



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 04:41 PM UTC

PDB ID : 7ET3 / pdb_00007et3
EMDB ID : EMD-31297
Title : C5 portal vertex in the enveloped virion capsid
Authors : Li, Z.; Yu, X.
Deposited on : 2021-05-12
Resolution : 4.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

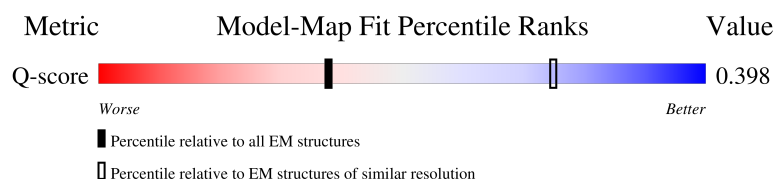
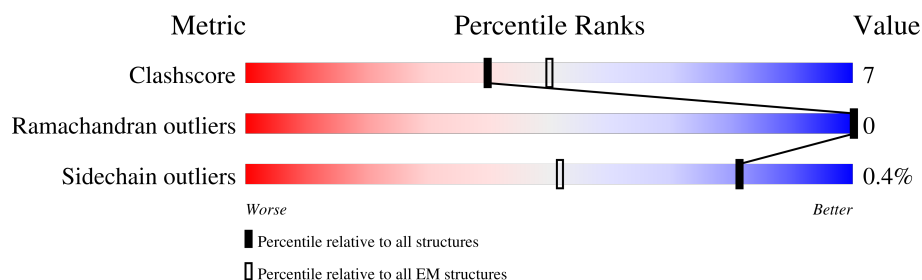
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 Å.

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



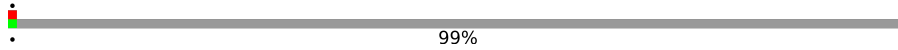
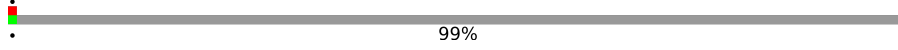
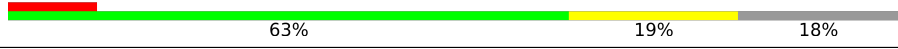
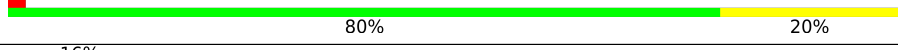
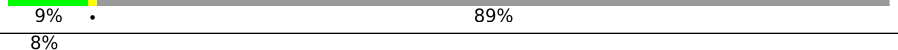
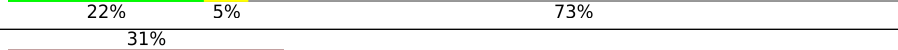
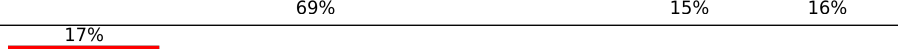
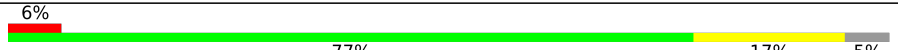
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5410 (3.70 - 4.70)

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

Mol	Chain	Length	Quality of chain
1	I	306	7% 75% 19% 7%
1	h	306	8% 75% 18% 7%
1	n	306	5% 81% 15% .
1	o	306	. 72% 20% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H	2241	
2	P	2241	
3	g	290	
3	m	290	
4	M	594	
5	N	642	
5	O	642	
6	1	1048	
7	R	75	
7	S	75	
7	T	75	
7	i	75	
7	j	75	
8	B	1370	
8	C	1370	
8	D	1370	
8	Y	1370	
8	Z	1370	
8	a	1370	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 86332 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 Triplex capsid protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	h	285	Total	C	N	O	S	0	0
			2258	1454	386	402	16		
1	I	285	Total	C	N	O	S	0	0
			2264	1454	389	404	17		
1	n	293	Total	C	N	O	S	0	0
			2322	1493	400	410	19		
1	o	282	Total	C	N	O	S	0	0
			2239	1442	382	397	18		

- Molecule 2 is a protein called Large tegument protein deneddylase.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	20	Total	C	N	O	S	0	0
			172	110	32	29	1		
2	P	20	Total	C	N	O	S	0	0
			172	110	32	29	1		

- Molecule 3 is a protein called Triplex capsid protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	g	237	Total	C	N	O	S	0	0
			1896	1218	332	335	11		
3	m	290	Total	C	N	O	S	0	0
			2325	1485	411	417	12		

- Molecule 4 is a protein called Capsid vertex component 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	468	Total	C	N	O	S	0	0
			3848	2408	740	686	14		

- Molecule 5 is a protein called Capsid vertex component 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	N	65	Total	C	N	O	S	0	0
			551	341	110	96	4		
5	O	69	Total	C	N	O	S	0	0
			589	371	113	102	3		

- Molecule 6 is a protein called ORFL92C_UL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	1	285	Total	C	N	O	S	0	0
			2328	1468	426	421	13		

- Molecule 7 is a protein called Small capsomere-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	R	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
7	S	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
7	T	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
7	i	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
7	j	63	Total	C	N	O	S	0	0
			513	321	97	91	4		

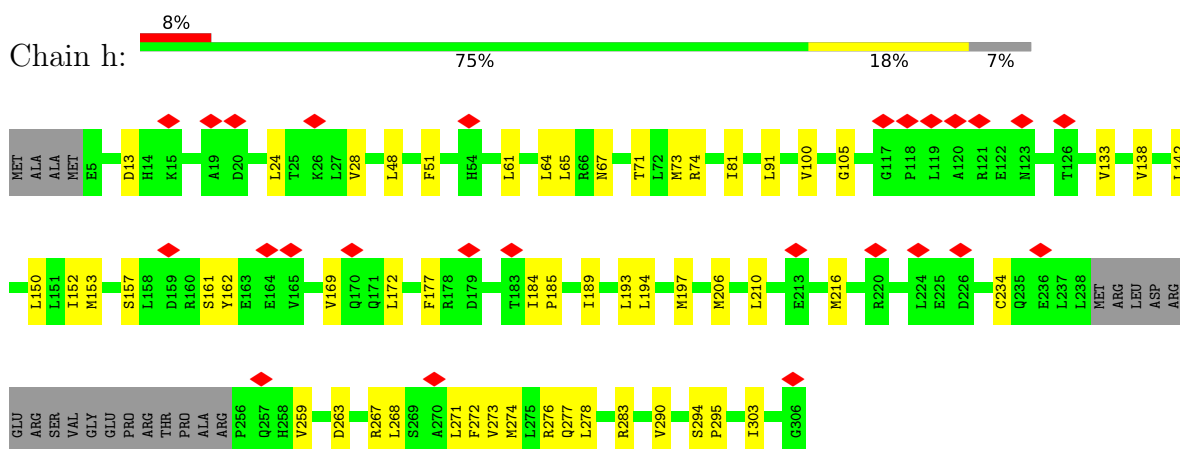
- Molecule 8 is a protein called Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	a	1286	Total	C	N	O	S	0	0
			10169	6469	1770	1871	59		
8	B	1332	Total	C	N	O	S	0	0
			10567	6728	1831	1947	61		
8	C	1330	Total	C	N	O	S	0	0
			10540	6713	1830	1936	61		
8	D	1297	Total	C	N	O	S	0	0
			10269	6538	1785	1887	59		
8	Y	1347	Total	C	N	O	S	0	0
			10676	6799	1850	1966	61		
8	Z	1337	Total	C	N	O	S	0	0
			10582	6740	1831	1952	59		

