K:1397:VAL:HG22	2:K:1407:CYS:HB2	1.87	0.57
1:D:624:ARG:NH1	1:D:685:ASP:O	2.26	0.57
1:F:538:VAL:HG22	1:F:546:VAL:HG23	1.87	0.57
1:A:713:ARG:NH2	1:C:501:PHE:CE2	2.40	0.56
1:C:500:VAL:HG11	1:C:518:LEU:HD23	1.87	0.56
1:D:761:LEU:HD21	1:D:767:VAL:HG11	1.87	0.56
2:L:1397:VAL:HG22	2:L:1407:CYS:HB2	1.87	0.56
2:N:1383:ALA:N	2:N:1419:ASP:O	2.35	0.56
1:B:991:ILE:HG21	1:B:1153:LEU:HD21	1.87	0.56
1:E:162:THR:OG1	1:G:948:GLY:O	2.17	0.56
1:H:1229:ASP:OD1	1:H:1230:VAL:N	2.38	0.56
1:A:896:VAL:HG22	1:A:1011:PHE:HD1	1.71	0.56
1:A:992:PHE:HD2	1:A:1193:LEU:HD13	1.70	0.56
1:B:137:GLN:HB3	1:D:946:THR:HA	1.86	0.56
1:B:178:ARG:HH22	1:D:956:LYS:HE3	1.71	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:427:VAL:HG22	1:B:433:ILE:HG12	1.85	0.56
1:B:719:ASP:OD2	1:B:722:CYS:HB3	2.06	0.56
1:B:992:PHE:HD2	1:B:1193:LEU:HD13	1.70	0.56
1:C:691:TYR:HA	1:C:694:ASN:HD22	1.70	0.56
1:E:178:ARG:HH22	1:G:956:LYS:HE3	1.71	0.56
1:E:538:VAL:HG22	1:E:546:VAL:HG23	1.87	0.56
1:F:573:PHE:HB2	1:F:580:VAL:HG13	1.87	0.56
1:F:719:ASP:OD1	1:F:722:CYS:HB3	2.06	0.56
2:I:1397:VAL:HG22	2:I:1407:CYS:HB2	1.87	0.56
1:A:299:CYS:HA	1:A:302:PHE:CD2	2.40	0.56
1:B:564:ASN:ND2	1:B:571:ASP:OD2	2.32	0.56
1:D:992:PHE:CD2	1:D:1193:LEU:HD13	2.39	0.56
1:F:137:GLN:HB3	1:H:946:THR:HA	1.86	0.56
1:F:250:LEU:HD12	1:F:251:PRO:HD2	1.87	0.56
2:I:1398:ASP:OD2	2:I:1406:MET:HB3	2.05	0.56
2:M:1383:ALA:N	2:M:1419:ASP:O	2.35	0.56
1:A:427:VAL:HB	1:A:546:VAL:HG12	1.86	0.56
1:B:178:ARG:HD2	1:B:179:LEU:HD23	1.87	0.56
1:B:896:VAL:HG22	1:B:1011:PHE:HD1	1.71	0.56
1:B:1088:LEU:HD22	1:B:1132:TYR:HD2	1.70	0.56
1:C:295:PRO:HD2	1:C:296:THR:N	2.18	0.56
2:N:1362:GLU:N	2:N:1362:GLU:OE1	2.39	0.56
1:A:961:SER:HB3	1:A:977:GLY:HA3	1.87	0.56
1:B:538:VAL:HG22	1:B:546:VAL:HG23	1.87	0.56
1:B:871:ARG:HH21	1:B:1140:GLY:HA2	1.71	0.56
1:C:798:MET:HE2	1:C:798:MET:O	2.06	0.56
1:D:986:ILE:HG12	1:D:995:ILE:HG12	1.86	0.56
1:F:345:THR:O	1:F:348:ASN:N	2.34	0.56
2:M:1362:GLU:OE1	2:M:1362:GLU:N	2.39	0.56
1:A:691:TYR:HA	1:A:694:ASN:HD22	1.70	0.56
1:A:1198:PRO:HB2	1:A:1214:CYS:SG	2.46	0.56
1:D:108:ARG:HB3	1:D:202:GLN:HA	1.87	0.56
1:D:500:VAL:HG11	1:D:518:LEU:HD23	1.87	0.56
1:A:923:GLN:HB3	1:A:936:ARG:HG2	1.87	0.56
1:A:992:PHE:CD2	1:A:1193:LEU:HD13	2.39	0.56
1:B:974:VAL:O	1:B:976:ARG:HG2	2.06	0.56
1:E:564:ASN:ND2	1:E:571:ASP:OD2	2.32	0.56
1:E:780:LYS:H	1:E:780:LYS:HD2	1.70	0.56
1:A:205:GLY:HA2	1:A:235:GLN:HG2	1.86	0.56
1:A:798:MET:HE2	1:A:798:MET:O	2.06	0.56
1:B:961:SER:HB3	1:B:977:GLY:HA3	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:345:THR:HB	1:C:371:LEU:HB3	1.88	0.56
1:F:632:PHE:HB3	1:F:669:TYR:HE2	1.71	0.56
2:J:1396:GLN:N	2:J:1412:GLN:OE1	2.33	0.56
1:A:700:ARG:HG2	1:A:735:PRO:HG3	1.88	0.56
1:B:108:ARG:HB3	1:B:202:GLN:HA	1.88	0.56
1:D:719:ASP:OD1	1:D:722:CYS:N	2.37	0.56
1:D:1229:ASP:OD1	1:D:1230:VAL:N	2.38	0.56
1:E:632:PHE:HB3	1:E:669:TYR:HE2	1.71	0.56
1:A:871:ARG:HH21	1:A:1140:GLY:HA2	1.71	0.55
1:A:955:ILE:HB	1:A:966:LEU:HB2	1.87	0.55
1:C:108:ARG:HB3	1:C:202:GLN:HA	1.88	0.55
1:C:299:CYS:HA	1:C:302:PHE:CD2	2.39	0.55
1:C:896:VAL:HG22	1:C:1011:PHE:HD1	1.71	0.55
1:E:137:GLN:HB3	1:G:946:THR:HA	1.86	0.55
1:E:719:ASP:OD1	1:E:722:CYS:HB3	2.06	0.55
1:B:780:LYS:H	1:B:780:LYS:HD2	1.70	0.55
1:B:1179:CYS:HB2	1:B:1208:ASN:HA	1.87	0.55
1:C:1088:LEU:HD22	1:C:1132:TYR:HD2	1.70	0.55
1:D:691:TYR:HA	1:D:694:ASN:HD22	1.71	0.55
1:D:753:PRO:HG3	2:J:1385:LEU:CD2	2.37	0.55
1:B:767:VAL:HG12	2:L:1416:LEU:CD1	2.32	0.55
1:D:401:ASN:HA	1:D:406:SER:HA	1.88	0.55
1:H:816:LEU:HD23	1:H:836:VAL:HG13	1.87	0.55
2:J:1362:GLU:OE1	2:J:1362:GLU:N	2.39	0.55
1:A:755:TYR:HE1	1:A:760:VAL:HG22	1.70	0.55
1:B:632:PHE:HB3	1:B:669:TYR:HE2	1.71	0.55
1:C:1043:SER:O	1:C:1043:SER:OG	2.25	0.55
1:D:345:THR:HB	1:D:371:LEU:HB3	1.88	0.55
1:D:816:LEU:HD23	1:D:836:VAL:HG13	1.87	0.55
1:F:500:VAL:HG11	1:F:518:LEU:HD23	1.89	0.55
1:A:236:LYS:NZ	1:A:238:ASP:OD1	2.30	0.55
1:A:974:VAL:O	1:A:976:ARG:HG2	2.06	0.55
1:B:573:PHE:HB2	1:B:580:VAL:HG13	1.87	0.55
1:B:798:MET:HE2	1:B:798:MET:O	2.05	0.55
1:C:763:PRO:CD	2:I:1385:LEU:HD21	2.36	0.55
1:D:911:TYR:HH	1:D:1051:PHE:HE2	1.55	0.55
1:E:108:ARG:HB3	1:E:202:GLN:HA	1.88	0.55
1:A:345:THR:HB	1:A:371:LEU:HB3	1.88	0.55
1:B:266:LEU:HD22	1:B:305:TYR:HD2	1.72	0.55
1:C:401:ASN:HA	1:C:406:SER:HA	1.88	0.55
1:A:1088:LEU:HD22	1:A:1132:TYR:HD2	1.71	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:754:CYS:HB2	1:B:781:LEU:HD23	1.88	0.55
1:B:250:LEU:HD12	1:B:251:PRO:HD2	1.87	0.55
1:B:1198:PRO:HB2	1:B:1214:CYS:SG	2.46	0.55
1:B:1229:ASP:OD1	1:B:1230:VAL:N	2.40	0.55
1:C:1133:ALA:O	1:C:1137:HIS:ND1	2.24	0.55
1:C:1229:ASP:OD1	1:C:1230:VAL:N	2.40	0.55
1:D:700:ARG:HG2	1:D:735:PRO:HG3	1.88	0.55
1:E:178:ARG:HD2	1:E:179:LEU:HD23	1.87	0.55
1:G:961:SER:HB3	1:G:977:GLY:HA3	1.89	0.55
1:B:500:VAL:HG11	1:B:518:LEU:HD23	1.89	0.55
1:E:250:LEU:HD12	1:E:251:PRO:HD2	1.87	0.55
1:F:108:ARG:HB3	1:F:202:GLN:HA	1.88	0.55
1:F:178:ARG:HH22	1:H:956:LYS:HE3	1.71	0.55
1:F:564:ASN:ND2	1:F:571:ASP:OD2	2.32	0.55
1:F:754:CYS:HB2	1:F:781:LEU:HD23	1.88	0.55
1:A:401:ASN:HA	1:A:406:SER:HA	1.88	0.55
1:A:624:ARG:NH1	1:A:685:ASP:O	2.26	0.54
1:C:194:GLU:OE2	1:C:311:HIS:NE2	2.40	0.54
1:C:1198:PRO:HB2	1:C:1214:CYS:SG	2.46	0.54
1:D:961:SER:HB3	1:D:977:GLY:HA3	1.89	0.54
1:E:266:LEU:HD22	1:E:305:TYR:HD2	1.72	0.54
1:E:754:CYS:HB2	1:E:781:LEU:HD23	1.88	0.54
1:F:266:LEU:HD22	1:F:305:TYR:HD2	1.72	0.54
2:K:1401:ARG:HG2	2:K:1402:MET:SD	2.48	0.54
1:A:108:ARG:HB3	1:A:202:GLN:HA	1.88	0.54
1:A:760:VAL:HG11	2:K:1388:MET:SD	2.47	0.54
1:C:974:VAL:O	1:C:976:ARG:HG2	2.06	0.54
1:F:97:GLY:HA2	1:F:247:PRO:HG3	1.89	0.54
1:G:816:LEU:HD11	1:G:843:SER:HB3	1.90	0.54
1:H:816:LEU:HD11	1:H:843:SER:HB3	1.90	0.54
1:D:194:GLU:OE2	1:D:311:HIS:NE2	2.40	0.54
1:D:295:PRO:HD2	1:D:296:THR:N	2.18	0.54
1:D:937:ILE:HG12	1:D:957:LEU:HD23	1.88	0.54
1:F:442:ASP:OD1	1:F:442:ASP:N	2.23	0.54
2:L:1399:CYS:HA	2:L:1404:GLY:O	2.08	0.54
1:F:178:ARG:HD2	1:F:179:LEU:HD23	1.87	0.54
1:A:194:GLU:OE2	1:A:311:HIS:NE2	2.40	0.54
1:B:97:GLY:HA2	1:B:247:PRO:HG3	1.89	0.54
1:C:700:ARG:HG2	1:C:735:PRO:HG3	1.88	0.54
1:D:166:VAL:HG12	1:D:175:VAL:HG13	1.89	0.54
2:I:1399:CYS:HA	2:I:1404:GLY:O	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1401:ARG:HG2	2:I:1402:MET:SD	2.48	0.54
2:L:1401:ARG:HG2	2:L:1402:MET:SD	2.48	0.54
1:A:659:GLU:HG2	1:A:690:LYS:HE2	1.90	0.54
1:D:659:GLU:HG2	1:D:690:LYS:HE2	1.90	0.54
1:E:500:VAL:HG11	1:E:518:LEU:HD23	1.89	0.54
1:H:937:ILE:HG12	1:H:957:LEU:HD23	1.88	0.54
2:K:1399:CYS:HA	2:K:1404:GLY:O	2.07	0.54
1:A:957:LEU:HD21	1:A:1002:VAL:HG21	1.89	0.54
1:C:871:ARG:HH21	1:C:1140:GLY:HA2	1.71	0.54
1:D:183:PHE:CZ	1:D:185:TRP:HB2	2.43	0.54
1:D:762:ALA:CB	2:J:1384:GLN:OE1	2.48	0.54
1:G:962:TYR:CE2	1:G:982:PRO:HA	2.43	0.54
1:H:962:TYR:CE2	1:H:982:PRO:HA	2.43	0.54
1:C:166:VAL:HG12	1:C:175:VAL:HG13	1.89	0.54
1:C:756:ALA:O	1:C:759:THR:OG1	2.20	0.54
1:D:763:PRO:HD2	2:J:1384:GLN:NE2	2.20	0.54
1:D:962:TYR:CE2	1:D:982:PRO:HA	2.43	0.54
1:F:361:ASP:OD1	1:F:362:GLY:N	2.41	0.54
1:G:1068:LYS:HE3	1:G:1073:ALA:HB2	1.90	0.54
1:H:1179:CYS:HB2	1:H:1208:ASN:HA	1.90	0.54
1:C:957:LEU:HD21	1:C:1002:VAL:HG21	1.89	0.53
1:E:361:ASP:OD1	1:E:362:GLY:N	2.41	0.53
1:H:1068:LYS:HE3	1:H:1073:ALA:HB2	1.90	0.53
1:A:936:ARG:HH21	1:A:958:PHE:HE2	1.57	0.53
1:A:1068:LYS:HD2	1:A:1073:ALA:HB2	1.91	0.53
1:A:1229:ASP:OD1	1:A:1230:VAL:N	2.40	0.53
1:B:468:LYS:NZ	1:B:470:GLY:O	2.25	0.53
1:C:1068:LYS:HD2	1:C:1073:ALA:HB2	1.91	0.53
1:G:937:ILE:HG12	1:G:957:LEU:HD23	1.88	0.53
2:N:1398:ASP:OD1	2:N:1398:ASP:N	2.42	0.53
1:C:183:PHE:CZ	1:C:185:TRP:HB2	2.43	0.53
2:J:1403:ARG:HD3	2:J:1406:MET:CE	2.38	0.53
2:N:1403:ARG:HD3	2:N:1406:MET:CE	2.38	0.53
1:A:763:PRO:CD	2:K:1385:LEU:HD21	2.38	0.53
1:B:796:ALA:HB3	1:B:798:MET:SD	2.49	0.53
1:B:957:LEU:HD21	1:B:1002:VAL:HG21	1.89	0.53
1:A:183:PHE:CZ	1:A:185:TRP:HB2	2.43	0.53
1:A:796:ALA:HB3	1:A:798:MET:SD	2.49	0.53
1:A:1056:LYS:NZ	1:A:1063:ASP:OD1	2.25	0.53
1:C:659:GLU:HG2	1:C:690:LYS:HE2	1.90	0.53
1:D:369:THR:O	1:D:369:THR:OG1	2.27	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:ASP:OD1	1:B:362:GLY:N	2.41	0.53
1:C:86:LYS:HE2	1:C:90:GLY:HA2	1.91	0.53
1:E:254:ASN:O	1:E:256:THR:N	2.41	0.53
1:E:485:LEU:HB3	1:E:490:THR:HB	1.91	0.53
2:M:1398:ASP:OD1	2:M:1398:ASP:N	2.42	0.53
1:B:485:LEU:HB3	1:B:490:THR:HB	1.91	0.53
1:B:1043:SER:O	1:B:1043:SER:OG	2.25	0.53
1:C:79:THR:HG22	1:C:120:ARG:HH21	1.74	0.53
1:C:690:LYS:HA	1:C:693:GLN:HG3	1.91	0.53
1:D:299:CYS:HA	1:D:302:PHE:CD2	2.40	0.53
1:H:961:SER:HB3	1:H:977:GLY:HA3	1.89	0.53
1:A:166:VAL:HG12	1:A:175:VAL:HG13	1.89	0.53
1:A:627:ASP:HB3	1:A:630:SER:HB3	1.91	0.53
1:F:271:PHE:HB3	1:F:274:CYS:HB2	1.91	0.53
1:G:819:CYS:SG	1:G:856:PRO:HD2	2.49	0.53
1:A:79:THR:HG22	1:A:120:ARG:HH21	1.74	0.52
1:A:126:ARG:HD3	1:A:127:PRO:HD2	1.92	0.52
1:A:479:LYS:HZ1	2:I:1413:SER:HB3	1.74	0.52
1:B:1005:ASP:OD1	1:B:1007:LYS:N	2.35	0.52
1:D:753:PRO:HG3	2:J:1385:LEU:HD21	1.89	0.52
1:D:816:LEU:HD11	1:D:843:SER:HB3	1.89	0.52
1:E:97:GLY:HA2	1:E:247:PRO:HG3	1.89	0.52
1:A:89:ASP:HB2	1:A:214:PRO:HA	1.92	0.52
1:B:767:VAL:CG1	2:L:1416:LEU:HD13	2.33	0.52
1:C:796:ALA:HB3	1:C:798:MET:SD	2.49	0.52
1:D:1179:CYS:HB2	1:D:1208:ASN:HA	1.90	0.52
2:J:1383:ALA:N	2:J:1419:ASP:O	2.35	0.52
2:M:1403:ARG:HD3	2:M:1406:MET:CE	2.38	0.52
1:B:254:ASN:O	1:B:256:THR:N	2.41	0.52
1:C:621:TRP:HB2	1:C:662:LEU:HD11	1.92	0.52
1:C:627:ASP:HB3	1:C:630:SER:HB3	1.92	0.52
1:D:893:GLY:O	1:D:1013:ARG:HA	2.09	0.52
1:E:205:GLY:HA2	1:E:235:GLN:HG2	1.92	0.52
1:D:126:ARG:HD3	1:D:127:PRO:HD2	1.92	0.52
1:E:194:GLU:OE2	1:E:311:HIS:NE2	2.43	0.52
1:A:1043:SER:O	1:A:1043:SER:OG	2.25	0.52
1:B:271:PHE:HB3	1:B:274:CYS:HB2	1.91	0.52
1:B:450:VAL:HA	1:B:463:LEU:HD23	1.92	0.52
1:D:123:VAL:HG23	1:D:128:VAL:HG21	1.91	0.52
1:D:297:CYS:N	1:D:298:PRO:HD3	2.24	0.52
1:D:819:CYS:SG	1:D:856:PRO:HD2	2.49	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:896:VAL:HG22	1:D:1011:PHE:HD1	1.75	0.52
1:G:1179:CYS:HB2	1:G:1208:ASN:HA	1.90	0.52
1:A:621:TRP:HB2	1:A:662:LEU:HD11	1.92	0.52
1:D:82:ASP:HA	1:D:127:PRO:HG3	1.92	0.52
1:F:670:VAL:HG11	1:F:683:TRP:CH2	2.45	0.52
1:A:468:LYS:NZ	1:A:470:GLY:O	2.29	0.52
1:C:89:ASP:HB2	1:C:214:PRO:HA	1.92	0.52
1:C:371:LEU:HD12	1:C:372:ASP:H	1.75	0.52
1:D:941:ASN:OD1	1:D:953:LYS:NZ	2.43	0.52
1:F:126:ARG:HD3	1:F:127:PRO:HD2	1.92	0.52
1:F:479:LYS:NZ	2:N:1413:SER:HB2	2.25	0.52
1:A:82:ASP:HA	1:A:127:PRO:HG3	1.92	0.52
1:C:126:ARG:HD3	1:C:127:PRO:HD2	1.92	0.52
1:C:297:CYS:N	1:C:298:PRO:HD3	2.24	0.52
1:D:79:THR:HG22	1:D:120:ARG:HH21	1.74	0.52
1:D:86:LYS:HE2	1:D:90:GLY:HA2	1.91	0.52
1:G:893:GLY:O	1:G:1013:ARG:HA	2.09	0.52
1:A:1172:GLY:HA3	1:A:1197:TYR:CZ	2.45	0.52
1:B:670:VAL:HG11	1:B:683:TRP:CH2	2.45	0.52
1:B:962:TYR:OH	1:B:980:GLY:O	2.28	0.52
1:D:690:LYS:HA	1:D:693:GLN:HG3	1.91	0.52
1:D:1068:LYS:HE3	1:D:1073:ALA:HB2	1.90	0.52
1:E:450:VAL:HA	1:E:463:LEU:HD23	1.92	0.52
1:E:594:GLN:HE21	1:G:828:SER:HB2	1.75	0.52
1:G:896:VAL:HG22	1:G:1011:PHE:HD1	1.75	0.52
1:H:819:CYS:SG	1:H:856:PRO:HD2	2.49	0.52
1:H:893:GLY:O	1:H:1013:ARG:HA	2.09	0.52
2:J:1398:ASP:OD2	2:J:1398:ASP:N	2.42	0.52
1:B:1068:LYS:HD2	1:B:1073:ALA:HB2	1.91	0.51
1:D:902:HIS:CD2	1:D:1108:ALA:HB1	2.46	0.51
1:G:902:HIS:CD2	1:G:1108:ALA:HB1	2.45	0.51
1:A:297:CYS:N	1:A:298:PRO:HD3	2.25	0.51
1:A:690:LYS:HA	1:A:693:GLN:HG3	1.91	0.51
1:B:594:GLN:HE21	1:D:828:SER:HB2	1.75	0.51
1:B:936:ARG:HH21	1:B:958:PHE:HE2	1.57	0.51
1:C:123:VAL:HG23	1:C:128:VAL:HG21	1.91	0.51
1:D:621:TRP:HB2	1:D:662:LEU:HD11	1.92	0.51
1:E:442:ASP:OD1	1:E:442:ASP:N	2.23	0.51
1:F:485:LEU:HB3	1:F:490:THR:HB	1.91	0.51
1:F:509:LEU:HD22	1:F:518:LEU:HB3	1.93	0.51
1:B:194:GLU:OE2	1:B:311:HIS:NE2	2.43	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:936:ARG:HH21	1:C:958:PHE:HE2	1.57	0.51
1:C:962:TYR:OH	1:C:980:GLY:O	2.28	0.51
1:F:194:GLU:OE2	1:F:311:HIS:NE2	2.43	0.51
1:A:369:THR:O	1:A:369:THR:OG1	2.27	0.51
1:A:1222:ASP:OD1	1:A:1224:ASP:N	2.44	0.51
1:B:479:LYS:NZ	2:J:1413:SER:HB2	2.25	0.51
1:C:607:PRO:HG2	1:C:654:ASN:HB2	1.93	0.51
1:F:621:TRP:HB2	1:F:662:LEU:HD11	1.93	0.51
1:G:941:ASN:OD1	1:G:953:LYS:NZ	2.43	0.51
1:A:962:TYR:OH	1:A:980:GLY:O	2.28	0.51
1:D:556:GLY:N	1:D:565:PHE:O	2.32	0.51
1:E:126:ARG:HD3	1:E:127:PRO:HD2	1.92	0.51
1:E:670:VAL:HG11	1:E:683:TRP:CH2	2.45	0.51
1:G:911:TYR:OH	1:G:1051:PHE:HE2	1.94	0.51
1:B:205:GLY:HA2	1:B:235:GLN:HG2	1.92	0.51
1:B:1222:ASP:OD1	1:B:1224:ASP:N	2.44	0.51
1:C:719:ASP:OD1	1:C:722:CYS:N	2.37	0.51
1:A:123:VAL:HG23	1:A:128:VAL:HG21	1.91	0.51
1:B:621:TRP:HB2	1:B:662:LEU:HD11	1.93	0.51
1:D:627:ASP:HB3	1:D:630:SER:HB3	1.91	0.51
1:F:114:PHE:HE1	1:F:199:TYR:CD1	2.28	0.51
1:C:82:ASP:HA	1:C:127:PRO:HG3	1.92	0.51
1:D:89:ASP:HB2	1:D:214:PRO:HA	1.92	0.51
1:D:236:LYS:NZ	1:D:238:ASP:OD1	2.31	0.51
1:E:114:PHE:HE1	1:E:199:TYR:CD1	2.28	0.51
1:E:271:PHE:HB3	1:E:274:CYS:HB2	1.91	0.51
1:E:556:GLY:N	1:E:565:PHE:O	2.40	0.51
1:H:896:VAL:HG22	1:H:1011:PHE:HD1	1.75	0.51
1:A:86:LYS:HE2	1:A:90:GLY:HA2	1.91	0.51
1:A:607:PRO:HG2	1:A:654:ASN:HB2	1.93	0.51
1:C:556:GLY:N	1:C:565:PHE:O	2.32	0.51
1:D:763:PRO:N	2:J:1384:GLN:HE22	2.09	0.51
1:F:205:GLY:HA2	1:F:235:GLN:HG2	1.92	0.51
1:H:1043:SER:O	1:H:1043:SER:OG	2.29	0.51
1:A:719:ASP:OD2	1:A:722:CYS:N	2.37	0.51
1:E:344:ASP:OD1	1:E:352:ALA:N	2.38	0.51
1:E:479:LYS:NZ	2:M:1413:SER:HB2	2.25	0.51
1:E:766:VAL:HG22	1:E:775:SER:HB2	1.93	0.51
1:F:594:GLN:HE21	1:H:828:SER:HB2	1.75	0.51
1:H:902:HIS:CD2	1:H:1108:ALA:HB1	2.46	0.51
2:N:1378:ILE:HG12	2:N:1401:ARG:HA	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:1380:CYS:SG	2:N:1405:LEU:HD12	2.51	0.51
1:A:816:LEU:HD23	1:A:836:VAL:HG22	1.94	0.50
1:B:114:PHE:HE1	1:B:199:TYR:CD2	2.28	0.50
1:B:822:LEU:HD22	1:B:882:ARG:NH1	2.27	0.50
1:B:939:THR:HG22	1:B:955:ILE:HG13	1.94	0.50
1:D:422:PRO:HA	1:D:552:PRO:HD3	1.93	0.50
1:E:509:LEU:HD22	1:E:518:LEU:HB3	1.92	0.50
1:E:766:VAL:HA	1:E:774:CYS:O	2.11	0.50
1:F:450:VAL:HA	1:F:463:LEU:HD23	1.92	0.50
1:A:904:ILE:HD11	1:A:1105:TYR:HE1	1.77	0.50
1:B:509:LEU:HD22	1:B:518:LEU:HB3	1.92	0.50
1:B:1172:GLY:HA3	1:B:1197:TYR:CZ	2.45	0.50
1:C:1172:GLY:HA3	1:C:1197:TYR:CZ	2.45	0.50
1:D:855:CYS:HB2	1:D:882:ARG:HG2	1.94	0.50
1:E:346:CYS:HA	1:E:349:PRO:HB3	1.93	0.50
1:F:254:ASN:O	1:F:256:THR:N	2.41	0.50
1:F:346:CYS:HA	1:F:349:PRO:HB3	1.93	0.50
2:J:1378:ILE:HG12	2:J:1401:ARG:HA	1.93	0.50
2:J:1380:CYS:SG	2:J:1405:LEU:HD12	2.51	0.50
2:M:1396:GLN:N	2:M:1412:GLN:OE1	2.33	0.50
1:A:556:GLY:N	1:A:565:PHE:O	2.32	0.50
1:A:670:VAL:HG21	1:A:683:TRP:CE2	2.47	0.50
1:B:126:ARG:HD3	1:B:127:PRO:HD2	1.92	0.50
1:B:766:VAL:HG22	1:B:775:SER:HB2	1.93	0.50
1:H:1145:TRP:CD1	1:H:1145:TRP:N	2.77	0.50
1:B:766:VAL:HA	1:B:774:CYS:O	2.12	0.50
1:C:822:LEU:HD22	1:C:882:ARG:NH1	2.27	0.50
1:E:621:TRP:HB2	1:E:662:LEU:HD11	1.93	0.50
1:F:766:VAL:HG22	1:F:775:SER:HB2	1.93	0.50
2:J:1378:ILE:HG22	2:J:1424:VAL:HA	1.94	0.50
1:B:991:ILE:HG23	1:B:1195:GLY:HA2	1.94	0.50
1:C:1222:ASP:OD1	1:C:1224:ASP:N	2.44	0.50
1:D:756:ALA:O	1:D:759:THR:OG1	2.20	0.50
1:D:911:TYR:OH	1:D:1051:PHE:HE2	1.94	0.50
1:D:1133:ALA:O	1:D:1137:HIS:ND1	2.26	0.50
1:G:807:SER:O	1:G:810:THR:HG23	2.12	0.50
2:M:1380:CYS:SG	2:M:1405:LEU:HD12	2.51	0.50
2:N:1396:GLN:N	2:N:1412:GLN:OE1	2.33	0.50
1:A:371:LEU:HD12	1:A:372:ASP:H	1.75	0.50
1:A:991:ILE:HG23	1:A:1195:GLY:HA2	1.94	0.50
1:C:904:ILE:HD11	1:C:1105:TYR:HE1	1.77	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:939:THR:HG22	1:C:955:ILE:HG13	1.94	0.50
1:D:805:ASN:OD1	1:D:806:SER:N	2.45	0.50
1:H:855:CYS:HB2	1:H:882:ARG:HG2	1.94	0.50
2:M:1378:ILE:HG12	2:M:1401:ARG:HA	1.93	0.50
1:A:422:PRO:HA	1:A:552:PRO:HD3	1.93	0.50
1:C:671:HIS:CD2	1:C:729:VAL:HG12	2.47	0.50
1:C:817:ARG:H	1:C:817:ARG:HD2	1.77	0.50
1:D:510:PRO:HA	1:D:518:LEU:O	2.12	0.50
1:D:671:HIS:CD2	1:D:729:VAL:HG12	2.47	0.50
1:F:766:VAL:HA	1:F:774:CYS:O	2.12	0.50
1:G:805:ASN:OD1	1:G:806:SER:N	2.45	0.50
1:G:957:LEU:HD21	1:G:1002:VAL:HG21	1.94	0.50
1:A:817:ARG:HD2	1:A:817:ARG:H	1.77	0.50
1:B:817:ARG:HH12	1:B:839:PRO:HA	1.77	0.50
1:B:904:ILE:HD11	1:B:910:ARG:HH11	1.77	0.50
1:B:958:PHE:CD1	1:B:963:GLU:HG2	2.47	0.50
1:C:816:LEU:HD23	1:C:836:VAL:HG22	1.94	0.50
1:C:991:ILE:HG23	1:C:1195:GLY:HA2	1.94	0.50
1:D:1145:TRP:CD1	1:D:1145:TRP:N	2.77	0.50
1:H:957:LEU:HD21	1:H:1002:VAL:HG21	1.94	0.50
1:A:671:HIS:CD2	1:A:729:VAL:HG12	2.47	0.50
1:B:447:CYS:SG	1:B:448:SER:N	2.85	0.50
1:B:479:LYS:HZ3	2:J:1413:SER:HB2	1.77	0.50
1:B:814:GLU:OE1	1:B:832:VAL:HG22	2.12	0.50
1:C:422:PRO:HA	1:C:552:PRO:HD3	1.93	0.50
1:C:624:ARG:NH1	1:C:685:ASP:O	2.26	0.50
1:D:607:PRO:HG2	1:D:654:ASN:HB2	1.93	0.50
1:H:805:ASN:OD1	1:H:806:SER:N	2.45	0.50
1:H:807:SER:O	1:H:810:THR:HG23	2.12	0.50
1:A:713:ARG:HD2	1:A:755:TYR:CE2	2.47	0.49
1:A:1005:ASP:OD1	1:A:1007:LYS:N	2.35	0.49
1:B:817:ARG:H	1:B:817:ARG:HD2	1.77	0.49
1:C:670:VAL:HG21	1:C:683:TRP:CE2	2.47	0.49
1:D:270:ALA:HA	1:D:317[B]:ARG:HB2	1.94	0.49
1:G:911:TYR:HH	1:G:1051:PHE:HE2	1.60	0.49
1:G:1058:SER:OG	1:G:1060:SER:OG	2.28	0.49
1:A:822:LEU:HD22	1:A:882:ARG:NH1	2.27	0.49
1:A:984:TYR:HA	1:A:996:GLU:O	2.12	0.49
1:B:427:VAL:HB	1:B:546:VAL:HG12	1.94	0.49
1:C:902:HIS:CD2	1:C:1108:ALA:HB1	2.47	0.49
1:C:904:ILE:HD11	1:C:910:ARG:HH11	1.77	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:371:LEU:HD12	1:D:372:ASP:H	1.75	0.49
1:D:713:ARG:HD2	1:D:755:TYR:CE2	2.47	0.49
1:F:447:CYS:SG	1:F:448:SER:N	2.85	0.49
1:G:855:CYS:HB2	1:G:882:ARG:HG2	1.94	0.49
1:H:798:MET:SD	1:H:835:CYS:HB3	2.53	0.49
1:H:1013:ARG:NH2	1:H:1138:ASP:OD2	2.46	0.49
1:A:904:ILE:HD11	1:A:910:ARG:HH11	1.77	0.49
1:A:958:PHE:CD1	1:A:963:GLU:HG2	2.47	0.49
1:B:984:TYR:HA	1:B:996:GLU:O	2.12	0.49
1:C:386:PRO:HA	1:C:396:PRO:HD3	1.94	0.49
1:C:817:ARG:HH12	1:C:839:PRO:HA	1.77	0.49
1:D:807:SER:O	1:D:810:THR:HG23	2.12	0.49
1:G:1043:SER:O	1:G:1043:SER:OG	2.29	0.49
1:G:1133:ALA:O	1:G:1137:HIS:ND1	2.26	0.49
1:A:817:ARG:HH12	1:A:839:PRO:HA	1.77	0.49
1:B:346:CYS:HA	1:B:349:PRO:HB3	1.93	0.49
1:B:904:ILE:HD11	1:B:1105:TYR:HE1	1.77	0.49
1:C:369:THR:O	1:C:369:THR:OG1	2.27	0.49
1:C:852:GLU:OE1	1:C:852:GLU:N	2.42	0.49
1:C:958:PHE:CD1	1:C:963:GLU:HG2	2.47	0.49
1:C:964:LEU:HD11	1:C:984:TYR:CE2	2.48	0.49
1:A:316:PRO:HG2	1:A:338:CYS:HB2	1.95	0.49
1:A:386:PRO:HA	1:A:396:PRO:HD3	1.94	0.49
1:A:814:GLU:OE1	1:A:832:VAL:HG22	2.12	0.49
1:B:700:ARG:NH1	1:B:735:PRO:HB3	2.28	0.49
1:B:816:LEU:HD23	1:B:836:VAL:HG22	1.94	0.49
1:D:1172:GLY:HA3	1:D:1197:TYR:CZ	2.48	0.49
1:E:700:ARG:NH1	1:E:735:PRO:HB3	2.28	0.49
2:M:1378:ILE:HG22	2:M:1424:VAL:HA	1.94	0.49
1:A:700:ARG:NH1	1:A:700:ARG:O	2.45	0.49
1:A:964:LEU:HD11	1:A:984:TYR:CE2	2.47	0.49
1:B:402:THR:N	1:B:405:SER:O	2.46	0.49
1:B:571:ASP:O	1:B:574:THR:OG1	2.23	0.49
1:C:920:ILE:HD13	1:C:923:GLN:OE1	2.13	0.49
1:C:984:TYR:HA	1:C:996:GLU:O	2.12	0.49
1:D:386:PRO:HA	1:D:396:PRO:HD3	1.93	0.49
1:F:446:ASP:OD1	1:F:467:ARG:NH1	2.36	0.49
1:G:1013:ARG:NH2	1:G:1138:ASP:OD2	2.46	0.49
1:H:941:ASN:OD1	1:H:953:LYS:NZ	2.43	0.49
1:H:1172:GLY:HA3	1:H:1197:TYR:CZ	2.48	0.49
2:I:1400:ASP:N	2:I:1400:ASP:OD1	2.46	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:1405:LEU:HD11	2:K:1420:TYR:HB3	1.95	0.49
1:A:402:THR:N	1:A:405:SER:O	2.42	0.49
1:A:706:ASP:HB3	1:A:728:PRO:HB3	1.95	0.49
1:C:316:PRO:HG2	1:C:338:CYS:HB2	1.94	0.49
1:C:814:GLU:OE1	1:C:832:VAL:HG22	2.12	0.49
1:D:670:VAL:HG21	1:D:683:TRP:CE2	2.47	0.49
1:D:1058:SER:OG	1:D:1060:SER:OG	2.28	0.49
1:A:871:ARG:NH2	1:A:1138:ASP:O	2.44	0.49
1:A:939:THR:HG22	1:A:955:ILE:HG13	1.94	0.49
1:B:166:VAL:HG12	1:B:175:VAL:HG22	1.95	0.49
1:F:79:THR:O	1:F:190:SER:HA	2.13	0.49
1:F:625:LEU:O	1:F:636:HIS:NE2	2.45	0.49
1:F:656:GLU:OE1	1:F:656:GLU:N	2.31	0.49
1:G:798:MET:SD	1:G:835:CYS:HB3	2.53	0.49
1:A:1145:TRP:CD1	1:A:1145:TRP:N	2.79	0.49
1:D:632:PHE:HB3	1:D:669:TYR:HE2	1.78	0.49
1:F:166:VAL:HG12	1:F:175:VAL:HG22	1.95	0.49
1:F:342:CYS:HB2	1:F:351:ARG:HG3	1.95	0.49
1:F:418:ASP:OD1	1:F:418:ASP:N	2.34	0.49
2:M:1375:LEU:HD11	2:M:1401:ARG:O	2.13	0.49
2:N:1375:LEU:HD11	2:N:1401:ARG:O	2.13	0.49
1:A:902:HIS:CD2	1:A:1108:ALA:HB1	2.47	0.49
1:B:902:HIS:CD2	1:B:1108:ALA:HB1	2.47	0.49
1:B:1056:LYS:NZ	1:B:1063:ASP:OD1	2.25	0.49
1:C:632:PHE:HB3	1:C:669:TYR:HE2	1.78	0.49
1:C:706:ASP:HB3	1:C:728:PRO:HB3	1.95	0.49
1:C:871:ARG:NH2	1:C:1138:ASP:O	2.44	0.49
2:L:1405:LEU:HD11	2:L:1420:TYR:HB3	1.95	0.49
1:B:119:ARG:HG2	1:B:130:THR:OG1	2.13	0.48
1:B:342:CYS:HB2	1:B:351:ARG:HG3	1.95	0.48
1:C:1005:ASP:OD1	1:C:1007:LYS:N	2.35	0.48
1:D:700:ARG:NH1	1:D:700:ARG:O	2.45	0.48
1:E:79:THR:O	1:E:190:SER:HA	2.13	0.48
1:E:402:THR:N	1:E:405:SER:O	2.46	0.48
1:F:270:ALA:HA	1:F:317[A]:ARG:HB2	1.95	0.48
1:F:700:ARG:NH1	1:F:735:PRO:HB3	2.28	0.48
1:G:1172:GLY:HA3	1:G:1197:TYR:CZ	2.48	0.48
1:H:853:GLU:OE1	1:H:881:ASN:ND2	2.47	0.48
2:I:1405:LEU:HD11	2:I:1420:TYR:HB3	1.95	0.48
2:J:1375:LEU:HD11	2:J:1401:ARG:O	2.12	0.48
1:A:270:ALA:HA	1:A:317[B]:ARG:HB2	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:THR:O	1:B:190:SER:HA	2.13	0.48
1:B:920:ILE:HD13	1:B:923:GLN:OE1	2.13	0.48
1:D:798:MET:SD	1:D:835:CYS:HB3	2.53	0.48
1:D:817:ARG:O	1:D:817:ARG:HG2	2.13	0.48
1:D:853:GLU:OE1	1:D:881:ASN:ND2	2.47	0.48
1:D:944:CYS:H	1:D:951:CYS:HB3	1.78	0.48
1:D:964:LEU:HD11	1:D:984:TYR:CE2	2.49	0.48
1:E:119:ARG:HG2	1:E:130:THR:OG1	2.13	0.48
1:E:342:CYS:HB2	1:E:351:ARG:HG3	1.95	0.48
2:N:1378:ILE:HG22	2:N:1424:VAL:HA	1.94	0.48
1:A:920:ILE:HD13	1:A:923:GLN:OE1	2.13	0.48
1:B:344:ASP:OD1	1:B:352:ALA:N	2.38	0.48
1:C:510:PRO:HA	1:C:518:LEU:O	2.12	0.48
1:D:706:ASP:HB3	1:D:728:PRO:HB3	1.95	0.48
1:D:957:LEU:HD21	1:D:1002:VAL:HG21	1.94	0.48
1:E:447:CYS:SG	1:E:448:SER:N	2.85	0.48
2:M:1414:PRO:O	2:M:1416:LEU:N	2.43	0.48
1:B:874:CYS:O	1:B:889:ARG:NH2	2.47	0.48
1:B:964:LEU:HD11	1:B:984:TYR:CE2	2.48	0.48
1:C:838:PRO:HG2	1:C:841:LEU:HD13	1.96	0.48
1:C:1215:VAL:HG22	1:C:1216:ALA:H	1.79	0.48
1:D:211:ASN:ND2	1:D:217:ASN:HD22	2.12	0.48
1:F:402:THR:N	1:F:405:SER:O	2.46	0.48
1:F:556:GLY:N	1:F:565:PHE:O	2.40	0.48
2:K:1396:GLN:HB2	2:K:1412:GLN:HE22	1.78	0.48
1:A:510:PRO:HA	1:A:518:LEU:O	2.12	0.48
1:A:757:HIS:CE1	1:A:830:HIS:CD2	3.01	0.48
1:A:989:MET:HB3	1:A:1193:LEU:HD11	1.96	0.48
1:B:1004:TRP:HD1	1:B:1010:VAL:HG22	1.78	0.48
1:C:700:ARG:NH1	1:C:700:ARG:O	2.45	0.48
1:C:713:ARG:HD2	1:C:755:TYR:CE2	2.47	0.48
1:C:874:CYS:O	1:C:889:ARG:NH2	2.47	0.48
1:C:1145:TRP:CD1	1:C:1145:TRP:N	2.79	0.48
1:F:517:THR:HG21	1:F:721:THR:HA	1.96	0.48
1:G:817:ARG:NH1	1:G:841:LEU:O	2.45	0.48
1:G:944:CYS:H	1:G:951:CYS:HB3	1.78	0.48
1:A:632:PHE:HB3	1:A:669:TYR:HE2	1.78	0.48
1:D:316:PRO:HG2	1:D:338:CYS:HB2	1.95	0.48
1:D:817:ARG:NH1	1:D:841:LEU:O	2.45	0.48
1:E:166:VAL:HG12	1:E:175:VAL:HG22	1.95	0.48
1:E:625:LEU:O	1:E:636:HIS:NE2	2.45	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:119:ARG:HG2	1:F:130:THR:OG1	2.13	0.48
1:G:817:ARG:O	1:G:817:ARG:HG2	2.13	0.48
1:G:920:ILE:HD13	1:G:923:GLN:OE1	2.13	0.48
1:H:911:TYR:OH	1:H:1051:PHE:HE2	1.94	0.48
1:H:920:ILE:HD13	1:H:923:GLN:OE1	2.13	0.48
1:B:806:SER:HB2	1:B:810:THR:HG21	1.96	0.48
1:B:989:MET:HB3	1:B:1193:LEU:HD11	1.96	0.48
1:C:745:ALA:HB3	2:I:1387:ASP:OD2	2.12	0.48
1:D:1013:ARG:NH2	1:D:1138:ASP:OD2	2.46	0.48
1:E:220:TYR:CE2	1:E:225:ARG:HB2	2.49	0.48
1:E:517:THR:HG21	1:E:721:THR:HA	1.96	0.48
1:A:1215:VAL:HG22	1:A:1216:ALA:H	1.79	0.48
1:B:99:CYS:HA	1:B:119:ARG:NH1	2.29	0.48
1:C:211:ASN:ND2	1:C:217:ASN:HD22	2.12	0.48
1:D:920:ILE:HD13	1:D:923:GLN:OE1	2.13	0.48
1:E:493:ARG:HH22	1:E:495:GLN:NE2	2.11	0.48
1:F:99:CYS:HA	1:F:119:ARG:NH1	2.29	0.48
1:G:853:GLU:OE1	1:G:881:ASN:ND2	2.47	0.48
1:H:964:LEU:HD11	1:H:984:TYR:CE2	2.49	0.48
2:L:1396:GLN:HB2	2:L:1412:GLN:HE22	1.78	0.48
1:A:874:CYS:O	1:A:889:ARG:NH2	2.47	0.48
1:A:1004:TRP:HD1	1:A:1010:VAL:HG22	1.78	0.48
1:B:346:CYS:HB3	1:B:370:VAL:HG21	1.95	0.48
1:B:1040:ARG:HG2	1:B:1055:TRP:CZ3	2.49	0.48
1:C:270:ALA:HA	1:C:317[B]:ARG:HB2	1.94	0.48
1:C:944:CYS:H	1:C:951:CYS:HB3	1.79	0.48
1:E:346:CYS:HB3	1:E:370:VAL:HG21	1.95	0.48
1:C:989:MET:HB3	1:C:1193:LEU:HD11	1.95	0.48
1:F:344:ASP:OD1	1:F:352:ALA:N	2.38	0.48
1:A:245:PRO:HD3	2:J:1403:ARG:NH1	2.29	0.47
1:B:656:GLU:OE1	1:B:656:GLU:N	2.31	0.47
1:E:178:ARG:HD2	1:E:179:LEU:CD2	2.44	0.47
1:E:427:VAL:HB	1:E:546:VAL:HG12	1.94	0.47
1:F:507:THR:HG21	1:F:511:LEU:HD13	1.96	0.47
1:G:955:ILE:HG21	1:G:966:LEU:HD22	1.96	0.47
1:G:964:LEU:HD11	1:G:984:TYR:CE2	2.49	0.47
1:H:817:ARG:HG2	1:H:817:ARG:O	2.13	0.47
1:H:944:CYS:H	1:H:951:CYS:HB3	1.78	0.47
1:H:1058:SER:OG	1:H:1060:SER:OG	2.28	0.47
1:B:1005:ASP:OD2	1:B:1009:SER:N	2.44	0.47
1:B:1215:VAL:HG22	1:B:1216:ALA:H	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:991:ILE:HG23	1:D:1195:GLY:HA2	1.97	0.47
1:D:1207:PHE:CZ	1:D:1209:GLU:HG3	2.49	0.47