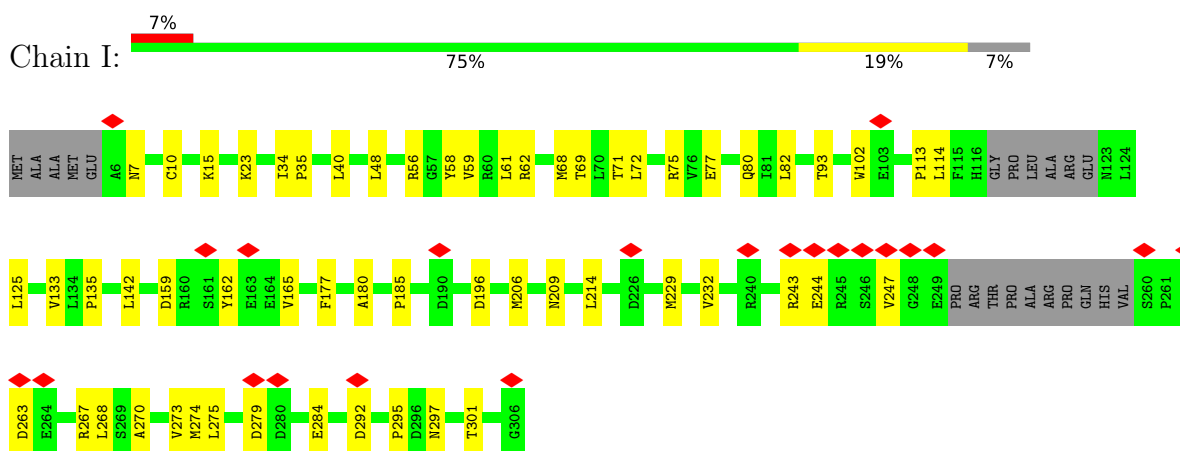
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

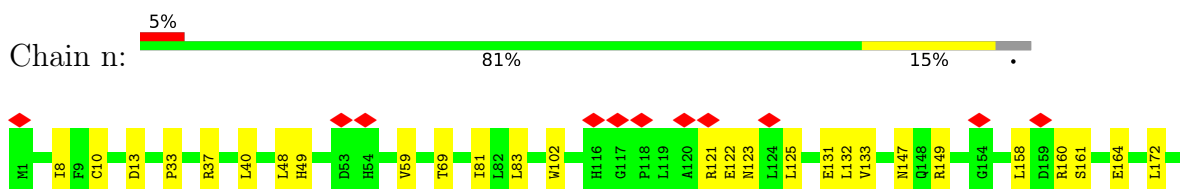
- Molecule 1: Triplex capsid protein 2

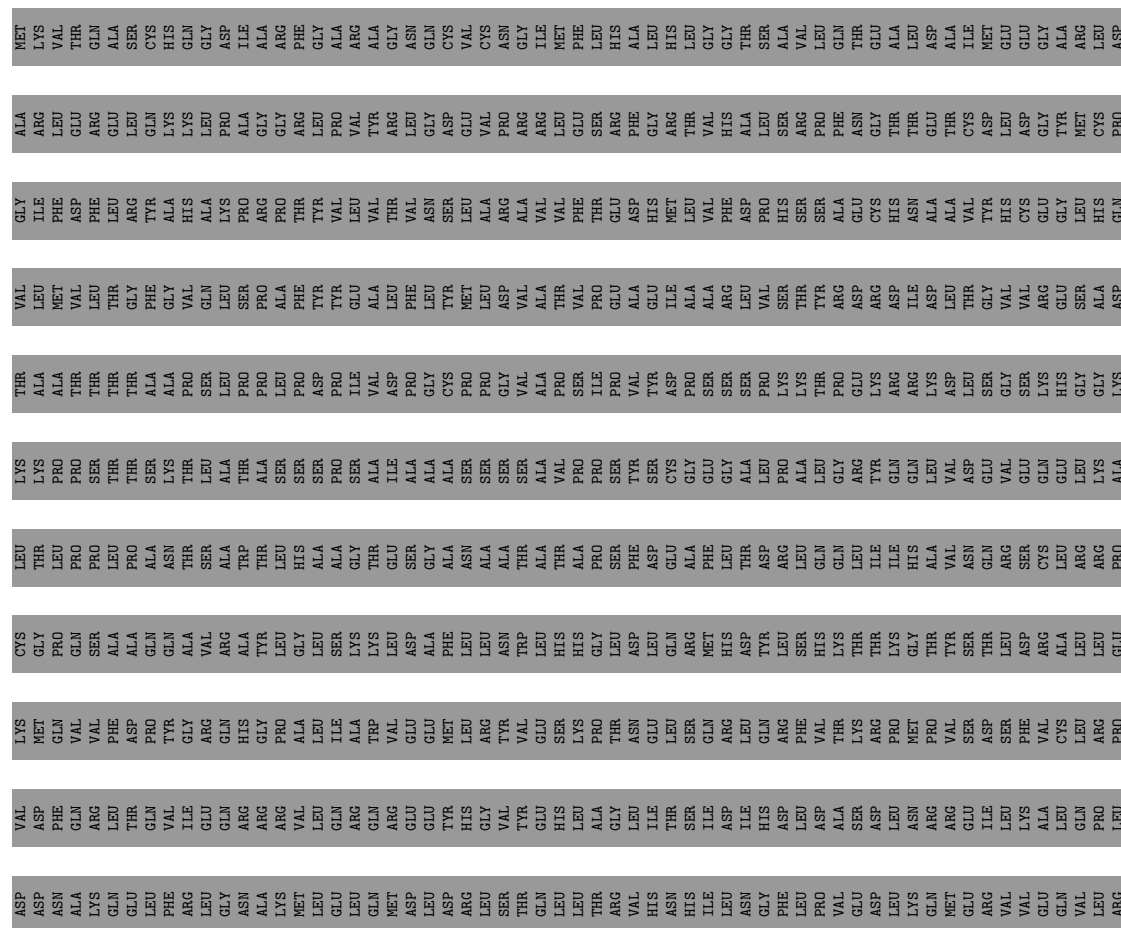


- Molecule 1: Triplex capsid protein 2



- Molecule 1: Triplex capsid protein 2

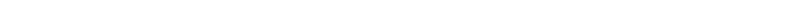






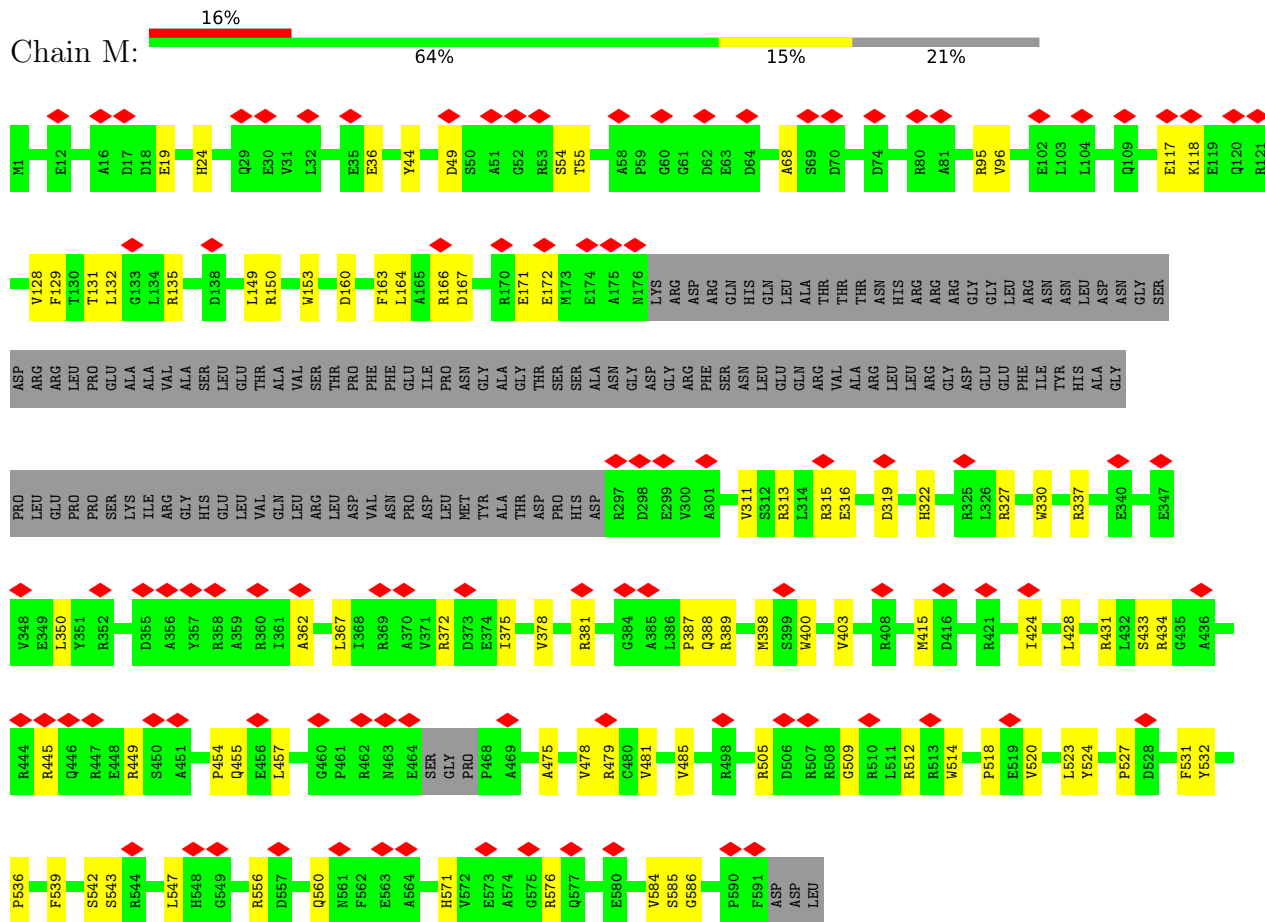
[illegible]