2:I:1396:GLN:HB2	2:I:1412:GLN:HE22	1.78	0.47
1:A:171:ASP:OD1	1:A:171:ASP:N	2.47	0.47
1:A:687:VAL:HG22	1:A:688:CYS:SG	2.54	0.47
1:A:838:PRO:HG2	1:A:841:LEU:HD13	1.96	0.47
1:B:178:ARG:HD2	1:B:179:LEU:CD2	2.44	0.47
1:C:237:LEU:HD11	1:E:611:SER:HB2	1.97	0.47
1:D:671:HIS:HD2	1:D:729:VAL:HG12	1.79	0.47
1:E:270:ALA:HA	1:E:317[B]:ARG:HB2	1.97	0.47
1:E:468:LYS:NZ	1:E:470:GLY:O	2.25	0.47
1:F:401:ASN:HA	1:F:406:SER:HA	1.96	0.47
1:A:767:VAL:HG12	2:K:1416:LEU:HD13	1.96	0.47
1:B:871:ARG:NH2	1:B:1138:ASP:O	2.44	0.47
1:B:944:CYS:H	1:B:951:CYS:HB3	1.79	0.47
1:D:293:ARG:NH1	1:D:297:CYS:SG	2.88	0.47
1:B:549:ARG:HB2	1:B:549:ARG:CZ	2.44	0.47
1:B:706:ASP:HA	1:B:728:PRO:HB3	1.96	0.47
1:C:266:LEU:HD22	1:C:305:TYR:HD2	1.80	0.47
1:D:266:LEU:HD22	1:D:305:TYR:HD2	1.80	0.47
1:E:83:PHE:CE2	1:E:127:PRO:HB3	2.49	0.47
1:E:270:ALA:HA	1:E:317[A]:ARG:HB2	1.95	0.47
1:F:346:CYS:HB3	1:F:370:VAL:HG21	1.95	0.47
1:F:427:VAL:HB	1:F:546:VAL:HG12	1.94	0.47
1:A:996:GLU:OE1	1:A:1187:LEU:HB2	2.15	0.47
1:A:1040:ARG:HG2	1:A:1055:TRP:CZ3	2.49	0.47
1:B:777:THR:O	1:B:780:LYS:HD2	2.15	0.47
1:C:171:ASP:N	1:C:171:ASP:OD1	2.47	0.47
1:C:245:PRO:HD3	2:M:1403:ARG:NH1	2.29	0.47
1:C:817:ARG:O	1:C:817:ARG:HG2	2.15	0.47
1:D:402:THR:N	1:D:405:SER:O	2.42	0.47
1:D:852:GLU:OE1	1:D:852:GLU:N	2.47	0.47
1:H:1207:PHE:CZ	1:H:1209:GLU:HG3	2.49	0.47
2:N:1342:SER:OG	2:N:1343:TRP:N	2.48	0.47
1:A:237:LEU:HD11	1:B:611:SER:HB2	1.97	0.47
1:A:266:LEU:HD22	1:A:305:TYR:HD2	1.80	0.47
1:A:536:LEU:HD22	1:A:548:VAL:HG22	1.97	0.47
1:A:806:SER:HB2	1:A:810:THR:HG21	1.96	0.47
1:A:944:CYS:H	1:A:951:CYS:HB3	1.79	0.47
1:B:270:ALA:HA	1:B:317[A]:ARG:HB2	1.96	0.47
1:B:507:THR:HG21	1:B:511:LEU:HD13	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:517:THR:HG21	1:B:721:THR:HA	1.96	0.47
1:B:752:CYS:SG	1:B:753:PRO:HD2	2.55	0.47
1:B:960:GLU:HB3	1:B:961:SER:H	1.58	0.47
1:B:1091:PRO:HA	1:B:1094:ALA:HB2	1.97	0.47
1:C:671:HIS:HD2	1:C:729:VAL:HG12	1.79	0.47
1:C:687:VAL:HG22	1:C:688:CYS:SG	2.54	0.47
1:C:996:GLU:OE1	1:C:1187:LEU:HB2	2.15	0.47
1:E:752:CYS:SG	1:E:753:PRO:HD2	2.55	0.47
1:G:1207:PHE:CZ	1:G:1209:GLU:HG3	2.50	0.47
1:A:211:ASN:ND2	1:A:217:ASN:HD22	2.12	0.47
1:B:838:PRO:HG2	1:B:841:LEU:HD13	1.96	0.47
1:B:996:GLU:OE1	1:B:1187:LEU:HB2	2.15	0.47
1:C:806:SER:HB2	1:C:810:THR:HG21	1.96	0.47
1:E:99:CYS:HA	1:E:119:ARG:NH1	2.29	0.47
1:E:507:THR:HG21	1:E:511:LEU:HD13	1.96	0.47
1:F:83:PHE:CE2	1:F:127:PRO:HB3	2.49	0.47
1:A:293:ARG:NH1	1:A:297:CYS:SG	2.88	0.47
1:A:1102:SER:HB3	1:A:1132:TYR:CZ	2.50	0.47
1:A:1199:LYS:HE2	1:A:1199:LYS:HB2	1.75	0.47
1:B:220:TYR:CE2	1:B:225:ARG:HB2	2.49	0.47
1:B:401:ASN:HA	1:B:406:SER:HA	1.96	0.47
1:B:446:ASP:OD1	1:B:467:ARG:NH1	2.36	0.47
1:C:293:ARG:NH1	1:C:297:CYS:SG	2.88	0.47
1:C:1005:ASP:OD2	1:C:1009:SER:N	2.44	0.47
1:C:1040:ARG:HG2	1:C:1055:TRP:CZ3	2.49	0.47
1:D:237:LEU:HD11	1:F:611:SER:HB2	1.97	0.47
1:D:536:LEU:HD22	1:D:548:VAL:HG22	1.97	0.47
1:D:1043:SER:O	1:D:1043:SER:OG	2.29	0.47
1:E:106:HIS:NE2	1:E:202:GLN:OE1	2.40	0.47
1:F:270:ALA:HA	1:F:317[B]:ARG:HB2	1.97	0.47
1:H:991:ILE:HG23	1:H:1195:GLY:HA2	1.97	0.47
1:A:1005:ASP:OD2	1:A:1009:SER:N	2.44	0.47
1:B:270:ALA:HA	1:B:317[B]:ARG:HB2	1.97	0.47
1:B:297:CYS:N	1:B:298:PRO:HD3	2.30	0.47
1:C:1004:TRP:HD1	1:C:1010:VAL:HG22	1.78	0.47
1:E:297:CYS:N	1:E:298:PRO:HD3	2.30	0.47
1:E:571:ASP:O	1:E:574:THR:OG1	2.23	0.47
1:F:220:TYR:CE2	1:F:225:ARG:HB2	2.49	0.47
1:H:1068:LYS:HD3	1:H:1068:LYS:C	2.35	0.47
1:H:1199:LYS:HE2	1:H:1199:LYS:HB2	1.69	0.47
2:M:1342:SER:OG	2:M:1343:TRP:N	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:1414:PRO:O	2:N:1416:LEU:N	2.43	0.47
1:A:167:GLU:HG3	1:A:169:SER:HB3	1.97	0.46
1:A:414:TRP:HB2	1:C:1041:SER:O	2.15	0.46
1:A:468:LYS:HA	1:A:476:ASN:HD22	1.81	0.46
1:B:607:PRO:HG2	1:B:654:ASN:HB2	1.98	0.46
1:B:852:GLU:OE1	1:B:852:GLU:N	2.42	0.46
1:C:219:PHE:O	1:C:225:ARG:HA	2.15	0.46
1:C:633:SER:HA	1:C:636:HIS:ND1	2.30	0.46
1:F:178:ARG:HD2	1:F:179:LEU:CD2	2.44	0.46
1:F:595:ALA:HB2	1:H:821:THR:OG1	2.15	0.46
1:F:700:ARG:HH11	1:F:735:PRO:HB3	1.80	0.46
1:G:817:ARG:HG2	1:G:842:VAL:HA	1.97	0.46
1:G:991:ILE:HG23	1:G:1195:GLY:HA2	1.97	0.46
2:J:1342:SER:OG	2:J:1343:TRP:N	2.48	0.46
2:K:1400:ASP:N	2:K:1400:ASP:OD1	2.46	0.46
1:D:167:GLU:HG3	1:D:169:SER:HB3	1.97	0.46
1:D:171:ASP:OD1	1:D:171:ASP:N	2.47	0.46
1:D:633:SER:HA	1:D:636:HIS:ND1	2.30	0.46
1:D:687:VAL:HG22	1:D:688:CYS:SG	2.54	0.46
1:F:777:THR:O	1:F:780:LYS:HD2	2.15	0.46
1:H:955:ILE:HG21	1:H:966:LEU:HD22	1.96	0.46
1:B:83:PHE:CE2	1:B:127:PRO:HB3	2.49	0.46
1:B:595:ALA:HB2	1:D:821:THR:OG1	2.15	0.46
1:F:607:PRO:HG2	1:F:654:ASN:HB2	1.98	0.46
1:F:752:CYS:SG	1:F:753:PRO:HD2	2.55	0.46
1:H:817:ARG:NH1	1:H:841:LEU:O	2.45	0.46
2:L:1400:ASP:N	2:L:1400:ASP:OD1	2.46	0.46
1:A:157:LEU:HD12	1:A:167:GLU:HA	1.97	0.46
1:A:800:TYR:HE1	1:A:833:SER:HB3	1.81	0.46
1:A:819:CYS:SG	1:A:856:PRO:HD2	2.55	0.46
1:B:1102:SER:HB3	1:B:1132:TYR:CZ	2.50	0.46
1:C:564:ASN:ND2	1:C:571:ASP:OD2	2.44	0.46
1:D:219:PHE:O	1:D:225:ARG:HA	2.15	0.46
1:D:757:HIS:HE1	1:D:830:HIS:CD2	2.15	0.46
1:A:219:PHE:O	1:A:225:ARG:HA	2.15	0.46
1:C:76:VAL:O	1:C:88:PHE:HA	2.16	0.46
1:C:479:LYS:HZ1	2:K:1413:SER:HB3	1.80	0.46
1:D:270:ALA:HA	1:D:317[A]:ARG:HB2	1.97	0.46
1:E:549:ARG:HB2	1:E:549:ARG:CZ	2.44	0.46
1:E:607:PRO:HG2	1:E:654:ASN:HB2	1.98	0.46
1:A:76:VAL:O	1:A:88:PHE:HA	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:ASN:ND2	1:A:571:ASP:OD2	2.44	0.46
1:A:937:ILE:HG12	1:A:957:LEU:HD23	1.98	0.46
1:B:76:VAL:O	1:B:88:PHE:HA	2.16	0.46
1:B:510:PRO:HA	1:B:518:LEU:O	2.16	0.46
1:B:700:ARG:HH11	1:B:735:PRO:HB3	1.80	0.46
1:C:762:ALA:HB1	2:I:1384:GLN:OE1	2.15	0.46
1:E:76:VAL:O	1:E:88:PHE:HA	2.16	0.46
1:E:446:ASP:OD1	1:E:467:ARG:NH1	2.36	0.46
1:E:700:ARG:HH11	1:E:735:PRO:HB3	1.80	0.46
1:E:706:ASP:HA	1:E:728:PRO:HB3	1.97	0.46
1:F:510:PRO:HA	1:F:518:LEU:O	2.16	0.46
1:F:706:ASP:HA	1:F:728:PRO:HB3	1.97	0.46
1:G:1068:LYS:C	1:G:1068:LYS:HD3	2.35	0.46
2:J:1333:CYS:HB3	2:J:1432:CYS:HB2	1.68	0.46
2:L:1348:ARG:HG3	2:L:1348:ARG:HH11	1.81	0.46
2:M:1400:ASP:OD1	2:M:1400:ASP:N	2.49	0.46
1:B:1058:SER:OG	1:B:1060:SER:OG	2.33	0.46
1:B:1207:PHE:CZ	1:B:1209:GLU:HG3	2.51	0.46
1:C:167:GLU:HG3	1:C:169:SER:HB3	1.97	0.46
1:C:270:ALA:HA	1:C:317[A]:ARG:HB2	1.97	0.46
1:C:536:LEU:HD22	1:C:548:VAL:HG22	1.97	0.46
1:C:1058:SER:OG	1:C:1060:SER:OG	2.33	0.46
1:C:1098:SER:OG	1:C:1099:GLN:OE1	2.33	0.46
1:D:1068:LYS:C	1:D:1068:LYS:HD3	2.35	0.46
1:E:401:ASN:HA	1:E:406:SER:HA	1.96	0.46
1:E:777:THR:O	1:E:780:LYS:HD2	2.15	0.46
1:F:549:ARG:CZ	1:F:549:ARG:HB2	2.44	0.46
2:J:1343:TRP:CZ3	2:J:1423:ARG:HD2	2.51	0.46
2:J:1397:VAL:HG21	2:J:1420:TYR:CZ	2.51	0.46
2:N:1343:TRP:CZ3	2:N:1423:ARG:HD2	2.51	0.46
1:A:754:CYS:HB3	1:A:781:LEU:HB2	1.98	0.46
1:A:817:ARG:O	1:A:817:ARG:HG2	2.15	0.46
1:A:1091:PRO:HA	1:A:1094:ALA:HB2	1.97	0.46
1:A:1207:PHE:CZ	1:A:1209:GLU:HG3	2.51	0.46
1:B:556:GLY:N	1:B:565:PHE:O	2.40	0.46
1:B:800:TYR:HE1	1:B:833:SER:HB3	1.81	0.46
1:B:1041:SER:O	1:D:414:TRP:HB2	2.15	0.46
1:C:1102:SER:HB3	1:C:1132:TYR:CZ	2.50	0.46
1:D:955:ILE:HG21	1:D:966:LEU:HD22	1.96	0.46
1:F:76:VAL:O	1:F:88:PHE:HA	2.16	0.46
1:F:297:CYS:N	1:F:298:PRO:HD3	2.30	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:1397:VAL:HG21	2:M:1420:TYR:CZ	2.51	0.46
1:A:83:PHE:CE2	1:A:127:PRO:HB3	2.51	0.46
1:A:278:VAL:HB	1:A:305:TYR:HE1	1.81	0.46
1:A:509:LEU:HD22	1:A:518:LEU:HB3	1.98	0.46
1:A:796:ALA:HB1	1:A:797:PRO:HD2	1.98	0.46
1:C:83:PHE:CE2	1:C:127:PRO:HB3	2.51	0.46
1:C:468:LYS:HA	1:C:476:ASN:HD22	1.81	0.46
1:C:1091:PRO:HA	1:C:1094:ALA:HB2	1.97	0.46
1:D:760:VAL:O	2:J:1418:HIS:NE2	2.49	0.46
1:D:1220:CYS:HB2	1:D:1250:ILE:HG13	1.98	0.46
1:E:510:PRO:HA	1:E:518:LEU:O	2.16	0.46
1:E:595:ALA:HB2	1:G:821:THR:OG1	2.15	0.46
1:F:756:ALA:O	1:F:759:THR:OG1	2.25	0.46
1:H:1220:CYS:HB2	1:H:1250:ILE:HG13	1.98	0.46
2:N:1395:GLN:OE1	2:N:1420:TYR:OH	2.33	0.46
2:N:1397:VAL:HG21	2:N:1420:TYR:CZ	2.51	0.46
1:A:671:HIS:HD2	1:A:729:VAL:HG12	1.80	0.46
1:B:582:ALA:HB2	1:D:860:ASN:ND2	2.31	0.46
1:B:819:CYS:SG	1:B:856:PRO:HD2	2.56	0.46
1:B:1230:VAL:HA	1:B:1245:CYS:HB3	1.97	0.46
1:C:178:ARG:CD	1:C:179:LEU:HD23	2.43	0.46
1:D:157:LEU:HD12	1:D:167:GLU:HA	1.97	0.46
1:E:425:CYS:SG	1:E:426:SER:N	2.89	0.46
1:H:817:ARG:HG2	1:H:842:VAL:HA	1.97	0.46
2:I:1348:ARG:HG3	2:I:1348:ARG:HH11	1.81	0.46
2:J:1400:ASP:OD1	2:J:1400:ASP:N	2.49	0.46
2:M:1395:GLN:OE1	2:M:1420:TYR:OH	2.33	0.46
1:A:270:ALA:HA	1:A:317[A]:ARG:HB2	1.97	0.45
1:A:860:ASN:ND2	1:C:582:ALA:HB2	2.31	0.45
1:B:262:CYS:O	1:B:266:LEU:HB2	2.16	0.45
1:B:636:HIS:CD2	1:B:641:PRO:HG3	2.51	0.45
1:C:800:TYR:HE1	1:C:833:SER:HB3	1.81	0.45
1:D:278:VAL:HB	1:D:305:TYR:HE1	1.81	0.45
1:F:768:HIS:HE1	1:F:771:GLY:HA2	1.81	0.45
2:J:1395:GLN:OE1	2:J:1420:TYR:OH	2.33	0.45
1:B:796:ALA:HB1	1:B:797:PRO:HD2	1.98	0.45
1:E:768:HIS:HE1	1:E:771:GLY:HA2	1.81	0.45
1:F:262:CYS:O	1:F:266:LEU:HB2	2.16	0.45
1:G:909:ASP:OD1	1:G:910:ARG:N	2.49	0.45
1:H:1049:LEU:HD12	1:H:1049:LEU:HA	1.83	0.45
1:H:1133:ALA:O	1:H:1137:HIS:ND1	2.26	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:1343:TRP:CZ3	2:M:1423:ARG:HD2	2.51	0.45
2:N:1400:ASP:N	2:N:1400:ASP:OD1	2.49	0.45
1:A:582:ALA:HB2	1:C:860:ASN:ND2	2.31	0.45
1:B:539:GLN:O	1:B:544:MET:HA	2.16	0.45
1:C:157:LEU:HD12	1:C:167:GLU:HA	1.97	0.45
1:C:341:PRO:HB3	1:C:360:VAL:HG21	1.98	0.45
1:C:509:LEU:HD22	1:C:518:LEU:HB3	1.98	0.45
1:C:819:CYS:SG	1:C:856:PRO:HD2	2.56	0.45
1:C:1035:ASN:HB2	1:C:1044:VAL:HG21	1.98	0.45
1:D:509:LEU:HD22	1:D:518:LEU:HB3	1.98	0.45
1:D:754:CYS:HB3	1:D:781:LEU:HB2	1.98	0.45
1:F:539:GLN:O	1:F:544:MET:HA	2.16	0.45
1:H:1078:LYS:HG2	1:H:1082:GLN:HE21	1.82	0.45
1:B:817:ARG:HG2	1:B:817:ARG:O	2.15	0.45
1:C:126:ARG:HE	1:C:293:ARG:HH12	1.65	0.45
1:D:1078:LYS:HG2	1:D:1082:GLN:HE21	1.81	0.45
1:E:266:LEU:HD22	1:E:305:TYR:CD2	2.52	0.45
1:F:493:ARG:HH22	1:F:495:GLN:NE2	2.11	0.45
1:F:582:ALA:HB2	1:H:860:ASN:ND2	2.31	0.45
1:F:604:PHE:N	1:F:605:GLU:OE2	2.48	0.45
1:G:1145:TRP:CD1	1:G:1145:TRP:N	2.77	0.45
2:M:1341:SER:OG	2:M:1344:TYR:OH	2.31	0.45
1:A:921:LEU:N	1:A:937:ILE:O	2.50	0.45
1:A:1041:SER:O	1:C:414:TRP:HB2	2.15	0.45
1:B:860:ASN:ND2	1:D:582:ALA:HB2	2.31	0.45
1:C:278:VAL:HB	1:C:305:TYR:HE1	1.81	0.45
1:F:425:CYS:SG	1:F:426:SER:N	2.89	0.45
1:G:817:ARG:HH12	1:G:839:PRO:HA	1.82	0.45
2:N:1341:SER:OG	2:N:1344:TYR:OH	2.31	0.45
1:B:768:HIS:HE1	1:B:771:GLY:HA2	1.81	0.45
1:B:937:ILE:HG12	1:B:957:LEU:HD23	1.98	0.45
1:E:582:ALA:HB2	1:G:860:ASN:ND2	2.31	0.45
1:F:636:HIS:CD2	1:F:641:PRO:HG3	2.51	0.45
1:G:907:ASP:OD1	1:G:1031:ASP:N	2.49	0.45
1:G:1220:CYS:HB2	1:G:1250:ILE:HG13	1.98	0.45
2:K:1348:ARG:HH11	2:K:1348:ARG:HG3	1.81	0.45
1:A:469:CYS:O	2:I:1411:GLN:HA	2.17	0.45
1:A:577:SER:HG	1:C:884:TRP:HD1	1.64	0.45
1:A:633:SER:HA	1:A:636:HIS:ND1	2.30	0.45
1:A:852:GLU:OE1	1:A:852:GLU:N	2.42	0.45
1:A:1230:VAL:HA	1:A:1245:CYS:HB3	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1230:VAL:HA	1:C:1245:CYS:HB3	1.98	0.45
1:D:245:PRO:HD3	2:N:1403:ARG:NH1	2.29	0.45
1:D:455:CYS:HB3	1:D:559:CYS:HB2	1.60	0.45
1:D:479:LYS:HZ1	2:L:1413:SER:HB3	1.81	0.45
1:E:539:GLN:O	1:E:544:MET:HA	2.16	0.45
1:E:636:HIS:CD2	1:E:641:PRO:HG3	2.51	0.45
2:I:1349:PRO:HG3	2:I:1418:HIS:O	2.17	0.45
1:A:126:ARG:HE	1:A:293:ARG:HH12	1.65	0.45
1:A:341:PRO:HB3	1:A:360:VAL:HG21	1.98	0.45
1:A:798:MET:HB3	1:A:837:CYS:HA	1.99	0.45
1:B:1199:LYS:HE2	1:B:1199:LYS:HB2	1.75	0.45
1:C:754:CYS:HB3	1:C:781:LEU:HB2	1.98	0.45
1:C:937:ILE:HG12	1:C:957:LEU:HD23	1.98	0.45
1:C:962:TYR:CE2	1:C:982:PRO:HA	2.51	0.45
1:E:262:CYS:O	1:E:266:LEU:HB2	2.16	0.45
1:E:592:LYS:NZ	1:E:599:ASN:OD1	2.48	0.45
1:H:852:GLU:OE1	1:H:852:GLU:N	2.47	0.45
1:H:1158:TYR:HB2	1:H:1166:TRP:CD1	2.52	0.45
1:B:493:ARG:HH22	1:B:495:GLN:NE2	2.11	0.45
1:B:625:LEU:O	1:B:636:HIS:NE2	2.45	0.45
1:B:962:TYR:CE2	1:B:982:PRO:HA	2.52	0.45
1:B:1035:ASN:HB2	1:B:1044:VAL:HG21	1.98	0.45
1:B:1156:ASP:HA	1:B:1159:ASN:HD22	1.82	0.45
1:D:76:VAL:O	1:D:88:PHE:HA	2.16	0.45
1:D:817:ARG:HG2	1:D:842:VAL:HA	1.97	0.45
1:D:1158:TYR:HB2	1:D:1166:TRP:CD1	2.52	0.45
1:G:1199:LYS:HB2	1:G:1199:LYS:HE2	1.69	0.45
1:A:1098:SER:OG	1:A:1099:GLN:OE1	2.33	0.45
1:B:106:HIS:NE2	1:B:202:GLN:OE1	2.40	0.45
1:B:425:CYS:SG	1:B:426:SER:N	2.89	0.45
1:B:798:MET:HB3	1:B:837:CYS:HA	1.99	0.45
1:C:159:TYR:HB3	1:C:166:VAL:HG22	1.99	0.45
1:C:447:CYS:SG	1:C:448:SER:N	2.90	0.45