- Molecule 2: Large tegument protein deneddylase

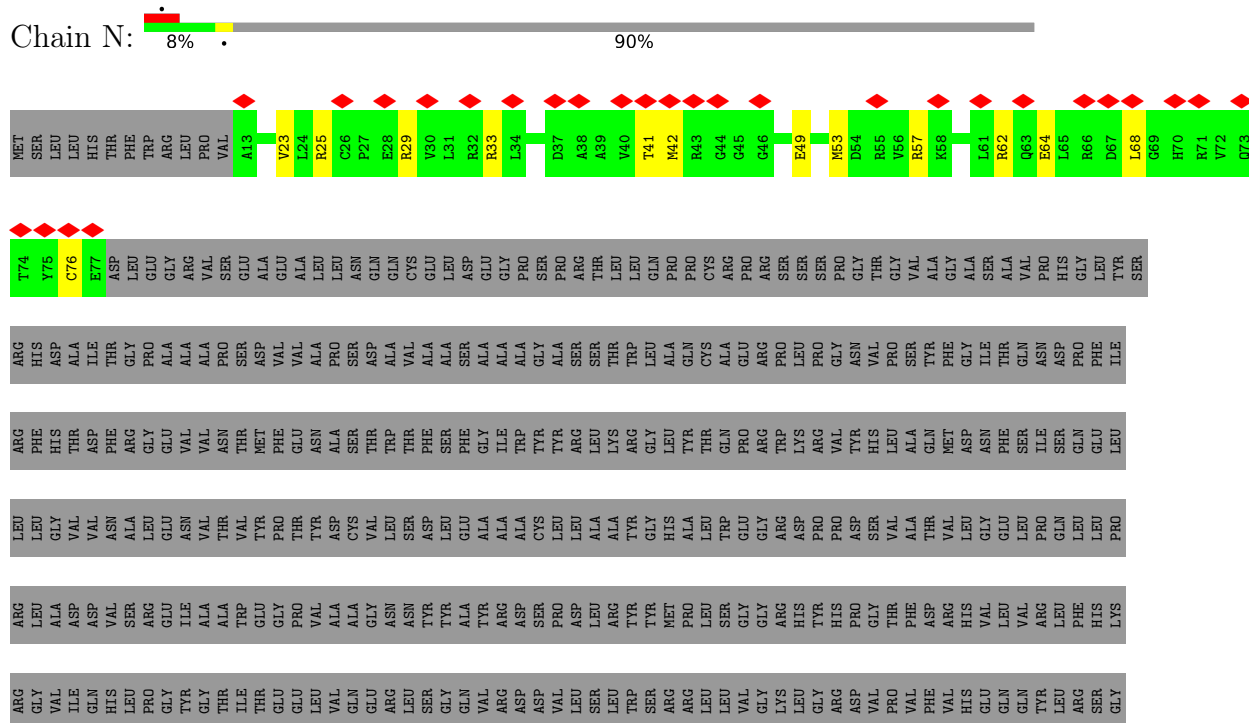
Chain P:  99%

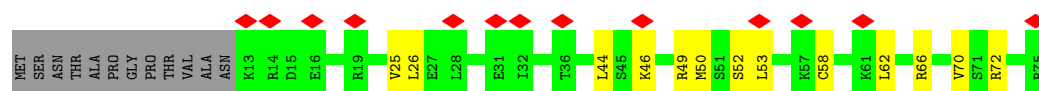
ASP	ASP	VAL	LYS	CYS	LEU	LYS	LYS	THR	VAL	GLY	ALA	MET
ASP	ASP	PHE	GLN	GLY	THR	THR	LYS	ALA	LEU	ILE	ARG	VAL
ALA	ASN	GLN	VAL	GLN	PRO	PRO	PRO	THR	VAL	PHE	GLU	GLN
LYS	ARG	LEU	PHE	SER	LEU	THR	THR	THR	THR	PHE	LEU	GLN
GLN	LEU	LEU	ALA	ALA	PRO	THR	THR	THR	THR	ARG	LEU	ALA
GLU	THR	THR	ASP	ALA	LEU	ALA	THR	THR	GLY	SER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



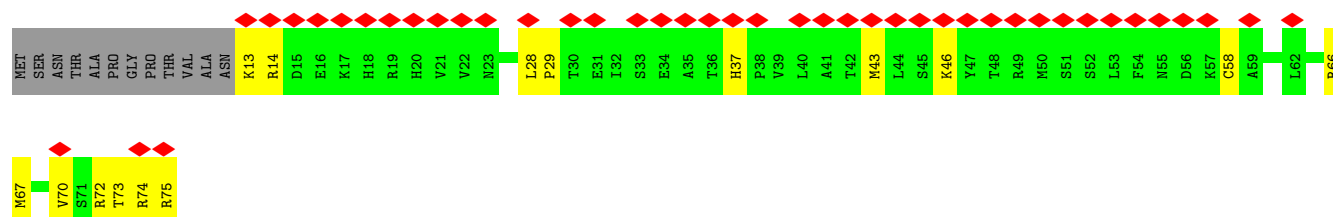


• Molecule 5: Capsid vertex component 2

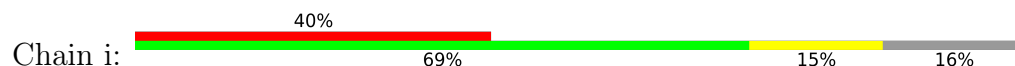




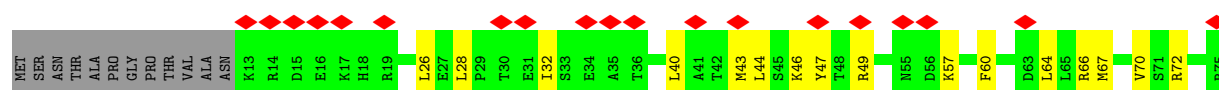
• Molecule 7: Small capsomere-interacting protein



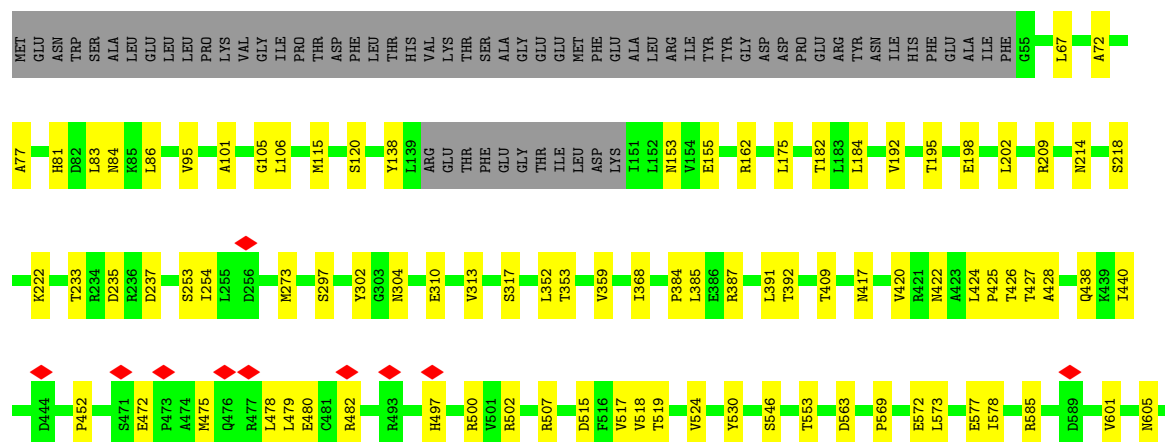
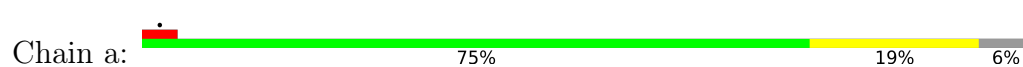
• Molecule 7: Small capsomere-interacting protein