1:C:853:GLU:OE1	1:C:881:ASN:ND2	2.50	0.45
1:C:1156:ASP:HA	1:C:1159:ASN:HD22	1.82	0.45
1:D:906:PHE:CZ	1:D:1014:LEU:HD12	2.52	0.45
1:E:371:LEU:HD12	1:E:372:ASP:H	1.82	0.45
1:G:1158:TYR:HB2	1:G:1166:TRP:CD1	2.52	0.45
2:I:1348:ARG:HG3	2:I:1348:ARG:NH1	2.32	0.45
1:A:740:LEU:HD12	1:A:740:LEU:O	2.17	0.44
1:A:853:GLU:OE1	1:A:881:ASN:ND2	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:962:TYR:CE2	1:A:982:PRO:HA	2.51	0.44
1:A:1058:SER:OG	1:A:1060:SER:OG	2.33	0.44
1:B:455:CYS:HB3	1:B:559:CYS:HB2	1.67	0.44
1:B:761:LEU:HD21	1:B:767:VAL:HG11	1.98	0.44
1:D:468:LYS:HA	1:D:476:ASN:HD22	1.81	0.44
1:D:909:ASP:OD1	1:D:910:ARG:N	2.49	0.44
1:H:1230:VAL:HA	1:H:1245:CYS:HB3	1.99	0.44
2:J:1414:PRO:O	2:J:1416:LEU:N	2.43	0.44
2:L:1349:PRO:HG3	2:L:1418:HIS:O	2.17	0.44
1:C:83:PHE:CZ	1:C:127:PRO:HB3	2.53	0.44
1:G:813:ALA:HB3	1:G:832:VAL:HG23	2.00	0.44
1:G:906:PHE:CZ	1:G:1014:LEU:HD12	2.52	0.44
2:K:1349:PRO:HG3	2:K:1418:HIS:O	2.17	0.44
2:M:1343:TRP:CE3	2:M:1423:ARG:HB3	2.53	0.44
1:A:625:LEU:HA	1:A:632:PHE:HD2	1.83	0.44
1:C:740:LEU:HD12	1:C:740:LEU:O	2.18	0.44
1:C:764:GLY:N	1:C:776:CYS:O	2.36	0.44
1:C:921:LEU:N	1:C:937:ILE:O	2.50	0.44
1:D:83:PHE:CZ	1:D:127:PRO:HB3	2.53	0.44
1:D:469:CYS:O	2:L:1411:GLN:HA	2.17	0.44
1:E:291:LEU:HD23	1:E:291:LEU:HA	1.84	0.44
1:F:295:PRO:CD	1:F:296:THR:N	2.80	0.44
1:H:1035:ASN:HB2	1:H:1044:VAL:HG21	2.00	0.44
2:M:1398:ASP:OD1	2:M:1406:MET:HB2	2.17	0.44
2:N:1398:ASP:OD1	2:N:1406:MET:HB2	2.17	0.44
1:A:1035:ASN:HB2	1:A:1044:VAL:HG21	1.98	0.44
1:B:295:PRO:CD	1:B:296:THR:N	2.80	0.44
1:D:447:CYS:SG	1:D:448:SER:N	2.90	0.44
1:E:263:HIS:O	1:E:267:LEU:HB2	2.18	0.44
1:F:651:ASP:O	1:F:655:CYS:N	2.47	0.44
2:N:1343:TRP:HA	2:N:1343:TRP:CE3	2.53	0.44
1:A:88:PHE:HE2	1:A:203:THR:HG21	1.82	0.44
1:A:763:PRO:O	2:K:1384:GLN:NE2	2.44	0.44
1:B:266:LEU:HD22	1:B:305:TYR:CD2	2.52	0.44
1:C:469:CYS:O	2:K:1411:GLN:HA	2.17	0.44
1:C:1207:PHE:CZ	1:C:1209:GLU:HG3	2.51	0.44
1:D:126:ARG:HE	1:D:293:ARG:HH12	1.65	0.44
1:D:341:PRO:HB3	1:D:360:VAL:HG21	1.98	0.44
1:D:740:LEU:HD12	1:D:740:LEU:O	2.17	0.44
1:G:1078:LYS:HG2	1:G:1082:GLN:HE21	1.81	0.44
2:J:1343:TRP:CE3	2:J:1423:ARG:HB3	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:606:ASP:OD2	1:A:608:CYS:HB2	2.18	0.44
1:B:891:CYS:H	1:B:1016:GLN:HE21	1.65	0.44
1:B:921:LEU:N	1:B:937:ILE:O	2.50	0.44
1:C:1083:LYS:HE2	1:C:1083:LYS:HB2	1.80	0.44
1:D:83:PHE:CE2	1:D:127:PRO:HB3	2.51	0.44
1:E:761:LEU:HD21	1:E:767:VAL:HG11	1.98	0.44
1:A:1156:ASP:HA	1:A:1159:ASN:HD22	1.82	0.44
1:B:216:PHE:O	1:B:216:PHE:CD1	2.71	0.44
1:B:1137:HIS:HA	1:B:1141:LEU:O	2.18	0.44
1:D:159:TYR:HB3	1:D:166:VAL:HG22	1.99	0.44
1:D:817:ARG:HH12	1:D:839:PRO:HA	1.82	0.44
1:E:216:PHE:O	1:E:216:PHE:CD1	2.71	0.44
1:F:263:HIS:O	1:F:267:LEU:HB2	2.17	0.44
1:H:813:ALA:HB3	1:H:832:VAL:HG23	2.00	0.44
2:I:1341:SER:HG	2:I:1424:VAL:H	1.66	0.44
2:M:1333:CYS:HB3	2:M:1432:CYS:HB2	1.68	0.44
1:A:447:CYS:SG	1:A:448:SER:N	2.90	0.44
1:A:1137:HIS:HA	1:A:1141:LEU:O	2.18	0.44
1:B:83:PHE:CZ	1:B:127:PRO:HB3	2.53	0.44
1:B:800:TYR:CE1	1:B:833:SER:HB3	2.53	0.44
1:B:853:GLU:OE1	1:B:881:ASN:ND2	2.50	0.44
1:C:796:ALA:HB1	1:C:797:PRO:HD2	1.98	0.44
1:C:891:CYS:H	1:C:1016:GLN:HE21	1.65	0.44
1:D:1102:SER:HB3	1:D:1132:TYR:CZ	2.53	0.44
1:E:604:PHE:N	1:E:605:GLU:OE2	2.48	0.44
1:F:266:LEU:HD22	1:F:305:TYR:CD2	2.52	0.44
1:F:448:SER:HA	1:F:465:GLU:HA	2.00	0.44
1:H:1057:LEU:HD23	1:H:1057:LEU:HA	1.75	0.44
1:H:1102:SER:HB3	1:H:1132:TYR:CZ	2.53	0.44
2:N:1340:TRP:CE3	2:N:1423:ARG:HG3	2.53	0.44
1:B:604:PHE:N	1:B:605:GLU:OE2	2.48	0.44
1:B:1098:SER:OG	1:B:1099:GLN:OE1	2.33	0.44
1:C:625:LEU:HA	1:C:632:PHE:HD2	1.83	0.44
1:D:813:ALA:HB3	1:D:832:VAL:HG23	2.00	0.44
1:E:83:PHE:CZ	1:E:127:PRO:HB3	2.53	0.44
1:F:83:PHE:CZ	1:F:127:PRO:HB3	2.53	0.44
1:F:455:CYS:HB3	1:F:559:CYS:HB2	1.67	0.44
1:F:592:LYS:NZ	1:F:599:ASN:OD1	2.48	0.44
1:H:909:ASP:OD1	1:H:910:ARG:N	2.49	0.44
2:J:1398:ASP:OD2	2:J:1406:MET:HB2	2.17	0.44
1:B:560:GLY:HA2	1:B:591:TRP:CE2	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:422:PRO:HA	1:C:550:LEU:O	2.18	0.43
1:C:606:ASP:OD2	1:C:608:CYS:HB2	2.18	0.43
1:C:1137:HIS:HA	1:C:1141:LEU:O	2.18	0.43
1:D:763:PRO:N	2:J:1384:GLN:NE2	2.66	0.43
1:E:394:TYR:HB3	1:E:398:THR:OG1	2.18	0.43
1:E:560:GLY:HA2	1:E:591:TRP:CE2	2.53	0.43
1:F:761:LEU:HD21	1:F:767:VAL:HG11	1.98	0.43
1:H:1168:TYR:HA	1:H:1196:CYS:HB3	2.00	0.43
2:J:1340:TRP:CE3	2:J:1423:ARG:HG3	2.53	0.43
2:N:1343:TRP:CE3	2:N:1423:ARG:HB3	2.53	0.43
1:A:83:PHE:CZ	1:A:127:PRO:HB3	2.53	0.43
1:A:656:GLU:H	1:A:656:GLU:CD	2.15	0.43
1:B:394:TYR:HB3	1:B:398:THR:OG1	2.18	0.43
1:C:893:GLY:O	1:C:1013:ARG:HA	2.19	0.43
1:D:88:PHE:HE2	1:D:203:THR:HG21	1.82	0.43
1:D:1057:LEU:HD23	1:D:1057:LEU:HA	1.75	0.43
1:E:295:PRO:CD	1:E:296:THR:N	2.80	0.43
1:E:448:SER:HA	1:E:465:GLU:HA	2.00	0.43
1:E:656:GLU:OE1	1:E:656:GLU:N	2.31	0.43
1:E:756:ALA:O	1:E:759:THR:OG1	2.25	0.43
1:F:216:PHE:CD1	1:F:216:PHE:O	2.71	0.43
1:F:318:ASN:OD1	1:F:318:ASN:N	2.51	0.43
1:F:560:GLY:HA2	1:F:591:TRP:CE2	2.53	0.43
1:H:906:PHE:CZ	1:H:1014:LEU:HD12	2.52	0.43
2:K:1348:ARG:HG3	2:K:1348:ARG:NH1	2.32	0.43
1:A:651:ASP:O	1:A:655:CYS:N	2.48	0.43
1:A:800:TYR:CE1	1:A:833:SER:HB3	2.53	0.43
1:B:201:ASN:HD22	4:B:2006:NAG:C7	2.31	0.43
1:C:200:ALA:O	1:C:202:GLN:HG3	2.18	0.43
1:F:162:THR:OG1	1:H:948:GLY:O	2.17	0.43
1:F:633:SER:HA	1:F:636:HIS:CE1	2.54	0.43
2:J:1343:TRP:CE3	2:J:1343:TRP:HA	2.53	0.43
1:A:891:CYS:H	1:A:1016:GLN:HE21	1.65	0.43
1:B:220:TYR:OH	1:B:225:ARG:HD2	2.18	0.43
1:B:633:SER:HA	1:B:636:HIS:CE1	2.54	0.43
1:B:893:GLY:O	1:B:1013:ARG:HA	2.19	0.43
1:C:1057:LEU:HA	1:C:1057:LEU:HD23	1.77	0.43
1:D:850:ILE:HG22	1:D:851:ALA:O	2.19	0.43
1:E:608:CYS:SG	1:E:649:MET:HG3	2.59	0.43
1:E:617:TYR:CE1	1:E:621:TRP:CD1	3.07	0.43
1:F:220:TYR:OH	1:F:225:ARG:HD2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:817:ARG:HH12	1:H:839:PRO:HA	1.82	0.43
1:B:318:ASN:N	1:B:318:ASN:OD1	2.51	0.43
1:B:891:CYS:O	1:B:1016:GLN:NE2	2.52	0.43
1:C:77:CYS:SG	1:C:193:LEU:HB2	2.59	0.43
1:C:867:GLY:H	1:C:880:ARG:HH21	1.67	0.43
1:D:77:CYS:SG	1:D:193:LEU:HB2	2.59	0.43
1:D:200:ALA:O	1:D:202:GLN:HG3	2.18	0.43
1:D:422:PRO:HA	1:D:550:LEU:O	2.18	0.43
1:F:371:LEU:HD12	1:F:372:ASP:H	1.82	0.43
1:H:850:ILE:HG22	1:H:851:ALA:O	2.19	0.43
1:B:608:CYS:SG	1:B:649:MET:HG3	2.59	0.43
1:B:852:GLU:OE2	1:B:853:GLU:HG2	2.19	0.43
1:C:798:MET:HB3	1:C:837:CYS:HA	1.99	0.43
1:D:651:ASP:O	1:D:655:CYS:N	2.48	0.43
1:G:1102:SER:HB3	1:G:1132:TYR:CZ	2.53	0.43
2:L:1333:CYS:SG	2:L:1334:VAL:N	2.92	0.43
2:M:1340:TRP:CE3	2:M:1423:ARG:HG3	2.53	0.43
1:A:422:PRO:HA	1:A:550:LEU:O	2.18	0.43
1:A:909:ASP:OD1	1:A:910:ARG:N	2.52	0.43
1:A:1057:LEU:HA	1:A:1057:LEU:HD23	1.77	0.43
1:B:448:SER:HA	1:B:465:GLU:HA	2.00	0.43
1:B:1168:TYR:HA	1:B:1196:CYS:HB3	2.00	0.43
1:E:220:TYR:OH	1:E:225:ARG:HD2	2.19	0.43
1:F:394:TYR:HB3	1:F:398:THR:OG1	2.18	0.43
1:F:447:CYS:HB2	1:F:597:CYS:HB3	1.97	0.43
1:F:617:TYR:CE1	1:F:621:TRP:CD1	3.07	0.43
1:G:1168:TYR:HA	1:G:1196:CYS:HB3	2.00	0.43
1:G:1180:ARG:O	1:G:1182:PRO:HD3	2.19	0.43
1:G:1230:VAL:HA	1:G:1245:CYS:HB3	1.99	0.43
1:G:1243:CYS:HA	1:G:1252:CYS:HB3	2.01	0.43
2:L:1348:ARG:HG3	2:L:1348:ARG:NH1	2.32	0.43
1:A:200:ALA:O	1:A:202:GLN:HG3	2.18	0.43
1:A:946:THR:HA	1:C:137:GLN:HB3	2.01	0.43
1:A:1168:TYR:HA	1:A:1196:CYS:HB3	2.00	0.43
1:B:592:LYS:NZ	1:B:599:ASN:OD1	2.48	0.43
1:B:909:ASP:OD1	1:B:910:ARG:N	2.52	0.43
1:B:1083:LYS:HE2	1:B:1083:LYS:HB2	1.80	0.43
1:C:455:CYS:HB3	1:C:559:CYS:HB2	1.60	0.43
1:C:800:TYR:CE1	1:C:833:SER:HB3	2.53	0.43
1:E:318:ASN:OD1	1:E:318:ASN:N	2.51	0.43
1:E:633:SER:HA	1:E:636:HIS:CE1	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:1333:CYS:SG	2:K:1334:VAL:N	2.92	0.43
1:B:236:LYS:NZ	1:B:238:ASP:OD1	2.36	0.43
1:B:907:ASP:OD1	1:B:1031:ASP:N	2.48	0.43
1:D:625:LEU:HA	1:D:632:PHE:HD2	1.83	0.43
1:D:1035:ASN:HB2	1:D:1044:VAL:HG21	2.00	0.43
2:M:1343:TRP:CE3	2:M:1343:TRP:HA	2.53	0.43
1:A:106:HIS:HB2	1:A:114:PHE:CE1	2.54	0.43
1:A:341:PRO:HB3	1:A:360:VAL:CG2	2.49	0.43
1:A:891:CYS:O	1:A:1016:GLN:NE2	2.52	0.43
1:A:1180:ARG:O	1:A:1182:PRO:HD3	2.19	0.43
1:B:263:HIS:O	1:B:267:LEU:HB2	2.18	0.43
1:C:88:PHE:HE2	1:C:203:THR:HG21	1.82	0.43
1:C:344:ASP:OD1	1:C:351:ARG:N	2.52	0.43
1:C:907:ASP:OD1	1:C:1031:ASP:N	2.49	0.43
1:D:341:PRO:HB3	1:D:360:VAL:CG2	2.49	0.43
1:D:907:ASP:OD1	1:D:1031:ASP:N	2.48	0.43
1:D:1243:CYS:HA	1:D:1252:CYS:HB3	2.01	0.43
2:L:1341:SER:HG	2:L:1424:VAL:H	1.67	0.43
1:A:77:CYS:SG	1:A:193:LEU:HB2	2.58	0.42
1:A:159:TYR:HB3	1:A:166:VAL:HG22	1.99	0.42
1:A:625:LEU:HD23	1:A:632:PHE:CD2	2.54	0.42
1:B:617:TYR:CE2	1:B:621:TRP:CD1	3.07	0.42
1:C:106:HIS:HB2	1:C:114:PHE:CE1	2.54	0.42
1:C:625:LEU:HD23	1:C:632:PHE:CD2	2.54	0.42
1:C:932:HIS:H	1:C:932:HIS:CD2	2.37	0.42
1:C:956:LYS:HB3	1:C:958:PHE:CE1	2.54	0.42
1:C:1168:TYR:HA	1:C:1196:CYS:HB3	2.00	0.42
1:G:1172:GLY:H	1:G:1193:LEU:H	1.67	0.42
1:G:1190:LEU:HD23	1:G:1190:LEU:HA	1.92	0.42
1:H:1154:PHE:CD1	1:H:1157:PHE:HB2	2.55	0.42
1:H:1243:CYS:HA	1:H:1252:CYS:HB3	2.01	0.42
1:B:89:ASP:O	1:B:214:PRO:HB3	2.19	0.42
1:C:852:GLU:OE2	1:C:853:GLU:HG2	2.19	0.42
1:D:606:ASP:OD2	1:D:608:CYS:HB2	2.18	0.42
1:D:1180:ARG:O	1:D:1182:PRO:HD3	2.19	0.42
1:G:850:ILE:HG22	1:G:851:ALA:O	2.19	0.42
1:H:907:ASP:OD1	1:H:1031:ASP:N	2.49	0.42
1:H:987:ARG:HD2	1:H:996:GLU:OE2	2.19	0.42
1:A:751:GLU:OE1	1:A:751:GLU:N	2.52	0.42
1:A:893:GLY:O	1:A:1013:ARG:HA	2.19	0.42
1:A:932:HIS:CD2	1:A:932:HIS:H	2.37	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:ASN:ND2	1:B:217:ASN:HD22	2.18	0.42
1:B:660:ASP:OD1	1:B:691:TYR:OH	2.35	0.42
1:D:115:ASN:HB3	1:D:135:LYS:HB3	2.02	0.42
1:D:625:LEU:HD23	1:D:632:PHE:CD2	2.54	0.42
1:D:987:ARG:HD2	1:D:996:GLU:OE2	2.19	0.42
1:D:1160:PRO:O	1:D:1160:PRO:HD2	2.20	0.42
1:D:1168:TYR:HA	1:D:1196:CYS:HB3	2.00	0.42
1:E:500:VAL:HG21	1:E:509:LEU:HD11	2.01	0.42
1:F:605:GLU:H	1:F:605:GLU:CD	2.19	0.42
1:G:1049:LEU:HD12	1:G:1049:LEU:HA	1.83	0.42
2:I:1333:CYS:SG	2:I:1334:VAL:N	2.92	0.42
1:A:344:ASP:OD1	1:A:351:ARG:N	2.52	0.42
1:B:371:LEU:HD12	1:B:372:ASP:H	1.82	0.42
1:B:447:CYS:HB2	1:B:597:CYS:HB3	1.97	0.42
1:C:700:ARG:HH21	1:C:735:PRO:HA	1.84	0.42
1:D:344:ASP:OD1	1:D:351:ARG:N	2.52	0.42
1:D:1230:VAL:HA	1:D:1245:CYS:HB3	1.99	0.42
1:E:536:LEU:HD22	1:E:548:VAL:HG22	2.02	0.42
1:F:201:ASN:HD22	4:F:1305:NAG:C7	2.31	0.42
1:F:500:VAL:HG21	1:F:509:LEU:HD11	2.01	0.42
1:G:987:ARG:HD2	1:G:996:GLU:OE2	2.19	0.42
1:H:1088:LEU:HD22	1:H:1132:TYR:CD2	2.52	0.42
2:M:1403:ARG:HD3	2:M:1406:MET:HE1	2.01	0.42
1:A:956:LYS:HB3	1:A:958:PHE:CE1	2.54	0.42
1:B:651:ASP:O	1:B:655:CYS:N	2.47	0.42
1:B:767:VAL:CG1	2:L:1416:LEU:HD22	2.49	0.42
1:B:911:TYR:OH	1:B:1051:PHE:HE2	2.03	0.42
1:B:932:HIS:H	1:B:932:HIS:CD2	2.37	0.42
1:D:184:LEU:HD22	1:D:307:ARG:HH12	1.84	0.42
1:E:479:LYS:HZ3	2:M:1413:SER:HB2	1.82	0.42
2:N:1403:ARG:HD3	2:N:1406:MET:HE1	2.01	0.42
1:B:697:LYS:O	1:B:698:SER:OG	2.35	0.42
1:C:115:ASN:N	1:C:135:LYS:O	2.53	0.42
1:C:341:PRO:HB3	1:C:360:VAL:CG2	2.49	0.42
1:C:621:TRP:CB	1:C:662:LEU:HD11	2.49	0.42
1:C:909:ASP:OD1	1:C:910:ARG:N	2.52	0.42
1:C:1004:TRP:CE3	1:C:1006:ARG:HA	2.55	0.42
1:D:751:GLU:N	1:D:751:GLU:OE1	2.52	0.42
1:D:1244:ASN:O	1:D:1250:ILE:HA	2.20	0.42
1:E:89:ASP:O	1:E:214:PRO:HB3	2.19	0.42
1:G:1035:ASN:HB2	1:G:1044:VAL:HG21	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1137:HIS:HA	1:G:1141:LEU:O	2.20	0.42
2:L:1333:CYS:HB3	2:L:1432:CYS:HB2	1.35	0.42
1:A:115:ASN:HB3	1:A:135:LYS:HB3	2.02	0.42
1:A:511:LEU:HD11	1:C:511:LEU:HD11	2.02	0.42
1:B:1004:TRP:CE3	1:B:1006:ARG:HA	2.55	0.42
1:C:960:GLU:HB3	1:C:961:SER:H	1.58	0.42
1:C:1180:ARG:O	1:C:1182:PRO:HD3	2.19	0.42
1:E:201:ASN:HD22	4:E:1305:NAG:C7	2.31	0.42
1:E:263:HIS:CE1	1:E:284:LEU:HD22	2.55	0.42
1:F:89:ASP:O	1:F:214:PRO:HB3	2.19	0.42
1:F:211:ASN:ND2	1:F:217:ASN:HD22	2.18	0.42
1:F:291:LEU:HD23	1:F:291:LEU:HA	1.84	0.42
1:F:536:LEU:HD22	1:F:548:VAL:HG22	2.02	0.42
1:G:1154:PHE:CD1	1:G:1157:PHE:HB2	2.54	0.42
1:B:615:GLU:OE1	1:B:615:GLU:HA	2.20	0.42
1:D:106:HIS:HB2	1:D:114:PHE:CE1	2.54	0.42
1:D:1172:GLY:H	1:D:1193:LEU:H	1.67	0.42
1:F:316:PRO:HG2	1:F:338:CYS:HB2	2.02	0.42
1:H:1137:HIS:HA	1:H:1141:LEU:O	2.20	0.42
1:H:1190:LEU:HD23	1:H:1190:LEU:HA	1.92	0.42
1:H:1244:ASN:O	1:H:1250:ILE:HA	2.20	0.42
2:K:1341:SER:HG	2:K:1424:VAL:H	1.65	0.42
1:A:137:GLN:HB3	1:C:946:THR:HA	2.01	0.42
1:A:424:THR:HA	1:A:548:VAL:O	2.20	0.42
1:B:235:GLN:OE1	1:B:235:GLN:N	2.53	0.42
1:C:891:CYS:O	1:C:1016:GLN:NE2	2.52	0.42
1:D:141:LEU:HD11	1:D:166:VAL:HG11	2.02	0.42
1:D:621:TRP:CB	1:D:662:LEU:HD11	2.49	0.42
1:D:921:LEU:N	1:D:937:ILE:O	2.53	0.42
1:D:1137:HIS:HA	1:D:1141:LEU:O	2.20	0.42
1:E:341:PRO:HG3	1:E:357:ASP:HB3	2.02	0.42
1:F:106:HIS:NE2	1:F:202:GLN:OE1	2.40	0.42
1:F:235:GLN:OE1	1:F:235:GLN:N	2.53	0.42
1:F:278:VAL:O	1:F:305:TYR:OH	2.22	0.42
1:F:532:LEU:HD13	1:F:532:LEU:HA	1.90	0.42
1:H:1180:ARG:O	1:H:1182:PRO:HD3	2.19	0.42
2:I:1378:ILE:C	2:I:1378:ILE:HD12	2.40	0.42
2:L:1340:TRP:CZ3	2:L:1425:LEU:HB2	2.55	0.42
1:A:189:ASP:N	1:A:189:ASP:OD1	2.53	0.42
1:B:867:GLY:H	1:B:880:ARG:HH21	1.67	0.42
1:B:956:LYS:HB3	1:B:958:PHE:CE1	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:424:THR:HA	1:C:548:VAL:O	2.20	0.42
1:E:422:PRO:HA	1:E:550:LEU:O	2.20	0.42
1:E:615:GLU:OE1	1:E:615:GLU:HA	2.20	0.42
1:F:608:CYS:SG	1:F:649:MET:HG3	2.59	0.42
1:F:615:GLU:OE1	1:F:615:GLU:HA	2.20	0.42
1:G:883:ARG:CZ	1:G:883:ARG:HB3	2.50	0.42
1:G:1153:LEU:HD12	1:G:1153:LEU:HA	1.93	0.42
1:H:921:LEU:N	1:H:937:ILE:O	2.53	0.42
1:H:1179:CYS:N	1:H:1207:PHE:O	2.52	0.42
2:I:1340:TRP:CZ3	2:I:1425:LEU:HB2	2.55	0.42
2:J:1343:TRP:CZ3	2:J:1423:ARG:HB3	2.55	0.42
2:K:1378:ILE:C	2:K:1378:ILE:HD12	2.40	0.42
2:M:1365:ARG:HE	2:M:1371:VAL:HB	1.85	0.42
2:N:1365:ARG:HE	2:N:1371:VAL:HB	1.85	0.42
1:A:700:ARG:HH21	1:A:735:PRO:HA	1.84	0.41
1:A:852:GLU:OE2	1:A:853:GLU:HG2	2.19	0.41
1:A:1034:ILE:H	1:A:1034:ILE:HG13	1.65	0.41
1:B:167:GLU:HG3	1:B:169:SER:HB3	2.02	0.41
1:B:278:VAL:O	1:B:305:TYR:OH	2.22	0.41
1:C:751:GLU:OE1	1:C:751:GLU:N	2.52	0.41
1:D:700:ARG:HH21	1:D:735:PRO:HA	1.85	0.41
1:D:1083:LYS:HE2	1:D:1083:LYS:HB2	1.87	0.41
1:H:816:LEU:HD22	1:H:817:ARG:N	2.35	0.41
2:J:1403:ARG:HD3	2:J:1406:MET:HE1	2.02	0.41
2:K:1333:CYS:HB3	2:K:1432:CYS:HB2	1.35	0.41
2:K:1414:PRO:O	2:K:1416:LEU:N	2.53	0.41
1:A:455:CYS:HB3	1:A:559:CYS:HB2	1.60	0.41
1:A:756:ALA:O	1:A:759:THR:OG1	2.20	0.41
1:A:1004:TRP:CE3	1:A:1006:ARG:HA	2.55	0.41
1:B:316:PRO:HG2	1:B:338:CYS:HB2	2.02	0.41
1:C:184:LEU:HD22	1:C:307:ARG:HH12	1.84	0.41
1:D:254:ASN:O	1:D:256:THR:N	2.53	0.41
1:D:454:LYS:HZ2	1:D:454:LYS:HG3	1.66	0.41
1:D:753:PRO:HG2	1:D:755:TYR:CZ	2.55	0.41
1:E:539:GLN:OE1	1:E:545:GLN:NE2	2.53	0.41
1:G:921:LEU:N	1:G:937:ILE:O	2.53	0.41
1:H:817:ARG:H	1:H:817:ARG:HD2	1.86	0.41
2:N:1343:TRP:CZ3	2:N:1423:ARG:HB3	2.55	0.41
1:A:184:LEU:HD22	1:A:307:ARG:HH12	1.84	0.41
1:B:1180:ARG:O	1:B:1182:PRO:HD3	2.19	0.41
1:C:141:LEU:HD11	1:C:166:VAL:HG11	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:VAL:O	1:C:154:ARG:HD2	2.21	0.41
1:C:1049:LEU:HD12	1:C:1049:LEU:HA	1.85	0.41
1:D:189:ASP:OD1	1:D:189:ASP:N	2.53	0.41
1:D:816:LEU:HD22	1:D:817:ARG:N	2.36	0.41
1:E:235:GLN:N	1:E:235:GLN:OE1	2.53	0.41
1:F:167:GLU:HG3	1:F:169:SER:HB3	2.02	0.41
1:G:1058:SER:HG	1:G:1060:SER:HG	1.63	0.41
1:A:148:VAL:O	1:A:154:ARG:HD2	2.21	0.41
1:A:254:ASN:O	1:A:256:THR:N	2.53	0.41
1:A:867:GLY:H	1:A:880:ARG:HH21	1.67	0.41
1:A:1109:CYS:HA	1:A:1128:ALA:HB1	2.02	0.41
1:C:526:ILE:HD11	1:C:540:LEU:HD11	2.03	0.41
1:C:802:ASP:OD2	1:C:804:SER:OG	2.26	0.41
1:D:1154:PHE:CD1	1:D:1157:PHE:HB2	2.55	0.41
1:E:77:CYS:SG	1:E:193:LEU:HB2	2.60	0.41
1:F:77:CYS:SG	1:F:193:LEU:HB2	2.60	0.41
1:F:183:PHE:HD1	1:F:193:LEU:CD2	2.33	0.41
1:G:1244:ASN:O	1:G:1250:ILE:HA	2.20	0.41
1:H:814:GLU:OE1	1:H:832:VAL:HG22	2.20	0.41
1:H:883:ARG:CZ	1:H:883:ARG:HB3	2.50	0.41
2:M:1343:TRP:CZ3	2:M:1423:ARG:HB3	2.55	0.41
1:A:400:PHE:CE1	1:A:407:CYS:HB2	2.56	0.41
1:B:183:PHE:HD1	1:B:193:LEU:CD2	2.34	0.41
1:B:263:HIS:CE1	1:B:284:LEU:HD22	2.55	0.41
1:B:594:GLN:HB2	1:B:597:CYS:SG	2.61	0.41
1:C:753:PRO:HG2	1:C:755:TYR:CZ	2.55	0.41
1:D:278:VAL:O	1:D:305:TYR:OH	2.28	0.41
1:D:656:GLU:H	1:D:656:GLU:CD	2.15	0.41
1:D:817:ARG:H	1:D:817:ARG:HD2	1.86	0.41
1:D:925:TYR:OH	1:D:934:THR:O	2.26	0.41
1:E:594:GLN:HB2	1:E:597:CYS:SG	2.61	0.41
1:G:1057:LEU:HA	1:G:1057:LEU:HD23	1.75	0.41
2:L:1378:ILE:C	2:L:1378:ILE:HD12	2.40	0.41
1:A:549:ARG:CZ	1:A:549:ARG:HB2	2.51	0.41
1:B:689:THR:HA	1:B:692:MET:HG2	2.02	0.41
1:B:946:THR:HA	1:D:137:GLN:HB3	2.01	0.41
1:C:115:ASN:HB3	1:C:135:LYS:HB3	2.02	0.41
1:C:1109:CYS:HA	1:C:1128:ALA:HB1	2.02	0.41
1:D:148:VAL:O	1:D:154:ARG:HD2	2.21	0.41
1:D:178:ARG:CD	1:D:179:LEU:HD23	2.43	0.41
1:D:400:PHE:CE1	1:D:407:CYS:HB2	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:424:THR:HA	1:D:548:VAL:O	2.20	0.41
1:D:479:LYS:NZ	2:L:1413:SER:HB3	2.35	0.41
1:D:564:ASN:ND2	1:D:571:ASP:OD2	2.44	0.41
1:D:629:ASN:C	1:D:629:ASN:OD1	2.59	0.41
1:E:211:ASN:ND2	1:E:217:ASN:HD22	2.18	0.41
1:G:838:PRO:HG2	1:G:841:LEU:HD13	2.03	0.41
1:G:1160:PRO:O	1:G:1160:PRO:HD2	2.20	0.41
1:H:1208:ASN:O	1:H:1212:MET:N	2.53	0.41
1:B:77:CYS:SG	1:B:193:LEU:HB2	2.60	0.41
1:B:1109:CYS:HA	1:B:1128:ALA:HB1	2.02	0.41
1:C:911:TYR:OH	1:C:1051:PHE:HE2	2.03	0.41
1:E:581:GLU:HG3	1:E:587:PHE:HA	2.03	0.41
1:F:341:PRO:HG3	1:F:357:ASP:HB3	2.02	0.41
1:F:594:GLN:HB2	1:F:597:CYS:SG	2.61	0.41
1:G:1208:ASN:O	1:G:1212:MET:N	2.53	0.41
1:H:1146:ARG:NH1	1:H:1151:CYS:HB3	2.36	0.41
1:H:1160:PRO:O	1:H:1160:PRO:HD2	2.20	0.41
1:H:1172:GLY:H	1:H:1193:LEU:H	1.67	0.41
1:A:334:GLN:HG3	1:A:336:GLN:HG2	2.03	0.41
1:A:353:GLN:HE22	1:C:930:THR:HG23	1.86	0.41
1:A:621:TRP:CB	1:A:662:LEU:HD11	2.49	0.41
1:A:629:ASN:OD1	1:A:629:ASN:C	2.59	0.41
1:A:821:THR:OG1	1:C:595:ALA:HB2	2.21	0.41
1:C:324:LEU:HD23	1:C:324:LEU:HA	1.90	0.41
1:D:539:GLN:O	1:D:544:MET:HA	2.21	0.41
1:D:814:GLU:OE1	1:D:832:VAL:HG22	2.20	0.41
1:E:80:TRP:CE3	1:E:304:GLU:HG2	2.56	0.41
1:E:689:THR:HA	1:E:692:MET:HG2	2.02	0.41
1:F:118:LEU:HD23	1:F:129:VAL:HG11	2.03	0.41
1:G:816:LEU:HD22	1:G:817:ARG:N	2.36	0.41
1:G:852:GLU:OE1	1:G:852:GLU:N	2.47	0.41
1:H:900:ASP:O	1:H:914:GLU:HG3	2.21	0.41
2:J:1365:ARG:HE	2:J:1371:VAL:HB	1.85	0.41
2:K:1340:TRP:CZ3	2:K:1425:LEU:HB2	2.55	0.41
1:A:539:GLN:O	1:A:544:MET:HA	2.21	0.41
1:A:753:PRO:HG2	1:A:755:TYR:CZ	2.55	0.41
1:A:1020:GLY:N	1:A:1029:PHE:O	2.54	0.41
1:B:189:ASP:OD1	1:B:190:SER:N	2.54	0.41
1:B:500:VAL:HG21	1:B:509:LEU:HD11	2.01	0.41
1:B:536:LEU:HD22	1:B:548:VAL:HG22	2.02	0.41
1:B:539:GLN:OE1	1:B:545:GLN:NE2	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:656:GLU:HG3	2:J:1411:GLN:OE1	2.21	0.41
1:B:802:ASP:OD2	1:B:804:SER:OG	2.26	0.41
1:B:821:THR:OG1	1:D:595:ALA:HB2	2.21	0.41
1:B:828:SER:HB2	1:D:594:GLN:HE21	1.86	0.41
1:C:263:HIS:O	1:C:267:LEU:HB2	2.21	0.41
1:C:327:ARG:HB2	1:C:335:HIS:CD2	2.56	0.41
1:C:400:PHE:CE1	1:C:407:CYS:HB2	2.56	0.41
1:C:454:LYS:HZ2	1:C:454:LYS:HG3	1.67	0.41
1:C:651:ASP:O	1:C:655:CYS:N	2.48	0.41
1:C:690:LYS:O	1:C:693:GLN:NE2	2.54	0.41
1:C:1199:LYS:HE2	1:C:1199:LYS:HB2	1.75	0.41
1:D:549:ARG:CZ	1:D:549:ARG:HB2	2.51	0.41
1:D:670:VAL:HG21	1:D:683:TRP:CD2	2.56	0.41
1:D:1208:ASN:O	1:D:1212:MET:N	2.53	0.41
1:E:260:GLY:O	1:E:264:ARG:N	2.44	0.41
1:E:316:PRO:HG2	1:E:338:CYS:HB2	2.02	0.41
1:E:660:ASP:OD1	1:E:691:TYR:OH	2.35	0.41
1:F:263:HIS:CE1	1:F:284:LEU:HD22	2.55	0.41
1:F:324:LEU:HD23	1:F:324:LEU:HA	1.91	0.41
1:F:454:LYS:HZ2	1:F:454:LYS:HG3	1.69	0.41
1:F:539:GLN:OE1	1:F:545:GLN:NE2	2.53	0.41
2:L:1381:ARG:HG2	2:L:1421:GLU:OE1	2.21	0.41
1:A:278:VAL:O	1:A:305:TYR:OH	2.28	0.41
1:A:595:ALA:HB2	1:C:821:THR:OG1	2.21	0.41
1:A:911:TYR:OH	1:A:1051:PHE:HE2	2.03	0.41
1:B:174:LYS:HE3	1:B:182:THR:HG23	2.03	0.41
1:B:1057:LEU:HD23	1:B:1057:LEU:HA	1.77	0.41
1:B:1068:LYS:HZ2	1:B:1069:ASP:HB3	1.86	0.41
1:C:166:VAL:HG12	1:C:175:VAL:HG22	2.03	0.41
1:C:479:LYS:NZ	2:K:1413:SER:HB3	2.35	0.41
1:C:539:GLN:O	1:C:544:MET:HA	2.21	0.41
1:C:1020:GLY:N	1:C:1029:PHE:O	2.54	0.41
1:D:99:CYS:H	1:D:101:TYR:HE1	1.69	0.41
1:D:690:LYS:O	1:D:693:GLN:NE2	2.54	0.41
1:D:745:ALA:HB3	2:J:1387:ASP:OD2	2.21	0.41
1:D:763:PRO:CD	2:J:1384:GLN:NE2	2.81	0.41
1:D:838:PRO:HG2	1:D:841:LEU:HD13	2.03	0.41
1:D:852:GLU:OE2	1:D:853:GLU:HG2	2.21	0.41
1:E:414:TRP:HD1	1:G:1041:SER:HG	1.65	0.41
1:E:656:GLU:HG3	2:M:1411:GLN:OE1	2.21	0.41
1:F:422:PRO:HA	1:F:550:LEU:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:689:THR:HA	1:F:692:MET:HG2	2.02	0.41
1:G:874:CYS:O	1:G:889:ARG:NH2	2.54	0.41
1:G:900:ASP:O	1:G:914:GLU:HG3	2.21	0.41
1:A:166:VAL:HG12	1:A:175:VAL:HG22	2.03	0.40
1:B:80:TRP:CE3	1:B:304:GLU:HG2	2.56	0.40
1:C:216:PHE:CD1	1:C:216:PHE:O	2.74	0.40
1:D:216:PHE:O	1:D:216:PHE:CD1	2.74	0.40
1:D:764:GLY:N	1:D:776:CYS:O	2.36	0.40
1:D:1146:ARG:NH1	1:D:1151:CYS:HB3	2.36	0.40
1:E:524:PHE:CD2	1:E:731:GLY:HA2	2.56	0.40
1:F:189:ASP:OD1	1:F:190:SER:N	2.54	0.40
1:F:660:ASP:OD1	1:F:691:TYR:OH	2.35	0.40
2:K:1381:ARG:HG2	2:K:1421:GLU:OE1	2.21	0.40
1:A:289:GLN:O	1:A:292:CYS:HB2	2.22	0.40
1:A:560:GLY:HA2	1:A:591:TRP:CE2	2.57	0.40
1:B:324:LEU:HD23	1:B:324:LEU:HA	1.91	0.40
1:B:581:GLU:HG3	1:B:587:PHE:HA	2.03	0.40
1:C:165:LEU:HG	1:C:167:GLU:OE1	2.21	0.40
1:C:752:CYS:O	1:C:763:PRO:HG3	2.21	0.40
1:D:324:LEU:HD23	1:D:324:LEU:HA	1.90	0.40
1:D:526:ILE:HD11	1:D:540:LEU:HD11	2.03	0.40
1:E:183:PHE:HD1	1:E:193:LEU:CD2	2.34	0.40
1:E:455:CYS:HB3	1:E:559:CYS:HB2	1.67	0.40
1:E:712:CYS:O	1:E:715:LEU:HG	2.22	0.40
1:F:751:GLU:OE1	1:F:751:GLU:N	2.54	0.40
1:G:814:GLU:OE1	1:G:832:VAL:HG22	2.20	0.40
1:H:802:ASP:HA	1:H:833:SER:OG	2.22	0.40
2:M:1381:ARG:CZ	2:M:1386:PRO:HB3	2.52	0.40
1:A:141:LEU:HD11	1:A:166:VAL:HG11	2.02	0.40
1:A:327:ARG:HB2	1:A:335:HIS:CD2	2.56	0.40
1:A:752:CYS:O	1:A:763:PRO:HG3	2.21	0.40
1:A:1068:LYS:HZ2	1:A:1069:ASP:HB3	1.86	0.40
1:B:118:LEU:HD23	1:B:129:VAL:HG11	2.03	0.40
1:B:422:PRO:HA	1:B:550:LEU:O	2.20	0.40
1:B:822:LEU:HD12	1:B:842:VAL:HG11	2.04	0.40
1:C:670:VAL:HG21	1:C:683:TRP:CD2	2.56	0.40
1:D:874:CYS:O	1:D:889:ARG:NH2	2.54	0.40
1:D:900:ASP:O	1:D:914:GLU:HG3	2.21	0.40
1:G:904:ILE:HA	1:G:909:ASP:O	2.22	0.40
2:L:1393:LEU:HB3	2:L:1395:GLN:HG2	2.04	0.40
1:A:88:PHE:CE1	1:A:195:LEU:HD23	2.57	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:958:PHE:CE1	1:A:963:GLU:HG2	2.57	0.40
1:B:341:PRO:HG3	1:B:357:ASP:HB3	2.02	0.40
1:B:524:PHE:CD2	1:B:731:GLY:HA2	2.56	0.40
1:B:751:GLU:N	1:B:751:GLU:OE1	2.54	0.40
1:C:183:PHE:HD1	1:C:193:LEU:CD2	2.34	0.40
1:C:245:PRO:HD3	2:M:1403:ARG:HH22	1.87	0.40
1:C:289:GLN:O	1:C:292:CYS:HB2	2.22	0.40
1:C:560:GLY:HA2	1:C:591:TRP:CE2	2.57	0.40
1:C:710:PRO:HB2	1:C:739:PHE:CD2	2.57	0.40
1:C:822:LEU:HD12	1:C:842:VAL:HG11	2.04	0.40
1:C:958:PHE:CE1	1:C:963:GLU:HG2	2.57	0.40
1:D:165:LEU:HG	1:D:167:GLU:OE1	2.21	0.40
1:D:327:ARG:HB2	1:D:335:HIS:CD2	2.56	0.40
1:D:710:PRO:HB2	1:D:739:PHE:CD2	2.57	0.40
1:D:1171:CYS:HB3	1:D:1192:GLY:HA3	2.03	0.40
1:E:751:GLU:N	1:E:751:GLU:OE1	2.54	0.40
1:F:80:TRP:CE3	1:F:304:GLU:HG2	2.56	0.40
1:F:581:GLU:HG3	1:F:587:PHE:HA	2.03	0.40
1:F:656:GLU:HG3	2:N:1411:GLN:OE1	2.21	0.40
1:H:1040:ARG:HG2	1:H:1055:TRP:CZ3	2.56	0.40
1:A:216:PHE:CD2	1:A:216:PHE:O	2.74	0.40
1:A:245:PRO:HD3	2:J:1403:ARG:HH22	1.86	0.40
1:A:700:ARG:HD2	1:A:701:TYR:O	2.22	0.40
1:B:1154:PHE:HB2	1:H:1152:PRO:CB	2.52	0.40
1:D:166:VAL:HG12	1:D:175:VAL:HG22	2.03	0.40
1:D:183:PHE:HD1	1:D:193:LEU:CD2	2.34	0.40
1:D:245:PRO:HD3	2:N:1403:ARG:HH22	1.87	0.40
1:D:747:VAL:HG23	1:D:748:PRO:O	2.22	0.40
1:D:904:ILE:HA	1:D:909:ASP:O	2.22	0.40
1:D:1040:ARG:HG2	1:D:1055:TRP:CZ3	2.56	0.40
1:D:1049:LEU:HA	1:D:1049:LEU:HD12	1.83	0.40
1:E:167:GLU:HG3	1:E:169:SER:HB3	2.02	0.40
1:F:524:PHE:CD2	1:F:731:GLY:HA2	2.56	0.40
1:G:1146:ARG:NH1	1:G:1151:CYS:HB3	2.36	0.40
1:H:874:CYS:O	1:H:889:ARG:NH2	2.54	0.40
1:H:904:ILE:HA	1:H:909:ASP:O	2.22	0.40
2:N:1381:ARG:CZ	2:N:1386:PRO:HB3	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	1164/1227 (95%)	1067 (92%)	97 (8%)	0	100	100
1	B	1164/1227 (95%)	1072 (92%)	92 (8%)	0	100	100
1	C	1164/1227 (95%)	1068 (92%)	96 (8%)	0	100	100
1	D	1164/1227 (95%)	1067 (92%)	97 (8%)	0	100	100
1	E	715/1227 (58%)	667 (93%)	48 (7%)	0	100	100
1	F	715/1227 (58%)	668 (93%)	47 (7%)	0	100	100
1	G	449/1227 (37%)	405 (90%)	44 (10%)	0	100	100
1	H	449/1227 (37%)	404 (90%)	45 (10%)	0	100	100
2	I	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
2	J	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
2	K	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
2	L	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
2	M	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
2	N	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
All	All	7572/10416 (73%)	6988 (92%)	584 (8%)	0	100	100