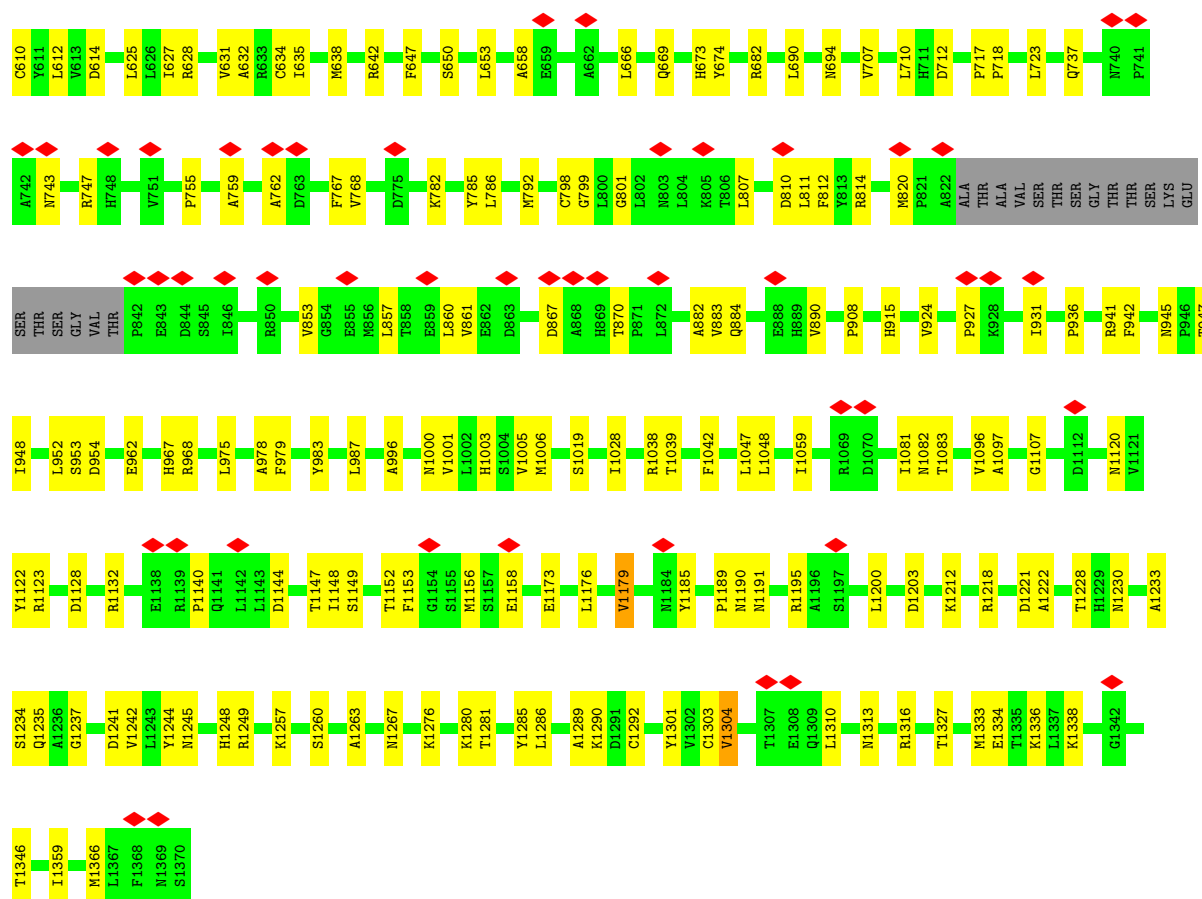


• Molecule 7: Small capsomere-interacting protein



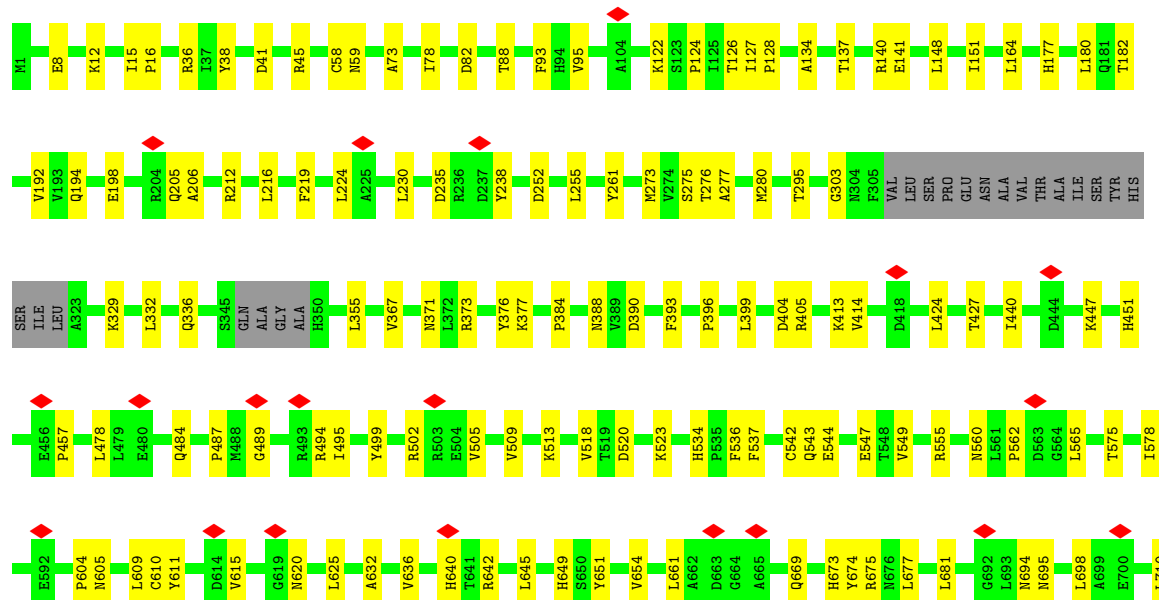
• Molecule 8: Major capsid protein

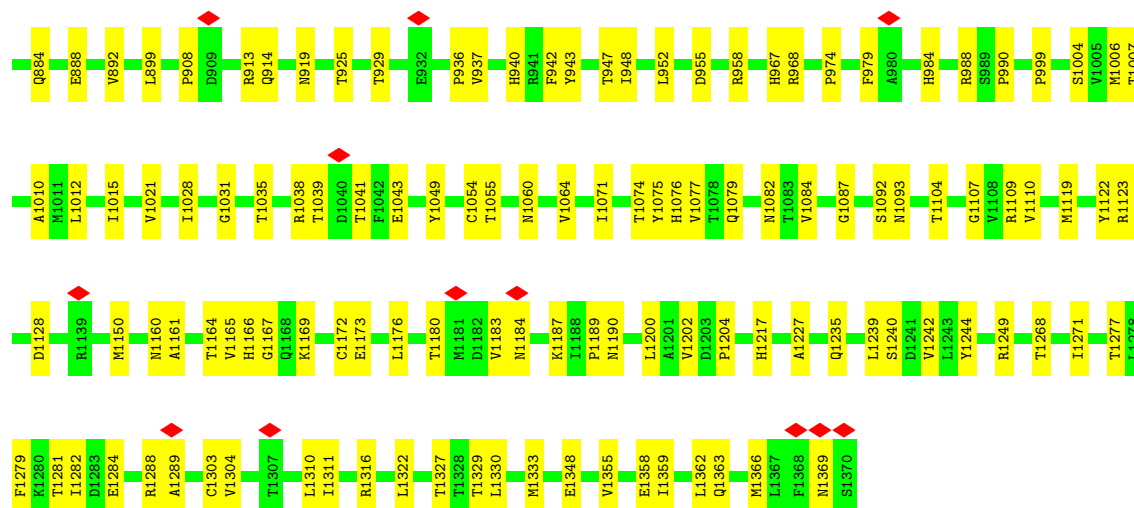




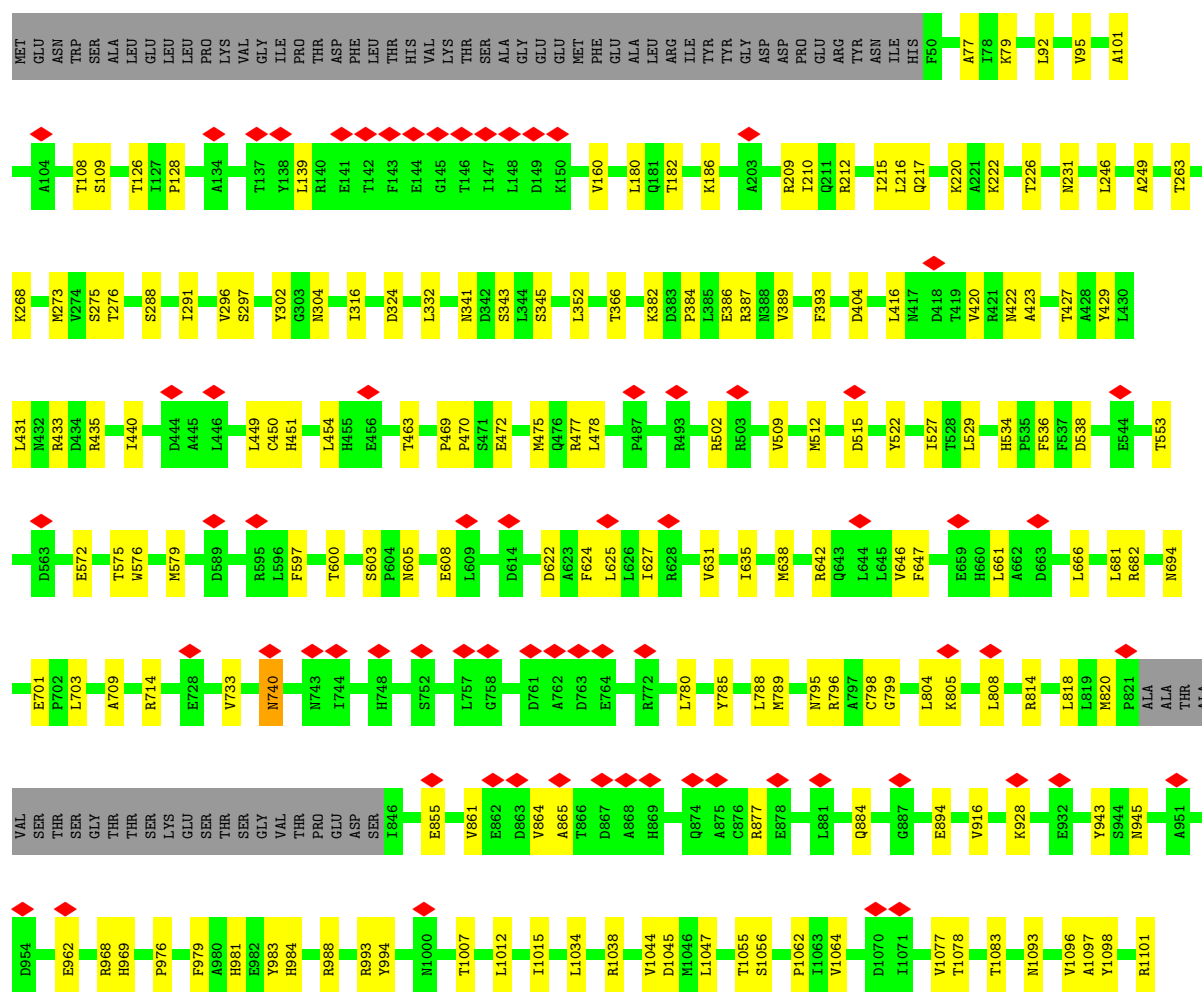