There are no Ramachandran outliers to report.

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	974/1023 (95%)	915 (94%)	59 (6%)	15	46
1	B	974/1023 (95%)	910 (93%)	64 (7%)	14	43
1	C	974/1023 (95%)	916 (94%)	58 (6%)	16	47
1	D	974/1023 (95%)	921 (95%)	53 (5%)	18	50
1	E	598/1023 (58%)	561 (94%)	37 (6%)	15	45
1	F	598/1023 (58%)	561 (94%)	37 (6%)	15	45
1	G	376/1023 (37%)	354 (94%)	22 (6%)	16	47
1	H	376/1023 (37%)	354 (94%)	22 (6%)	16	47
2	I	86/88 (98%)	79 (92%)	7 (8%)	9	34
2	J	86/88 (98%)	81 (94%)	5 (6%)	17	48
2	K	86/88 (98%)	79 (92%)	7 (8%)	9	34
2	L	86/88 (98%)	79 (92%)	7 (8%)	9	34
2	M	86/88 (98%)	81 (94%)	5 (6%)	17	48
2	N	86/88 (98%)	80 (93%)	6 (7%)	12	41
All	All	6360/8712 (73%)	5971 (94%)	389 (6%)	18	46

All (389) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	LYS
1	A	89	ASP
1	A	99	CYS
1	A	116	VAL
1	A	126	ARG
1	A	131	ARG
1	A	139	LEU
1	A	145	ASN
1	A	167	GLU
1	A	171	ASP
1	A	179	LEU
1	A	186	ASN
1	A	210	PHE
1	A	216	PHE
1	A	219	PHE
1	A	226	LEU
1	A	255	CYS
1	A	293	ARG
1	A	294	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	324	LEU
1	A	345	THR
1	A	361	ASP
1	A	479	LYS
1	A	511	LEU
1	A	571	ASP
1	A	604	PHE
1	A	611	SER
1	A	700	ARG
1	A	711	THR
1	A	741	ASN
1	A	752	CYS
1	A	768	HIS
1	A	794	CYS
1	A	798	MET
1	A	817	ARG
1	A	820	HIS
1	A	855	CYS
1	A	871	ARG
1	A	905	THR
1	A	932	HIS
1	A	940	GLU
1	A	1000	MET
1	A	1003	SER
1	A	1019	LYS
1	A	1021	ARG
1	A	1031	ASP
1	A	1035	ASN
1	A	1036	ASP
1	A	1042	ARG
1	A	1061	CYS
1	A	1083	LYS
1	A	1145	TRP
1	A	1156	ASP
1	A	1158	TYR
1	A	1164	CYS
1	A	1165	GLU
1	A	1179	CYS
1	A	1196	CYS
1	A	1220	CYS
1	B	87	THR
1	B	89	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	99	CYS
1	B	116	VAL
1	B	120	ARG
1	B	122	LEU
1	B	125	SER
1	B	145	ASN
1	B	171	ASP
1	B	172	TYR
1	B	186	ASN
1	B	210	PHE
1	B	216	PHE
1	B	219	PHE
1	B	318	ASN
1	B	340	SER
1	B	388	THR
1	B	418	ASP
1	B	426	SER
1	B	442	ASP
1	B	472	THR
1	B	479	LYS
1	B	571	ASP
1	B	583	THR
1	B	603	SER
1	B	604	PHE
1	B	611	SER
1	B	697	LYS
1	B	709	GLN
1	B	711	THR
1	B	719	ASP
1	B	720	VAL
1	B	742	ASP
1	B	768	HIS
1	B	773	VAL
1	B	780	LYS
1	B	781	LEU
1	B	794	CYS
1	B	798	MET
1	B	817	ARG
1	B	820	HIS
1	B	855	CYS
1	B	871	ARG
1	B	905	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	932	HIS
1	B	940	GLU
1	B	1000	MET
1	B	1003	SER
1	B	1019	LYS
1	B	1021	ARG
1	B	1031	ASP
1	B	1035	ASN
1	B	1036	ASP
1	B	1042	ARG
1	B	1061	CYS
1	B	1083	LYS
1	B	1145	TRP
1	B	1156	ASP
1	B	1158	TYR
1	B	1164	CYS
1	B	1165	GLU
1	B	1179	CYS
1	B	1196	CYS
1	B	1220	CYS
1	C	86	LYS
1	C	89	ASP
1	C	99	CYS
1	C	116	VAL
1	C	126	ARG
1	C	131	ARG
1	C	139	LEU
1	C	145	ASN
1	C	167	GLU
1	C	171	ASP
1	C	179	LEU
1	C	186	ASN
1	C	210	PHE
1	C	219	PHE
1	C	226	LEU
1	C	255	CYS
1	C	293	ARG
1	C	294	CYS
1	C	324	LEU
1	C	345	THR
1	C	361	ASP
1	C	479	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	511	LEU
1	C	571	ASP
1	C	604	PHE
1	C	611	SER
1	C	700	ARG
1	C	711	THR
1	C	741	ASN
1	C	752	CYS
1	C	768	HIS
1	C	794	CYS
1	C	798	MET
1	C	817	ARG
1	C	820	HIS
1	C	855	CYS
1	C	871	ARG
1	C	905	THR
1	C	932	HIS
1	C	940	GLU
1	C	1000	MET
1	C	1003	SER
1	C	1019	LYS
1	C	1021	ARG
1	C	1031	ASP
1	C	1035	ASN
1	C	1036	ASP
1	C	1042	ARG
1	C	1061	CYS
1	C	1083	LYS
1	C	1145	TRP
1	C	1156	ASP
1	C	1158	TYR
1	C	1164	CYS
1	C	1165	GLU
1	C	1179	CYS
1	C	1196	CYS
1	C	1220	CYS
1	D	86	LYS
1	D	89	ASP
1	D	99	CYS
1	D	116	VAL
1	D	126	ARG
1	D	131	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	139	LEU
1	D	145	ASN
1	D	167	GLU
1	D	171	ASP
1	D	179	LEU
1	D	186	ASN
1	D	210	PHE
1	D	219	PHE
1	D	226	LEU
1	D	255	CYS
1	D	293	ARG
1	D	294	CYS
1	D	324	LEU
1	D	345	THR
1	D	361	ASP
1	D	479	LYS
1	D	511	LEU
1	D	571	ASP
1	D	604	PHE
1	D	611	SER
1	D	700	ARG
1	D	711	THR
1	D	741	ASN
1	D	752	CYS
1	D	768	HIS
1	D	798	MET
1	D	816	LEU
1	D	817	ARG
1	D	820	HIS
1	D	932	HIS
1	D	940	GLU
1	D	976	ARG
1	D	987	ARG
1	D	998	HIS
1	D	1000	MET
1	D	1003	SER
1	D	1019	LYS
1	D	1031	ASP
1	D	1042	ARG
1	D	1061	CYS
1	D	1077	ARG
1	D	1083	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	1145	TRP
1	D	1179	CYS
1	D	1210	ASP
1	D	1220	CYS
1	D	1222	ASP
1	E	87	THR
1	E	89	ASP
1	E	99	CYS
1	E	116	VAL
1	E	120	ARG
1	E	122	LEU
1	E	125	SER
1	E	145	ASN
1	E	171	ASP
1	E	172	TYR
1	E	186	ASN
1	E	210	PHE
1	E	216	PHE
1	E	219	PHE
1	E	318	ASN
1	E	340	SER
1	E	388	THR
1	E	418	ASP
1	E	426	SER
1	E	442	ASP
1	E	472	THR
1	E	479	LYS
1	E	571	ASP
1	E	583	THR
1	E	603	SER
1	E	604	PHE
1	E	611	SER
1	E	697	LYS
1	E	709	GLN
1	E	711	THR
1	E	719	ASP
1	E	720	VAL
1	E	742	ASP
1	E	768	HIS
1	E	773	VAL
1	E	780	LYS
1	E	781	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	87	THR
1	F	89	ASP
1	F	99	CYS
1	F	116	VAL
1	F	120	ARG
1	F	122	LEU
1	F	125	SER
1	F	145	ASN
1	F	171	ASP
1	F	172	TYR
1	F	186	ASN
1	F	210	PHE
1	F	216	PHE
1	F	219	PHE
1	F	318	ASN
1	F	340	SER
1	F	388	THR
1	F	418	ASP
1	F	426	SER
1	F	442	ASP
1	F	472	THR
1	F	479	LYS
1	F	571	ASP
1	F	583	THR
1	F	603	SER
1	F	604	PHE
1	F	611	SER
1	F	697	LYS
1	F	709	GLN
1	F	711	THR
1	F	719	ASP
1	F	720	VAL
1	F	742	ASP
1	F	768	HIS
1	F	773	VAL
1	F	780	LYS
1	F	781	LEU
1	G	798	MET
1	G	816	LEU
1	G	817	ARG
1	G	820	HIS
1	G	932	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	940	GLU
1	G	976	ARG
1	G	987	ARG
1	G	998	HIS
1	G	1000	MET
1	G	1003	SER
1	G	1019	LYS
1	G	1031	ASP
1	G	1042	ARG
1	G	1061	CYS
1	G	1077	ARG
1	G	1083	LYS
1	G	1145	TRP
1	G	1179	CYS
1	G	1210	ASP
1	G	1220	CYS
1	G	1222	ASP
1	H	798	MET
1	H	816	LEU
1	H	817	ARG
1	H	820	HIS
1	H	932	HIS
1	H	940	GLU
1	H	976	ARG
1	H	987	ARG
1	H	998	HIS
1	H	1000	MET
1	H	1003	SER
1	H	1019	LYS
1	H	1031	ASP
1	H	1042	ARG
1	H	1061	CYS
1	H	1077	ARG
1	H	1083	LYS
1	H	1145	TRP
1	H	1179	CYS
1	H	1210	ASP
1	H	1220	CYS
1	H	1222	ASP
2	I	1363	ASN
2	I	1375	LEU
2	I	1399	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	I	1401	ARG
2	I	1406	MET
2	I	1421	GLU
2	I	1422	LEU
2	J	1336	GLU
2	J	1343	TRP
2	J	1388	MET
2	J	1406	MET
2	J	1422	LEU
2	K	1363	ASN
2	K	1375	LEU
2	K	1399	CYS
2	K	1401	ARG
2	K	1406	MET
2	K	1421	GLU
2	K	1422	LEU
2	L	1363	ASN
2	L	1375	LEU
2	L	1399	CYS
2	L	1401	ARG
2	L	1406	MET
2	L	1421	GLU
2	L	1422	LEU
2	M	1336	GLU
2	M	1343	TRP
2	M	1375	LEU
2	M	1406	MET
2	M	1422	LEU
2	N	1336	GLU
2	N	1343	TRP
2	N	1375	LEU
2	N	1388	MET
2	N	1406	MET
2	N	1422	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	168	GLN
1	A	217	ASN
1	A	332	ASN
1	A	476	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	545	GLN
1	A	569	GLN
1	A	654	ASN
1	A	694	ASN
1	A	757	HIS
1	A	881	ASN
1	A	998	HIS
1	B	217	ASN
1	B	476	ASN
1	B	495	GLN
1	B	545	GLN
1	B	569	GLN
1	B	594	GLN
1	B	616	ASN
1	B	654	ASN
1	B	881	ASN
1	C	168	GLN
1	C	217	ASN
1	C	332	ASN
1	C	476	ASN
1	C	545	GLN
1	C	569	GLN
1	C	654	ASN
1	C	694	ASN
1	C	757	HIS
1	C	881	ASN
1	C	998	HIS
1	D	168	GLN
1	D	217	ASN
1	D	332	ASN
1	D	476	ASN
1	D	545	GLN
1	D	569	GLN
1	D	594	GLN
1	D	654	ASN
1	D	694	ASN
1	D	757	HIS
1	D	881	ASN
1	D	929	ASN
1	E	217	ASN
1	E	476	ASN
1	E	495	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	545	GLN
1	E	569	GLN
1	E	594	GLN
1	E	616	ASN
1	E	654	ASN
1	F	217	ASN
1	F	476	ASN
1	F	495	GLN
1	F	545	GLN
1	F	569	GLN
1	F	594	GLN
1	F	616	ASN
1	F	654	ASN
1	G	881	ASN
1	G	929	ASN
1	H	881	ASN
1	H	929	ASN
2	I	1418	HIS
2	J	1363	ASN
2	K	1418	HIS
2	L	1418	HIS
2	M	1363	ASN
2	N	1363	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 51 ligands modelled in this entry, 24 are monoatomic - leaving 27 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	B	2007	1	14,14,15	0.39	0	17,19,21	0.61	0
4	NAG	B	2004	1	14,14,15	0.23	0	17,19,21	0.55	0
4	NAG	E	1306	1	14,14,15	0.40	0	17,19,21	0.61	0
4	NAG	C	2008	1	14,14,15	0.32	0	17,19,21	0.43	0
4	NAG	D	2006	1	14,14,15	0.31	0	17,19,21	0.49	0
4	NAG	F	1304	1	14,14,15	0.20	0	17,19,21	0.53	0
4	NAG	A	2008	1	14,14,15	0.32	0	17,19,21	0.42	0
4	NAG	F	1305	1	14,14,15	0.35	0	17,19,21	0.59	0
4	NAG	D	2005	1	14,14,15	0.32	0	17,19,21	0.55	0
4	NAG	C	2005	1	14,14,15	0.30	0	17,19,21	0.54	0
4	NAG	F	1303	1	14,14,15	0.23	0	17,19,21	0.54	0
4	NAG	A	2004	1	14,14,15	0.23	0	17,19,21	0.50	0
4	NAG	A	2005	1	14,14,15	0.31	0	17,19,21	0.55	0
4	NAG	B	2006	1	14,14,15	0.35	0	17,19,21	0.59	0
4	NAG	C	2006	1	14,14,15	0.30	0	17,19,21	0.49	0
4	NAG	D	2004	1	14,14,15	0.23	0	17,19,21	0.50	0
4	NAG	A	2006	1	14,14,15	0.30	0	17,19,21	0.49	0
4	NAG	F	1306	1	14,14,15	0.39	0	17,19,21	0.61	0
4	NAG	C	2007	1	14,14,15	0.37	0	17,19,21	0.61	0
4	NAG	C	2004	1	14,14,15	0.23	0	17,19,21	0.50	0
4	NAG	A	2007	1	14,14,15	0.38	0	17,19,21	0.61	0
4	NAG	D	2007	1	14,14,15	0.37	0	17,19,21	0.61	0
4	NAG	E	1303	1	14,14,15	0.24	0	17,19,21	0.54	0
4	NAG	E	1305	1	14,14,15	0.36	0	17,19,21	0.59	0
4	NAG	E	1304	1	14,14,15	0.21	0	17,19,21	0.52	0
4	NAG	B	2005	1	14,14,15	0.21	0	17,19,21	0.53	0
4	NAG	B	2008	1	14,14,15	0.32	0	17,19,21	0.43	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	2007	1	-	4/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	2004	1	-	2/6/23/26	0/1/1/1
4	NAG	E	1306	1	-	4/6/23/26	0/1/1/1
4	NAG	C	2008	1	-	0/6/23/26	0/1/1/1
4	NAG	D	2006	1	-	2/6/23/26	0/1/1/1
4	NAG	F	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2008	1	-	0/6/23/26	0/1/1/1
4	NAG	F	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	D	2005	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2005	1	-	2/6/23/26	0/1/1/1
4	NAG	F	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2004	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2005	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2006	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2006	1	-	2/6/23/26	0/1/1/1
4	NAG	D	2004	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2006	1	-	2/6/23/26	0/1/1/1
4	NAG	F	1306	1	-	4/6/23/26	0/1/1/1
4	NAG	C	2007	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2004	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2007	1	-	2/6/23/26	0/1/1/1
4	NAG	D	2007	1	-	2/6/23/26	0/1/1/1
4	NAG	E	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	E	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	E	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2005	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2008	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	2006	NAG	C4-C5-C6-O6
4	E	1305	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	F	1305	NAG	C4-C5-C6-O6
4	A	2006	NAG	C4-C5-C6-O6
4	C	2006	NAG	C4-C5-C6-O6
4	D	2006	NAG	C4-C5-C6-O6
4	B	2006	NAG	O5-C5-C6-O6
4	F	1305	NAG	O5-C5-C6-O6
4	E	1305	NAG	O5-C5-C6-O6
4	A	2006	NAG	O5-C5-C6-O6
4	C	2006	NAG	O5-C5-C6-O6
4	D	2006	NAG	O5-C5-C6-O6
4	A	2004	NAG	C8-C7-N2-C2
4	A	2004	NAG	O7-C7-N2-C2
4	B	2004	NAG	C8-C7-N2-C2
4	B	2004	NAG	O7-C7-N2-C2
4	C	2004	NAG	C8-C7-N2-C2
4	C	2004	NAG	O7-C7-N2-C2
4	D	2004	NAG	C8-C7-N2-C2
4	D	2004	NAG	O7-C7-N2-C2
4	E	1303	NAG	C8-C7-N2-C2
4	E	1303	NAG	O7-C7-N2-C2
4	F	1303	NAG	C8-C7-N2-C2
4	F	1303	NAG	O7-C7-N2-C2
4	E	1306	NAG	C4-C5-C6-O6
4	B	2007	NAG	C4-C5-C6-O6
4	F	1306	NAG	C4-C5-C6-O6
4	A	2005	NAG	C1-C2-N2-C7
4	B	2005	NAG	C1-C2-N2-C7
4	B	2007	NAG	C1-C2-N2-C7
4	C	2005	NAG	C1-C2-N2-C7
4	D	2005	NAG	C1-C2-N2-C7
4	E	1304	NAG	C1-C2-N2-C7
4	E	1306	NAG	C1-C2-N2-C7
4	F	1304	NAG	C1-C2-N2-C7
4	F	1306	NAG	C1-C2-N2-C7
4	A	2005	NAG	C3-C2-N2-C7
4	A	2007	NAG	C3-C2-N2-C7
4	C	2005	NAG	C3-C2-N2-C7
4	C	2007	NAG	C3-C2-N2-C7
4	D	2005	NAG	C3-C2-N2-C7
4	D	2007	NAG	C3-C2-N2-C7
4	B	2007	NAG	O5-C5-C6-O6
4	E	1306	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	F	1306	NAG	O5-C5-C6-O6
4	A	2007	NAG	C1-C2-N2-C7
4	C	2007	NAG	C1-C2-N2-C7
4	D	2007	NAG	C1-C2-N2-C7
4	B	2005	NAG	C3-C2-N2-C7
4	B	2007	NAG	C3-C2-N2-C7
4	E	1304	NAG	C3-C2-N2-C7
4	E	1306	NAG	C3-C2-N2-C7
4	F	1304	NAG	C3-C2-N2-C7
4	F	1306	NAG	C3-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	1305	NAG	1	0
4	B	2006	NAG	1	0
4	E	1305	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