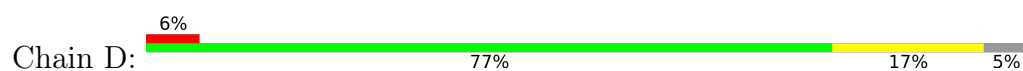
• Molecule 8: Major capsid protein

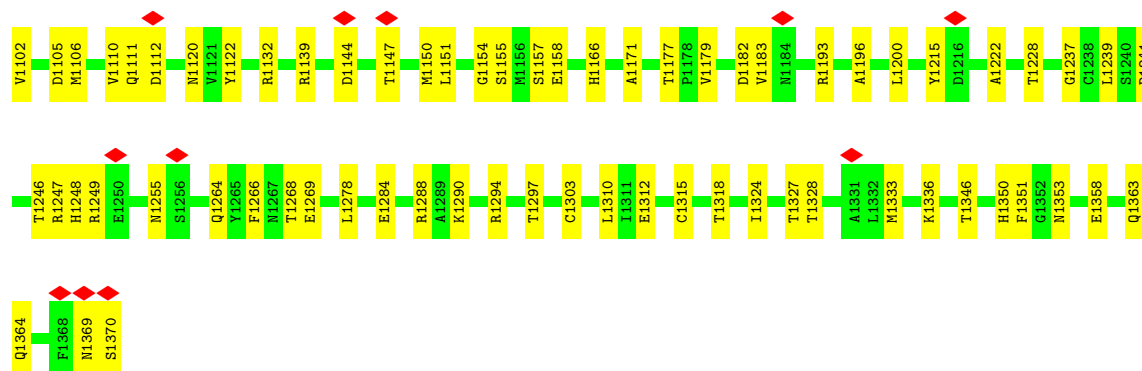
Chain B: 76% 21%



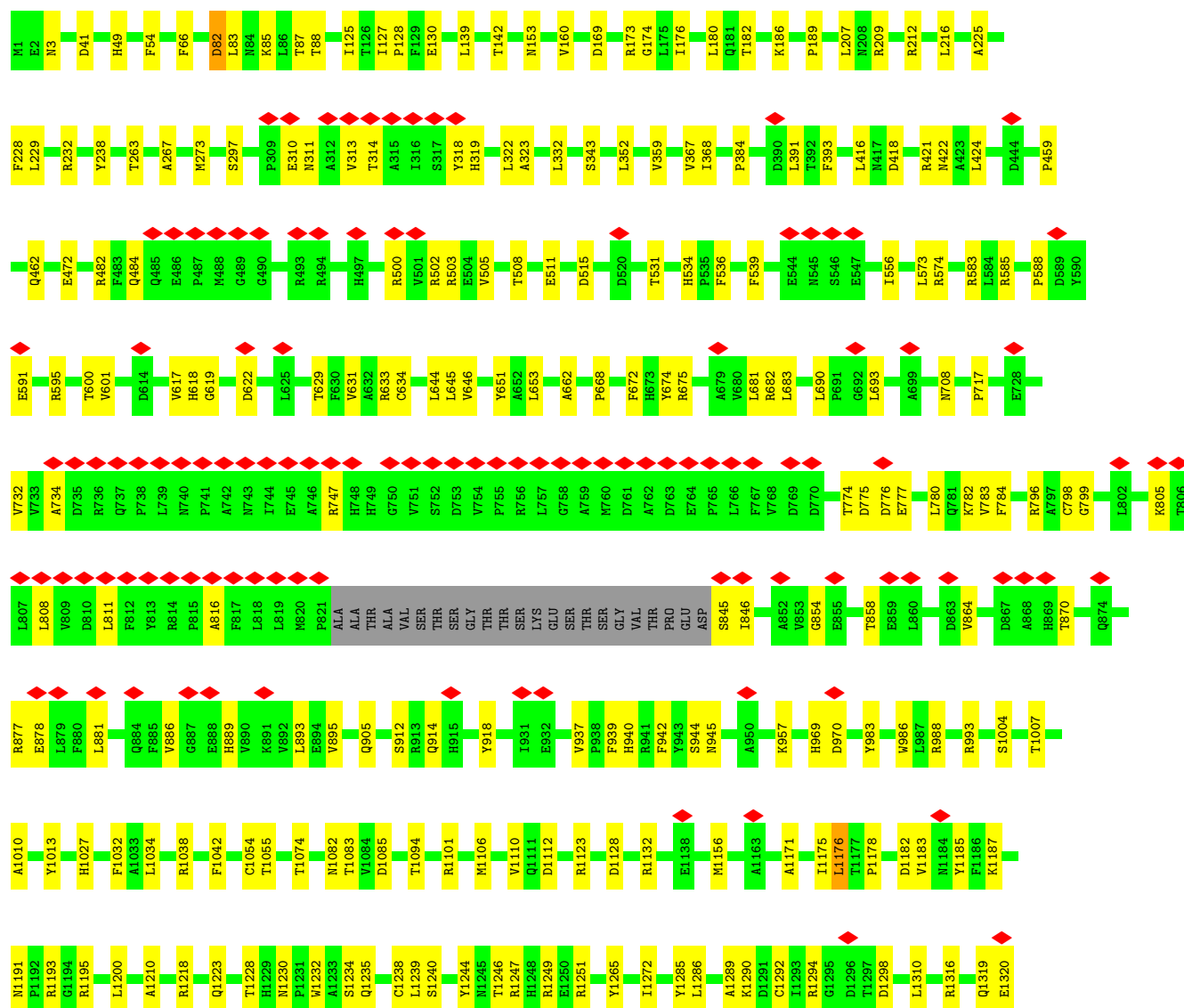
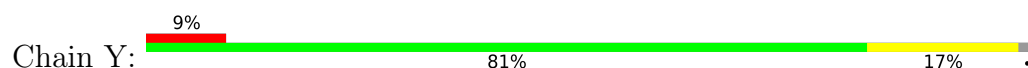