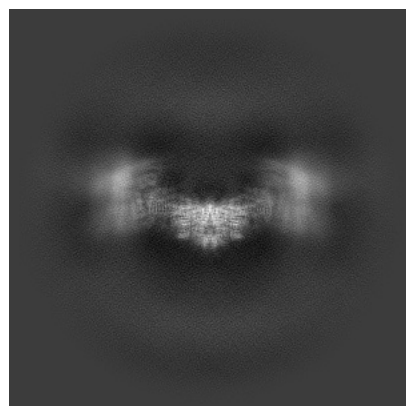
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16808. These allow visual inspection of the internal detail of the map and identification of artifacts.

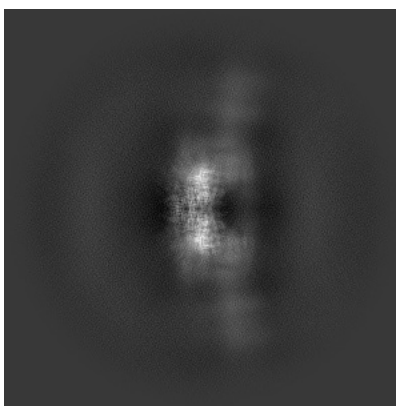
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

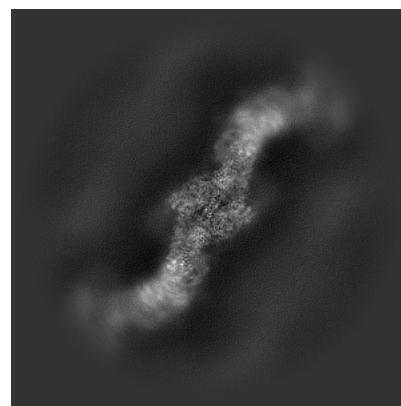
6.1.1 Primary map



X

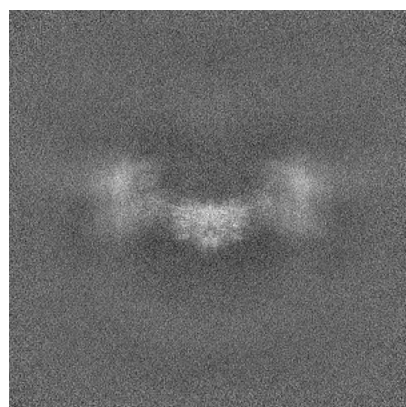


Y

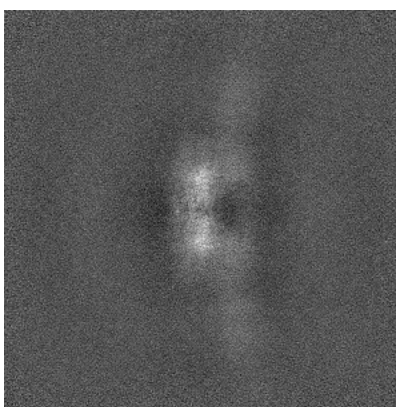


Z

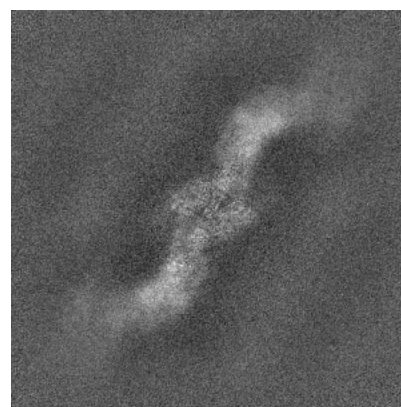
6.1.2 Raw map



X



Y

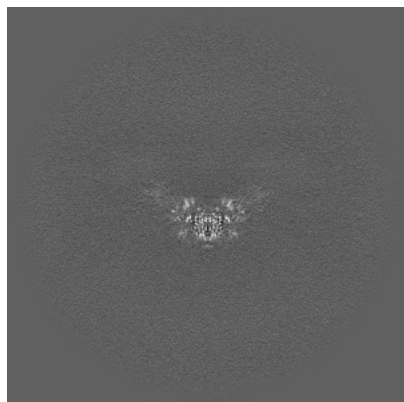


Z

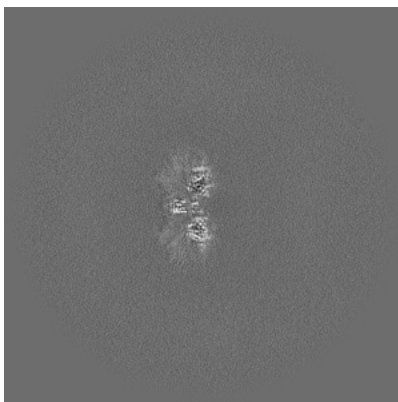
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

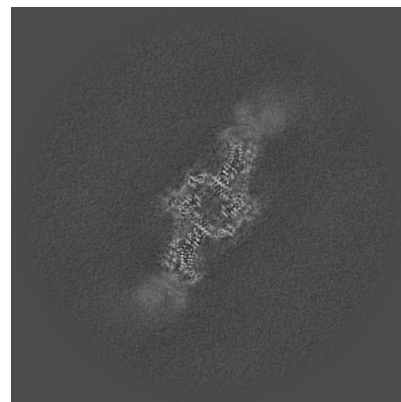
6.2.1 Primary map



X Index: 350

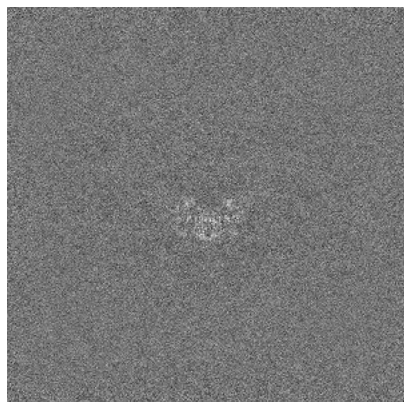


Y Index: 350

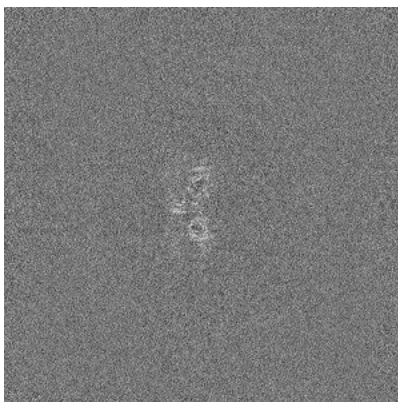


Z Index: 350

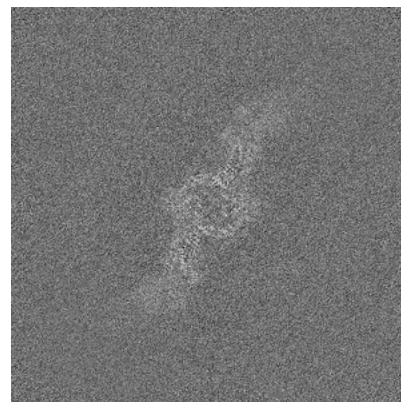
6.2.2 Raw map



X Index: 350



Y Index: 350

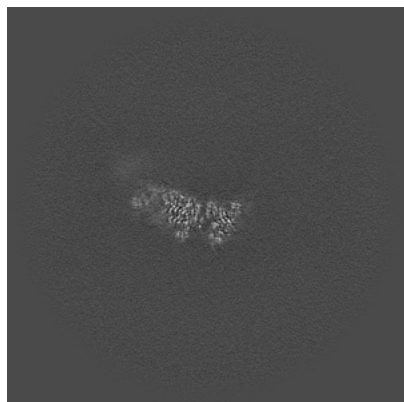


Z Index: 350

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

6.3 Largest variance slices [i](#)

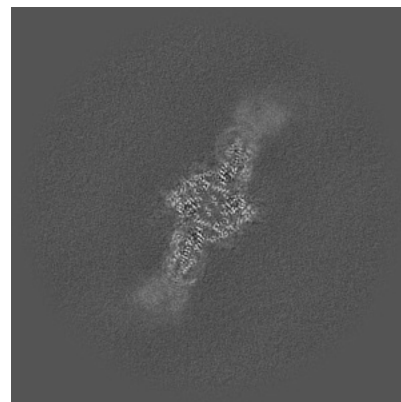
6.3.1 Primary map



X Index: 328

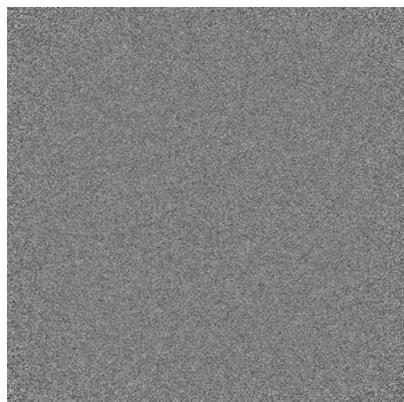


Y Index: 353

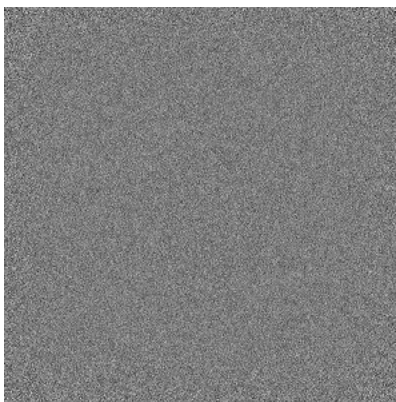


Z Index: 343

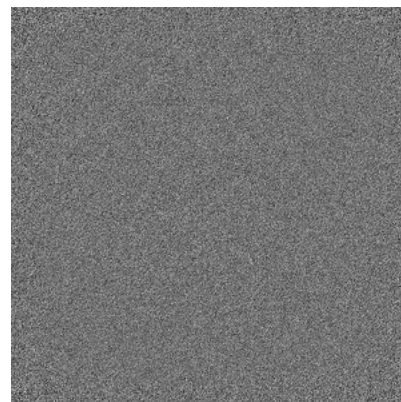
6.3.2 Raw map



X Index: 0



Y Index: 0

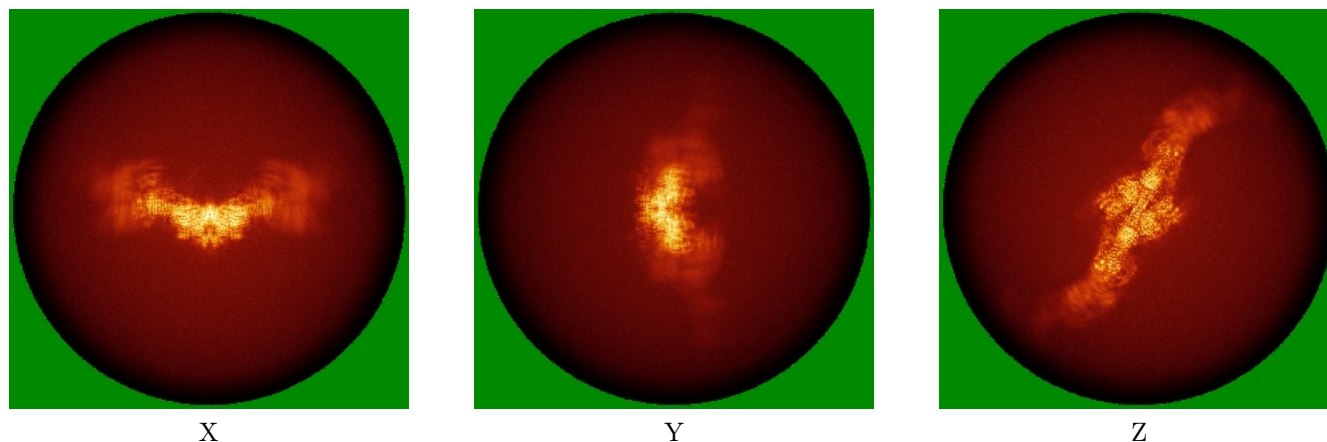


Z Index: 0

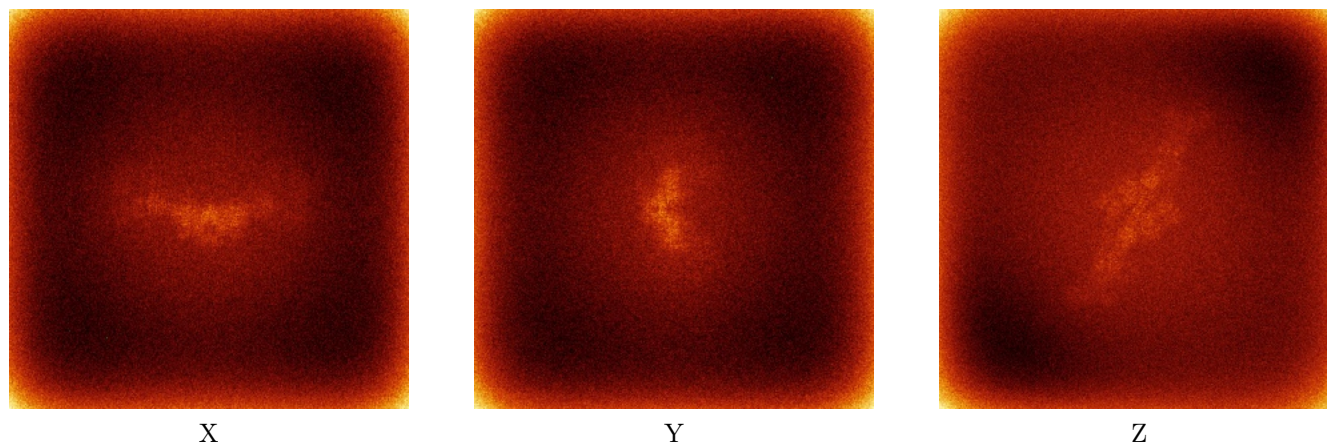
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



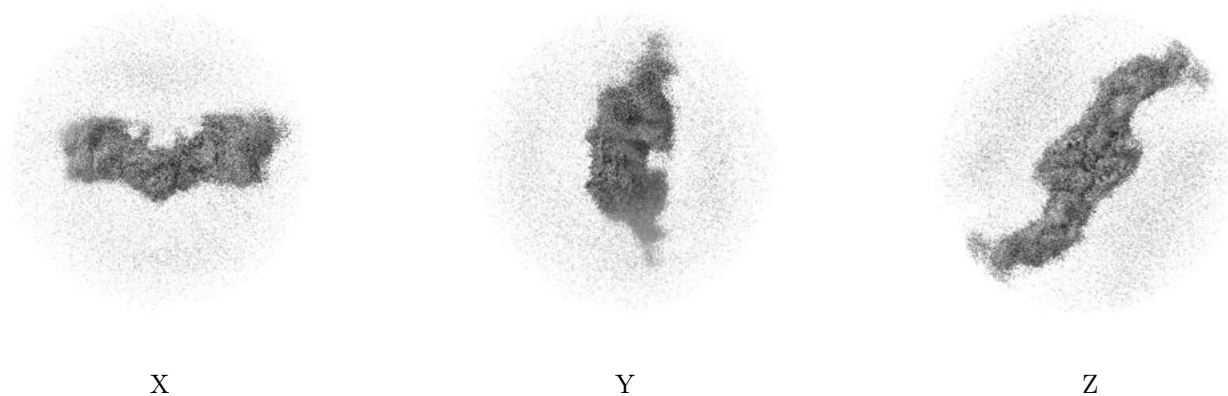
6.4.2 Raw map



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

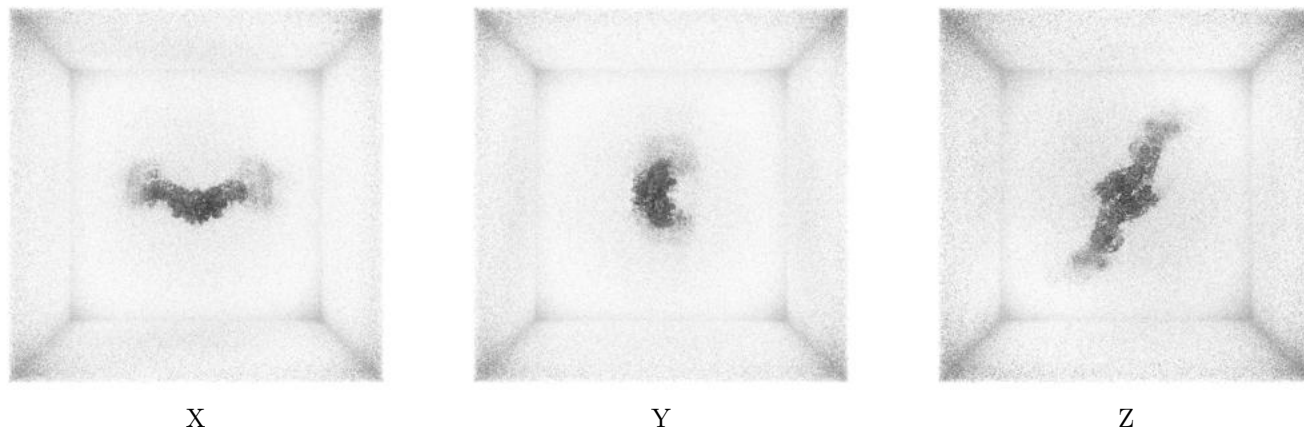
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.056. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

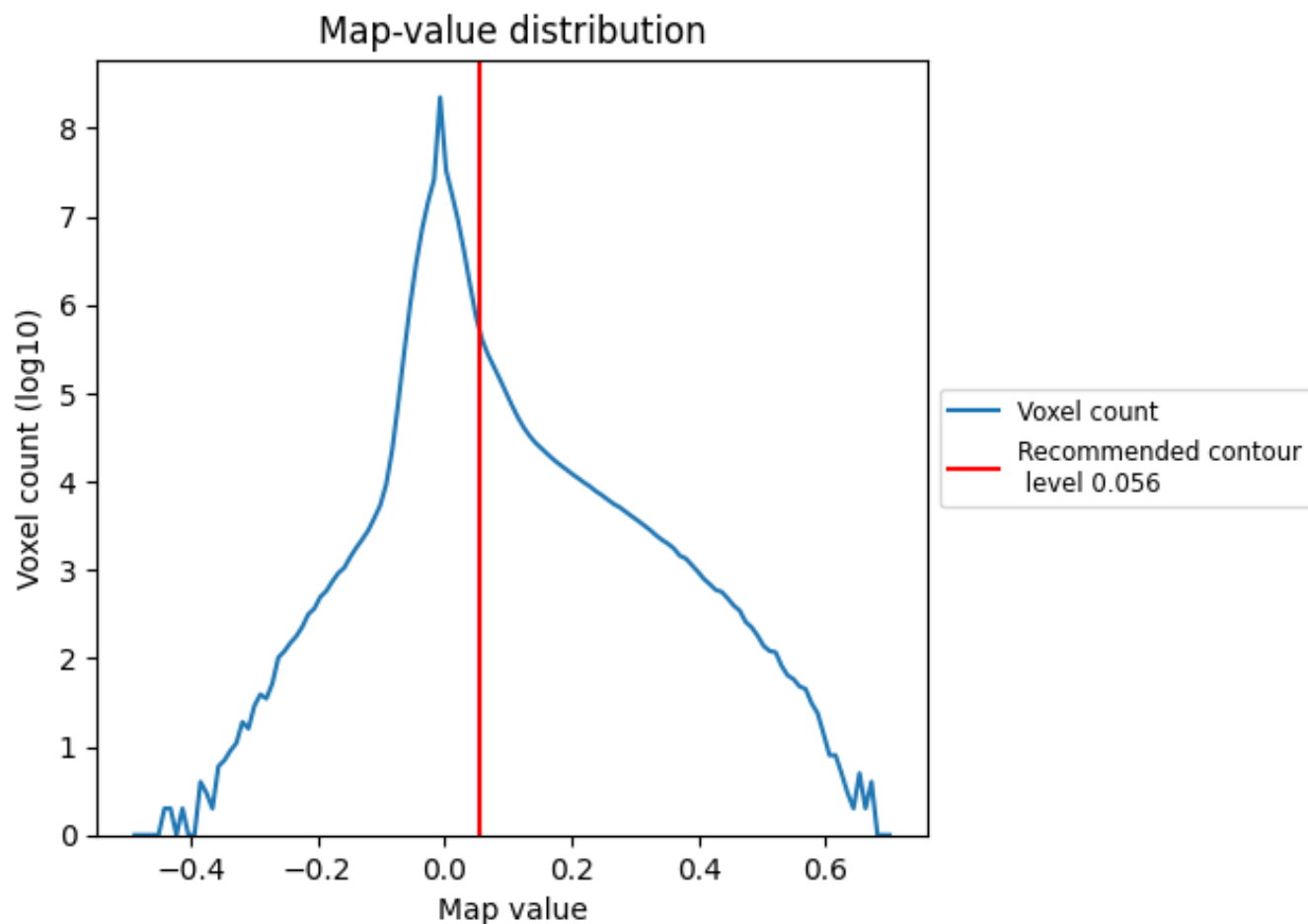
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