• Molecule 8: Major capsid protein



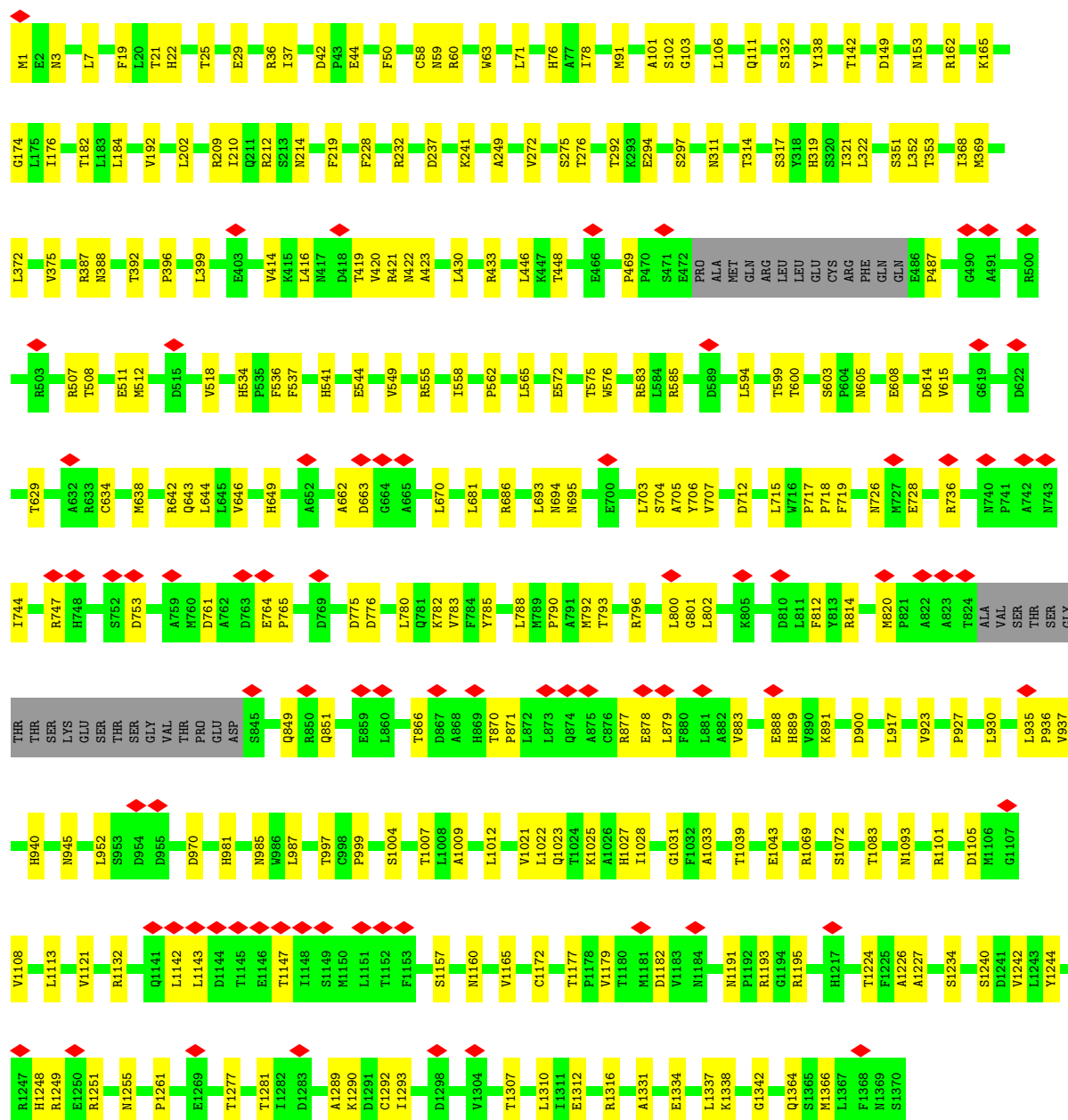
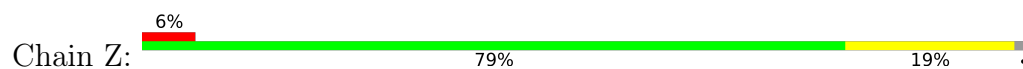


• Molecule 8: Major capsid protein





• Molecule 8: Major capsid protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	23136	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 ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.075	Depositor
Minimum map value	-0.051	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	416.0, 416.0, 416.0	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.625, 1.625, 1.625	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	I	0.23	0/2304	0.57	2/3125 (0.1%)
1	h	0.21	0/2302	0.54	0/3128
1	n	0.22	0/2366	0.55	0/3212
1	o	0.26	1/2279 (0.0%)	0.49	0/3092
2	H	0.21	0/174	0.48	0/233
2	P	0.22	0/174	0.54	0/233
3	g	0.20	0/1936	0.52	0/2625
3	m	0.21	0/2374	0.51	0/3221
4	M	0.22	0/3935	0.52	0/5331
5	N	0.24	0/560	0.57	0/751
5	O	0.22	0/600	0.59	0/808
6	l	0.23	0/2366	0.57	0/3192
7	R	0.18	0/520	0.50	0/697
7	S	0.20	0/520	0.55	0/697
7	T	0.22	0/520	0.54	0/697
7	i	0.22	0/520	0.58	0/697
7	j	0.21	0/520	0.48	0/697
8	B	0.23	1/10819 (0.0%)	0.51	0/14733
8	C	0.22	0/10790	0.49	0/14695
8	D	0.21	0/10513	0.50	1/14322 (0.0%)
8	Y	0.21	0/10932	0.50	0/14892
8	Z	0.21	0/10835	0.50	0/14762
8	a	0.22	0/10410	0.51	1/14183 (0.0%)
All	All	0.22	2/88269 (0.0%)	0.51	4/120023 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	l	0	1
8	Y	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
8	a	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	754	VAL	C-N	7.46	1.41	1.33
1	o	47	GLY	C-O	7.01	1.27	1.24

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	a	883	VAL	N-CA-C	-7.71	105.20	112.83
1	I	295	PRO	CA-C-N	5.29	131.64	121.54
1	I	295	PRO	C-N-CA	5.29	131.64	121.54
8	D	527	ILE	N-CA-C	-5.11	107.85	112.96

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	l	69	HIS	Peptide
8	Y	585	ARG	Peptide
8	a	585	ARG	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	2264	0	2350	39	0
1	h	2258	0	2342	35	0
1	n	2322	0	2418	34	0
1	o	2239	0	2331	41	0
2	H	172	0	176	4	0
2	P	172	0	176	5	0
3	g	1896	0	1934	35	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	m	2325	0	2363	41	0
4	M	3848	0	3773	55	0
5	N	551	0	548	10	0
5	O	589	0	587	8	0
6	l	2328	0	2363	34	0
7	R	513	0	539	8	0
7	S	513	0	539	9	0
7	T	513	0	539	12	0
7	i	513	0	539	7	0
7	j	513	0	539	9	0
8	B	10567	0	10501	173	0
8	C	10540	0	10495	166	0
8	D	10269	0	10227	143	0
8	Y	10676	0	10618	143	0
8	Z	10582	0	10521	177	0
8	a	10169	0	10124	163	0
All	All	86332	0	86542	1219	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 7.

All (1219) 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)
8:C:782:LYS:O	8:C:786:LEU:HB2	1.80	0.81
8:a:782:LYS:O	8:a:786:LEU:HB2	1.82	0.78
3:g:45:ALA:HA	3:g:151:ARG:O	1.83	0.78
8:Y:130:GLU:H	8:Z:111:GLN:HE22	1.34	0.75
8:a:1292:CYS:SG	8:a:1303:CYS:N	2.63	0.72
8:C:575:THR:HG21	8:C:1007:THR:HA	1.73	0.70
1:I:102:TRP:H	1:I:297:ASN:HD21	1.38	0.69
8:D:575:THR:HG21	8:D:1007:THR:HA	1.75	0.69
6:1:60:LEU:HD22	6:1:268:LEU:HB2	1.76	0.68
8:B:578:ILE:HG12	8:B:1028:ILE:HD12	1.77	0.67
8:C:1327:THR:HG21	8:C:1333:MET:HB2	1.76	0.67
8:B:212:ARG:HH22	8:B:1203:ASP:HA	1.61	0.66
3:g:185:VAL:HA	3:g:205:LEU:O	1.95	0.66
8:Y:482:ARG:HB3	8:Y:484:GLN:HE22	1.61	0.66
8:B:534:HIS:HD2	8:B:536:PHE:H	1.44	0.66
3:g:224:ALA:HA	3:g:227:ARG:HD3	1.78	0.66
8:a:578:ILE:HG22	8:a:1028:ILE:HD12	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:1101:ARG:HE	8:C:199:ASN:HD21	1.45	0.65
8:Y:182:THR:HG21	8:Y:1083:THR:HG21	1.78	0.65
8:Z:849:GLN:HE22	8:Z:871:PRO:HB2	1.62	0.65
8:C:1041:THR:HG22	8:C:1104:THR:HG23	1.79	0.65
8:a:642:ARG:NH2	8:Z:663:ASP:O	2.31	0.64
4:M:163:PHE:HB3	4:M:319:ASP:HA	1.80	0.64
8:Y:583:ARG:HH21	8:Z:997:THR:HG23	1.63	0.64
4:M:455:GLN:NE2	8:C:1119:MET:SD	2.72	0.63
8:Z:102:SER:HB2	8:Z:106:LEU:HD23	1.80	0.63
8:C:1172:CYS:SG	8:C:1173:GLU:N	2.71	0.63
8:a:798:CYS:SG	8:a:799:GLY:N	2.71	0.63
8:C:1244:TYR:HA	8:C:1249:ARG:HH21	1.63	0.63
7:j:66:ARG:NH2	8:a:884:GLN:O	2.32	0.62
8:Z:600:THR:HG22	8:Z:644:LEU:HB2	1.81	0.62
1:I:114:LEU:HD23	1:I:185:PRO:HD2	1.82	0.62
4:M:481:VAL:HG21	5:O:34:LEU:HD22	1.81	0.62
8:D:139:LEU:HD22	8:D:160:VAL:HG21	1.80	0.62
8:a:86:LEU:HA	8:Z:50:PHE:HB2	1.82	0.61
8:Y:216:LEU:HD11	8:Y:1200:LEU:HG	1.82	0.61
7:S:25:VAL:HG13	7:S:26:LEU:HD12	1.82	0.61
8:B:1327:THR:HG23	8:B:1355:VAL:HG12	1.83	0.61
3:m:136:LYS:HG3	3:m:137:THR:HG23	1.83	0.61
1:n:102:TRP:H	1:n:297:ASN:HD21	1.49	0.61
8:C:446:LEU:HD11	8:C:1021:VAL:HG22	1.82	0.61
6:1:174:VAL:HG13	6:1:175:ARG:HH12	1.65	0.61
8:a:518:VAL:HG23	8:a:519:THR:HG23	1.82	0.61
8:C:1279:PHE:HA	8:C:1282:ILE:HD12	1.83	0.61
8:B:900:ASP:HB3	8:B:903:GLN:H	1.66	0.60
8:B:58:CYS:SG	8:B:59:ASN:N	2.74	0.60
8:Y:1106:MET:SD	8:Y:1363:GLN:NE2	2.74	0.60
8:C:716:TRP:O	8:C:914:GLN:NE2	2.34	0.60
4:M:524:TYR:HB2	4:M:532:TYR:HB2	1.83	0.60
6:1:240:ARG:HA	6:1:251:ARG:HH21	1.66	0.60
8:a:182:THR:HG21	8:a:1083:THR:HG21	1.83	0.60
8:B:555:ARG:HB3	8:B:560:ASN:HB3	1.84	0.60
8:B:786:LEU:HD11	8:B:987:LEU:HG	1.82	0.60
3:m:188:ILE:HG12	3:m:248:ILE:HG22	1.84	0.60
7:S:58:CYS:SG	8:C:805:LYS:NZ	2.73	0.60
8:B:632:ALA:HB2	8:B:661:LEU:HD11	1.83	0.59
3:m:66:LEU:HB2	3:m:84:LEU:HB2	1.84	0.59
8:C:514:GLN:HE22	8:C:990:PRO:HD3	1.67	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:663:ASP:O	8:D:642:ARG:NH2	2.34	0.59
8:a:690:LEU:H	8:a:694:ASN:HD21	1.50	0.59
8:B:329:LYS:HE3	8:B:1077:VAL:HG11	1.83	0.59
8:D:682:ARG:HE	8:D:780:LEU:HD11	1.66	0.59
8:a:1122:TYR:HB2	8:a:1128:ASP:HB2	1.82	0.59
8:B:390:ASP:HB2	8:B:1313:ASN:HB3	1.83	0.59
8:Z:76:HIS:HD2	8:Z:78:ILE:HD11	1.67	0.59
8:C:988:ARG:HB2	8:C:990:PRO:HD2	1.85	0.59
8:a:95:VAL:HG12	8:Z:59:ASN:HB2	1.85	0.59
8:C:174:GLY:HA3	8:D:101:ALA:HB3	1.85	0.59
8:Z:1244:TYR:HA	8:Z:1249:ARG:HH21	1.68	0.59
8:a:605:ASN:HB3	8:Z:662:ALA:HB1	1.85	0.59
8:C:130:GLU:HG2	8:C:1074:THR:HG22	1.83	0.59
8:Z:534:HIS:O	8:Z:555:ARG:NH1	2.36	0.59
1:h:206:MET:HE1	3:g:234:ARG:HG2	1.85	0.58
4:M:514:TRP:HB2	4:M:520:VAL:HG21	1.84	0.58
8:Y:459:PRO:HA	8:Y:462:GLN:HG2	1.86	0.58
8:B:177:HIS:HD1	8:B:376:TYR:HH	1.52	0.58
8:Y:1292:CYS:HB3	8:Y:1310:LEU:HD23	1.84	0.58
1:h:67:ASN:ND2	8:a:1147:THR:OG1	2.37	0.58
8:B:1264:GLN:NE2	8:B:1315:CYS:SG	2.77	0.58
4:M:330:TRP:HB3	4:M:337:ARG:HH12	1.69	0.58
7:R:26:LEU:O	8:B:813:TYR:OH	2.21	0.58
4:M:117:GLU:HG2	4:M:118:LYS:HG2	1.84	0.58
8:a:120:SER:OG	8:a:1082:ASN:OD1	2.21	0.58
2:P:2230:ASP:OD1	5:O:71:ARG:NH1	2.36	0.58
7:S:50:MET:HE3	8:C:754:VAL:HG11	1.85	0.58
8:Y:708:ASN:HA	8:Y:1013:TYR:HA	1.86	0.58
8:Y:1244:TYR:HA	8:Y:1249:ARG:HH21	1.67	0.58
2:H:2225:ALA:HB1	5:N:76:CYS:HB2	1.85	0.58
1:h:272:PHE:HB3	1:h:276:ARG:HH11	1.69	0.57
8:B:1172:CYS:SG	8:B:1173:GLU:N	2.77	0.57
8:Z:1342:GLY:H	8:Z:1364:GLN:HE21	1.52	0.57