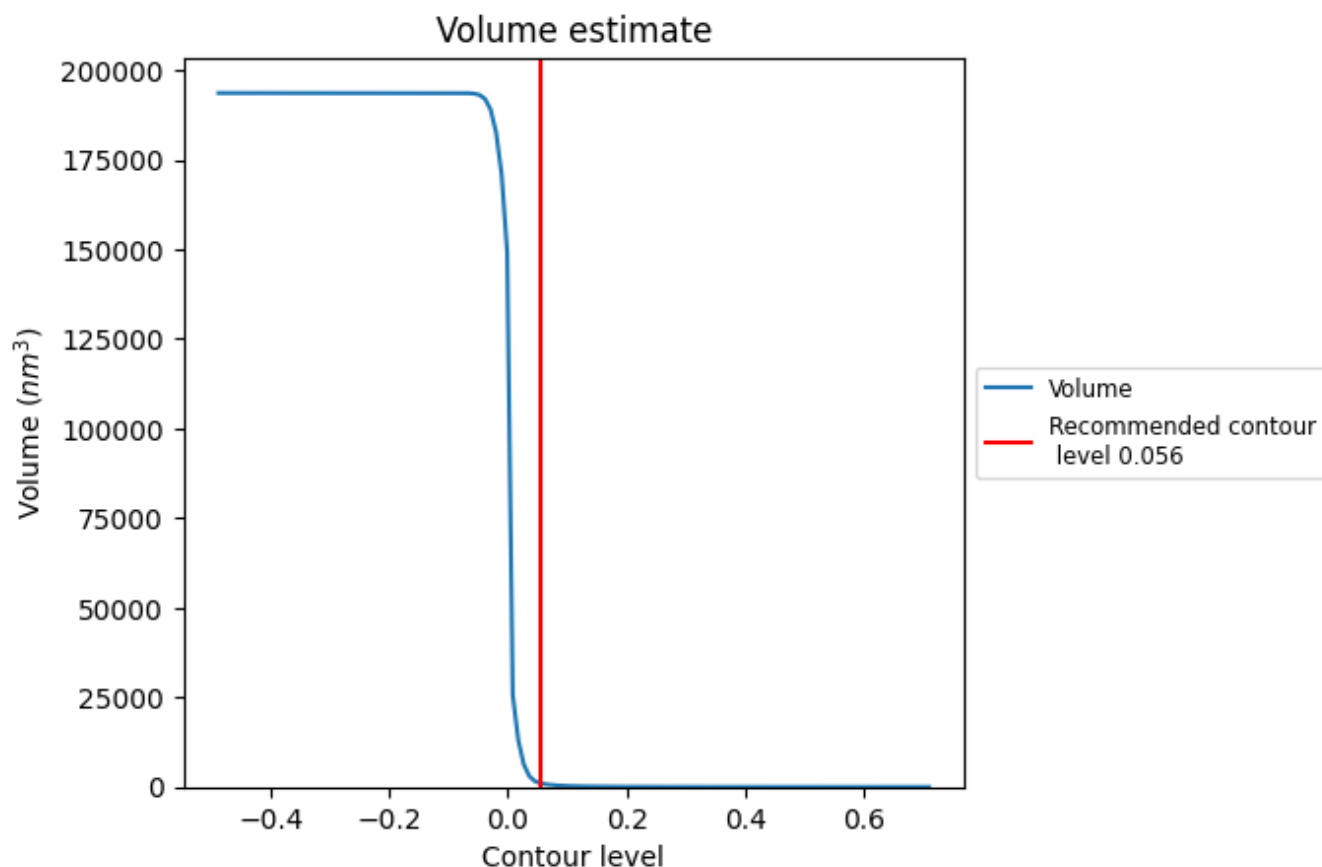
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

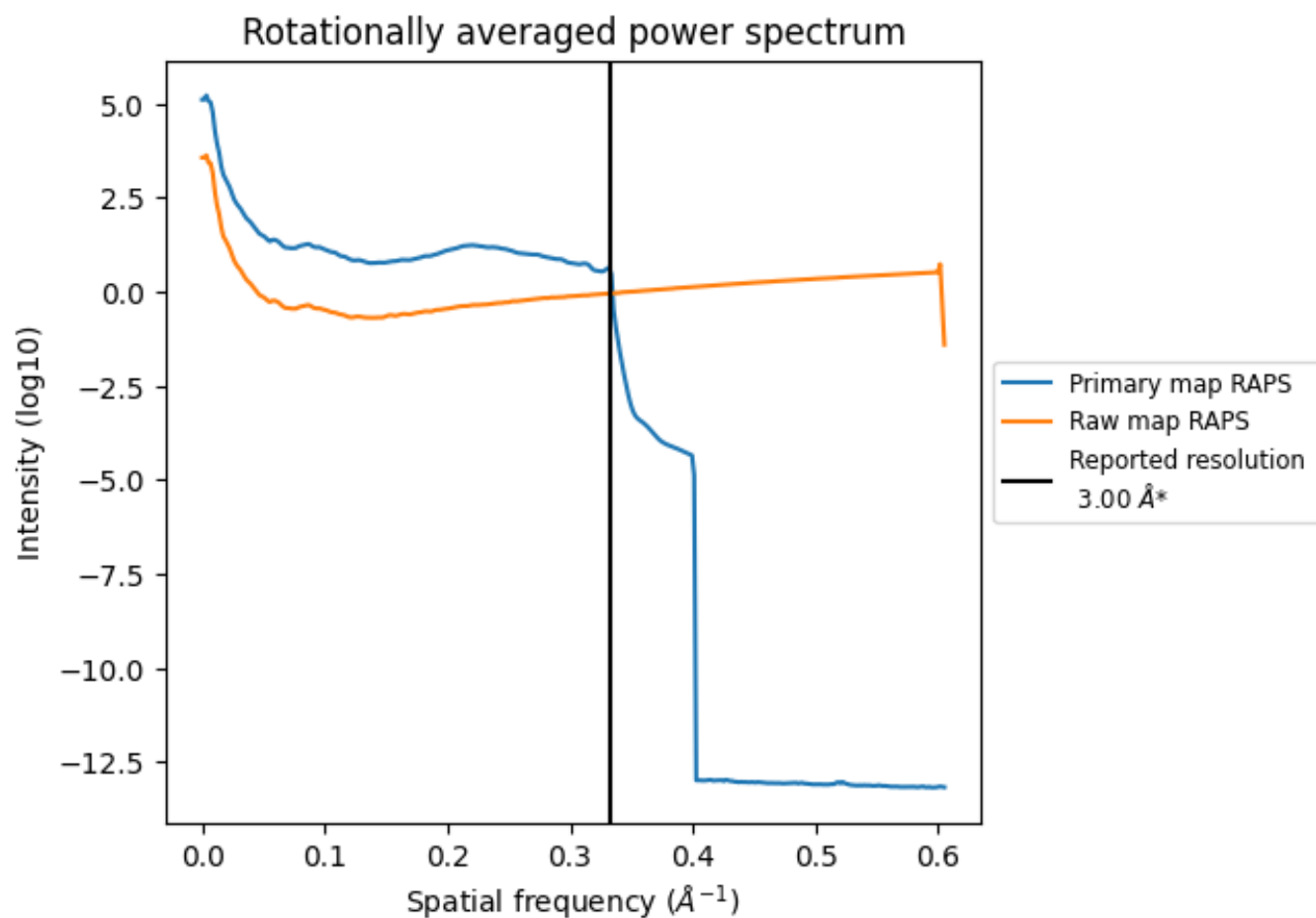
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 988 nm³; this corresponds to an approximate mass of 892 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

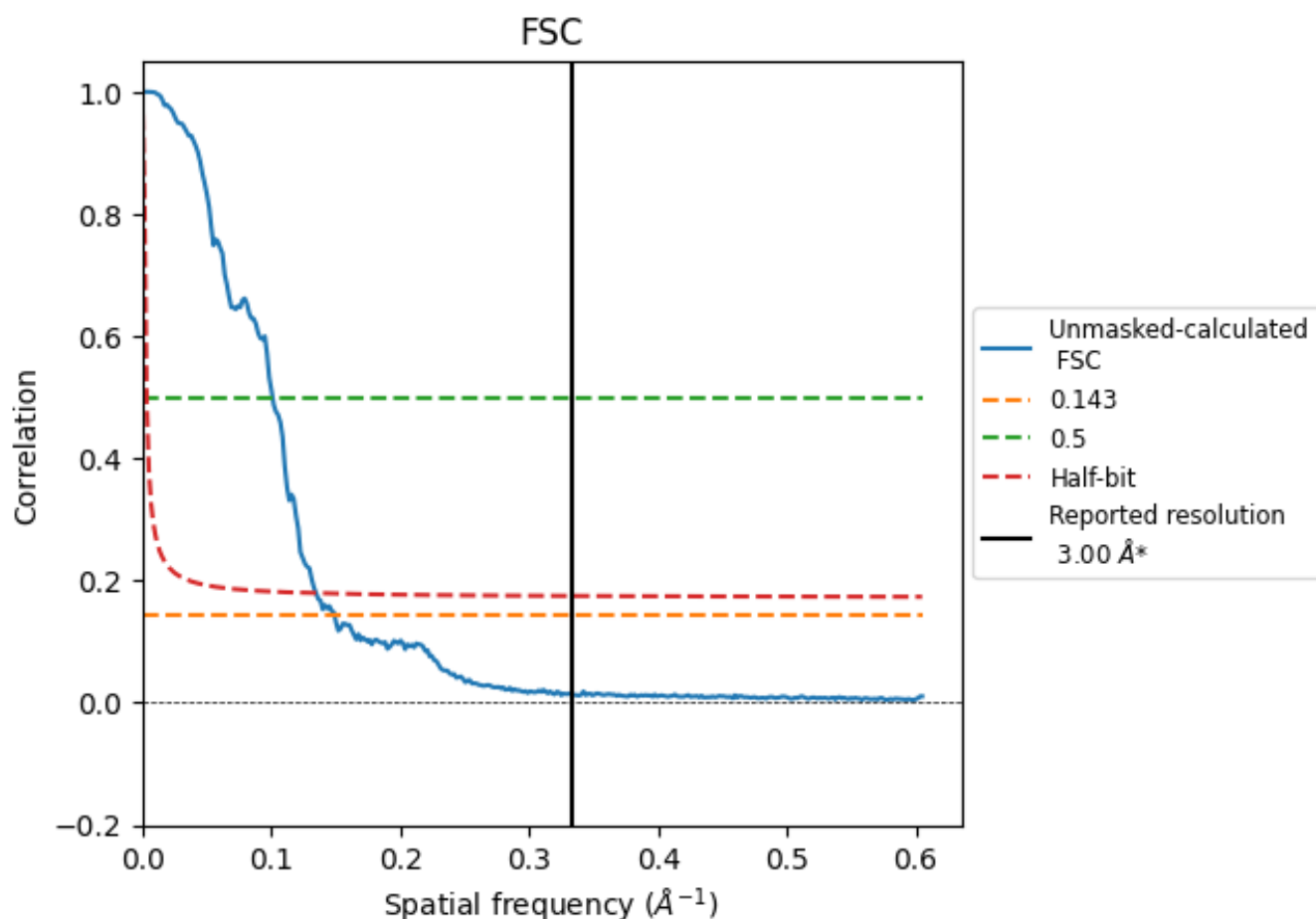


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.333 \AA^{-1}

8.2 Resolution estimates [i](#)

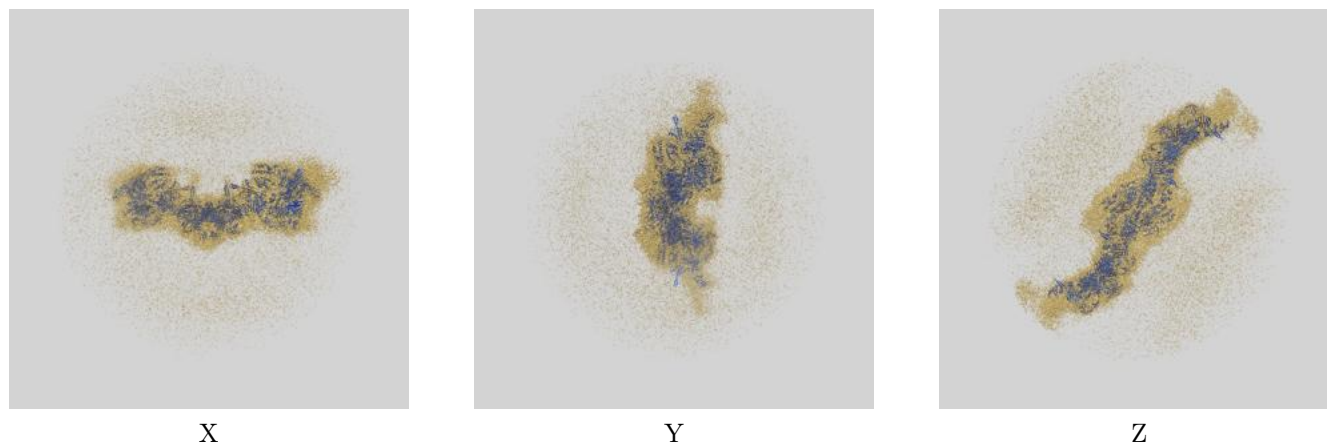
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.71	9.90	7.41

*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 6.71 differs from the reported value 3.0 by more than 10 %

9 Map-model fit [i](#)

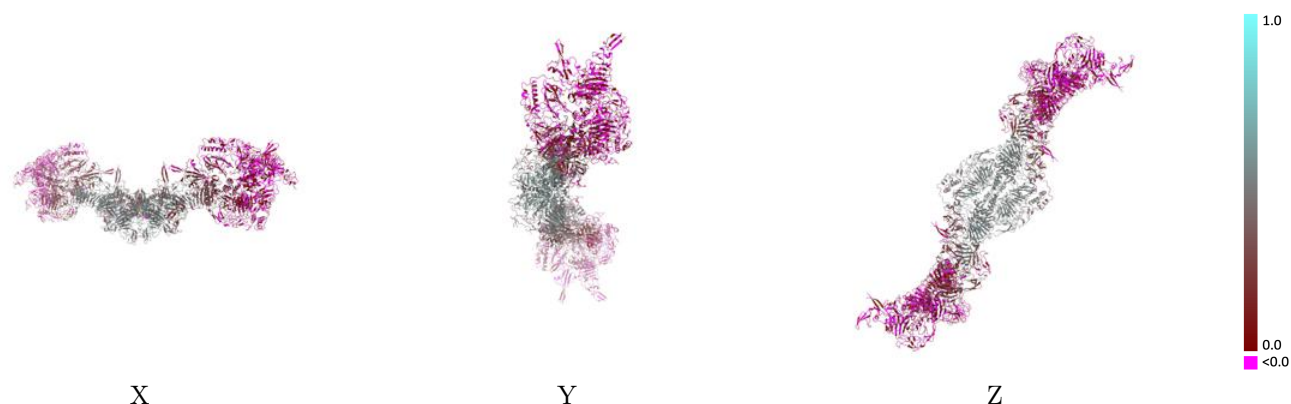
This section contains information regarding the fit between EMDB map EMD-16808 and PDB model 8OES. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



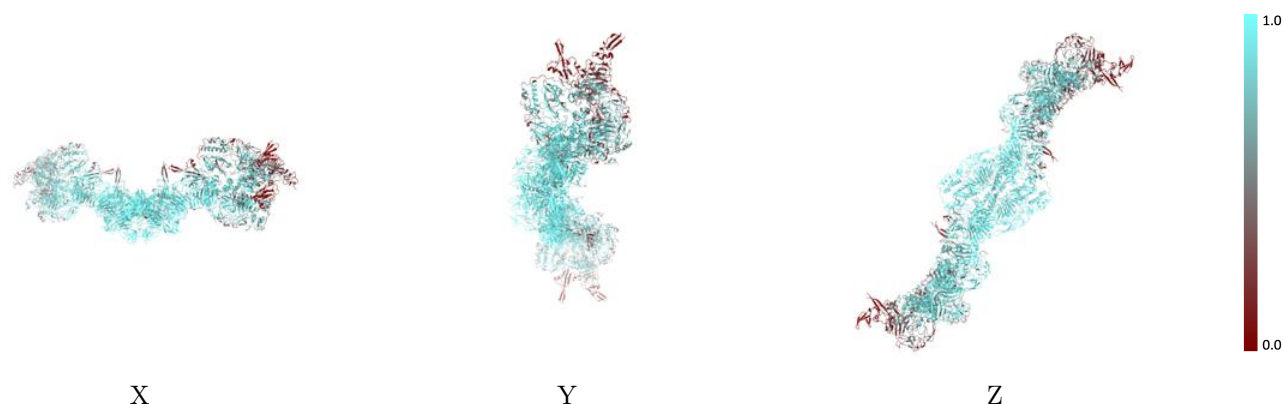
The images above show the 3D surface view of the map at the recommended contour level 0.056 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



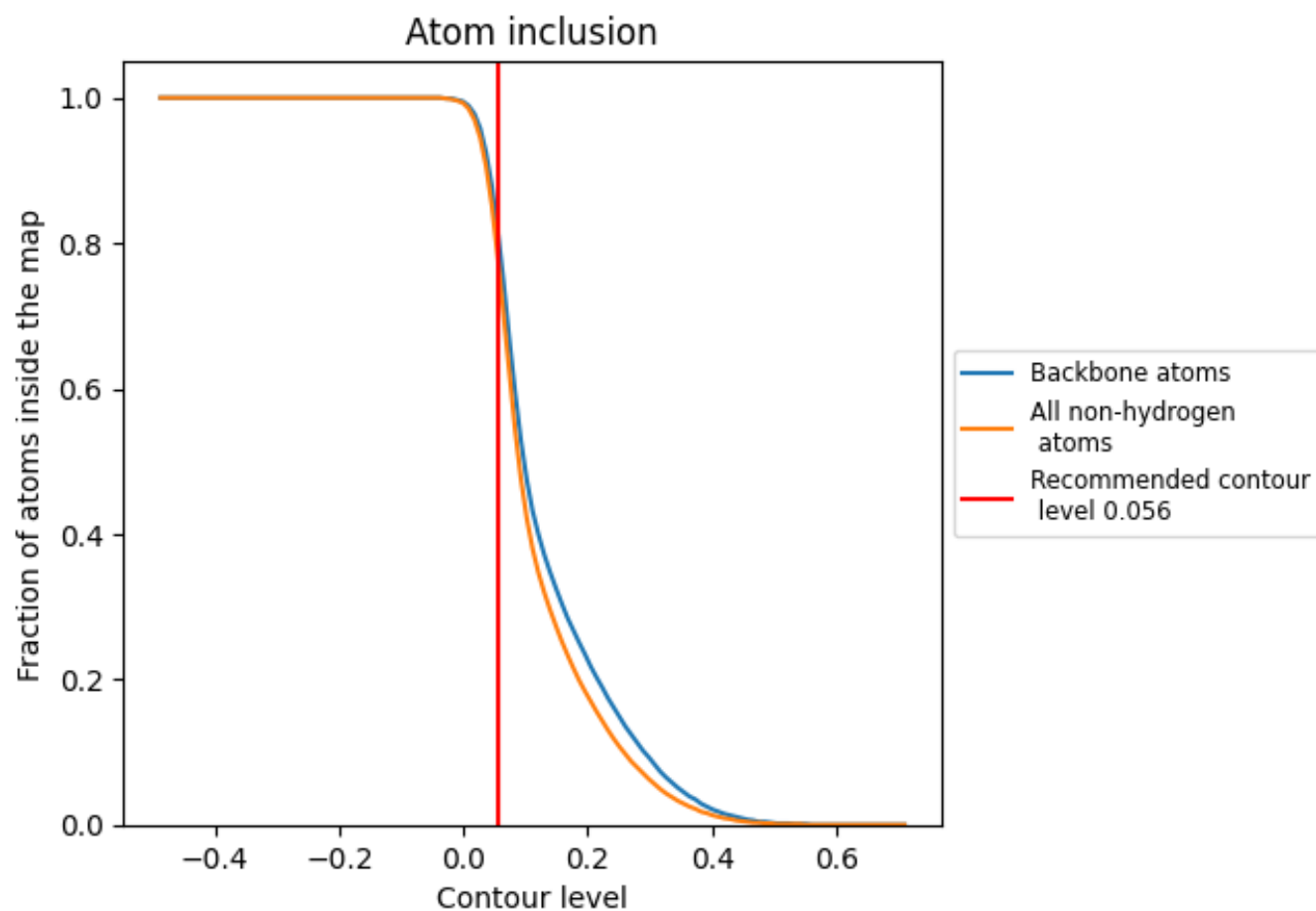
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.056).































9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 77% 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 (0.056) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7730	 0.2290
A	 0.9100	 0.3310
B	 0.9320	 0.3650
C	 0.8640	 0.2840
D	 0.8870	 0.3150
E	 0.5260	 0.0330
F	 0.6140	 0.0840
G	 0.6390	 0.0310
H	 0.6860	 0.0570
I	 0.7350	 0.3610
J	 0.7620	 0.3840
K	 0.4570	 0.1090
L	 0.5740	 0.2130
M	 0.0930	 0.0060
N	 0.0880	 -0.0230