8:B:277:ALA:HA	8:B:371:ASN:HD21	1.67	0.57
8:B:1038:ARG:NH1	8:B:1107:GLY:O	2.37	0.57
8:B:1156:MET:SD	8:B:1294:ARG:NH2	2.76	0.57
8:Y:1101:ARG:HH21	8:Z:202:LEU:HG	1.69	0.57
8:Z:1069:ARG:NH2	8:Z:1072:SER:OG	2.37	0.57
1:h:48:LEU:HD21	1:h:65:LEU:HD13	1.87	0.57
8:a:198:GLU:O	8:Z:1101:ARG:NH1	2.38	0.57
8:a:409:THR:OG1	8:Z:1338:LYS:NZ	2.38	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:575:THR:HG21	8:B:1007:THR:HA	1.85	0.57
8:C:807:LEU:O	8:C:811:LEU:HB2	2.05	0.57
8:Z:58:CYS:SG	8:Z:59:ASN:N	2.75	0.57
8:B:499:TYR:O	8:B:502:ARG:NH1	2.38	0.57
1:n:59:VAL:HG21	1:n:193:LEU:HB2	1.87	0.57
1:I:7:ASN:HB3	1:I:82:LEU:HD11	1.87	0.57
8:a:945:ASN:ND2	8:a:947:THR:OG1	2.38	0.57
8:a:1228:THR:HG22	8:a:1230:ASN:H	1.69	0.57
8:Y:631:VAL:HA	8:Y:634:CYS:HB3	1.87	0.57
8:Z:634:CYS:O	8:Z:638:MET:HB2	2.05	0.57
6:1:177:ASN:ND2	6:1:180:CYS:SG	2.78	0.57
7:j:43:MET:HA	7:j:46:LYS:HE2	1.85	0.57
1:I:214:LEU:HD21	1:I:267:ARG:HD3	1.87	0.56
1:I:214:LEU:HD11	1:I:267:ARG:HB3	1.86	0.56
4:M:150:ARG:NH1	4:M:160:ASP:OD2	2.38	0.56
8:Z:210:ILE:O	8:Z:214:ASN:ND2	2.37	0.56
8:a:202:LEU:HD11	8:Z:1043:GLU:HG2	1.86	0.56
8:a:747:ARG:HB2	8:a:767:PHE:HB3	1.87	0.56
8:B:544:GLU:HB3	8:B:547:GLU:HB3	1.87	0.56
8:C:8:GLU:HB3	8:C:45:ARG:HH11	1.70	0.56
8:C:212:ARG:HH22	8:C:1204:PRO:HD3	1.69	0.56
8:C:1064:VAL:HG22	8:C:1077:VAL:HG12	1.87	0.56
1:I:93:THR:HG22	1:I:301:THR:HG22	1.88	0.56
3:m:93:ASN:ND2	3:m:170:ASP:O	2.38	0.56
6:1:73:LEU:HD13	6:1:214:ARG:HH21	1.69	0.56
8:a:317:SER:O	8:Z:3:ASN:ND2	2.38	0.56
8:D:1064:VAL:HG22	8:D:1077:VAL:HG12	1.87	0.56
8:Y:747:ARG:NH2	8:Y:918:TYR:OH	2.38	0.56
8:Y:816:ALA:O	8:Y:877:ARG:NH2	2.38	0.56
1:o:101:THR:OG1	1:o:297:ASN:ND2	2.38	0.56
8:B:1239:LEU:O	8:B:1243:LEU:HB2	2.05	0.56
8:D:297:SER:HB2	8:D:352:LEU:HD12	1.87	0.56
8:Z:275:SER:OG	8:Z:276:THR:N	2.38	0.56
8:Z:820:MET:SD	8:Z:877:ARG:NH1	2.78	0.56
4:M:388:GLN:HA	4:M:539:PHE:HA	1.88	0.56
8:a:480:GLU:HB3	8:a:482:ARG:HH12	1.71	0.56
8:a:524:VAL:O	8:a:1218:ARG:NH1	2.37	0.56
8:a:669:GLN:O	8:a:673:HIS:ND1	2.35	0.56
8:B:694:ASN:ND2	8:B:695:ASN:OD1	2.38	0.56
8:C:231:ASN:O	8:C:1369:ASN:ND2	2.39	0.56
8:C:605:ASN:O	8:C:642:ARG:NH2	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:538:ASP:OD2	8:D:988:ARG:NH1	2.39	0.56
8:Y:1193:ARG:NH1	8:Y:1195:ARG:O	2.39	0.56
1:o:106:ASP:OD1	3:m:69:ARG:NH2	2.39	0.56
7:i:19:ARG:HD2	7:i:23:ASN:HD21	1.71	0.56
7:i:65:LEU:HB3	8:Z:883:VAL:HG11	1.86	0.56
8:a:807:LEU:O	8:a:811:LEU:HB2	2.05	0.56
8:Y:1289:ALA:O	8:Y:1316:ARG:NH1	2.38	0.56
1:n:149:ARG:NH1	1:n:172:LEU:O	2.39	0.56
7:T:58:CYS:HB2	8:D:805:LYS:HE3	1.86	0.56
8:a:712:ASP:O	8:a:782:LYS:NZ	2.38	0.56
8:a:915:HIS:NE2	8:a:978:ALA:O	2.38	0.56
8:Y:1327:THR:HG21	8:Y:1333:MET:HG2	1.88	0.56
1:n:160:ARG:NH1	1:n:164:GLU:OE2	2.39	0.56
8:a:101:ALA:HB3	8:Z:174:GLY:HA3	1.88	0.56
8:a:1059:ILE:HG22	8:a:1081:ILE:HG12	1.88	0.56
8:C:687:ILE:HG12	8:C:1006:MET:HE1	1.88	0.56
8:D:638:MET:HE3	8:D:864:VAL:HA	1.87	0.56
8:Y:174:GLY:HA3	8:Z:101:ALA:HB3	1.86	0.56
4:M:95:ARG:HB3	4:M:129:PHE:HB2	1.88	0.56
1:h:274:MET:HE1	3:g:290:VAL:HG21	1.86	0.56
1:I:62:ARG:NH2	1:I:284:GLU:OE1	2.39	0.56
3:g:165:LEU:N	3:g:276:LEU:O	2.39	0.56
3:g:254:CYS:SG	3:g:255:LEU:N	2.78	0.56
8:B:1041:THR:HG23	8:B:1103:ARG:HB3	1.87	0.56
8:Z:565:LEU:HD22	8:Z:1177:THR:HG21	1.88	0.56
8:C:936:PRO:HB3	8:C:952:LEU:HD13	1.88	0.55
8:D:451:HIS:HE1	8:D:1120:ASN:HB2	1.71	0.55
1:h:150:LEU:HD21	1:h:184:ILE:HG12	1.88	0.55
8:B:192:VAL:HA	8:B:219:PHE:HE1	1.72	0.55
8:B:505:VAL:HG11	8:B:974:PRO:HB3	1.87	0.55
8:C:445:ALA:HA	8:C:1110:VAL:HG11	1.88	0.55
8:D:1327:THR:HG21	8:D:1333:MET:HB2	1.88	0.55
8:Y:3:ASN:ND2	8:Z:317:SER:O	2.40	0.55
8:Z:575:THR:HG21	8:Z:1007:THR:HA	1.88	0.55
8:Z:889:HIS:O	8:Z:891:LYS:NZ	2.38	0.55
8:Z:1195:ARG:NH1	8:Z:1227:ALA:O	2.39	0.55
8:C:947:THR:HG22	8:C:967:HIS:HE1	1.71	0.55
8:Y:1156:MET:SD	8:Y:1294:ARG:NH1	2.80	0.55
8:Y:1285:TYR:HA	8:Y:1289:ALA:HB3	1.86	0.55
1:n:277:GLN:HE22	3:m:220:ARG:HH21	1.55	0.55
8:D:79:LYS:HE3	8:D:304:ASN:HB3	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Y:1247:ARG:O	8:Y:1251:ARG:NH1	2.40	0.55
8:Z:558:ILE:HD11	8:Z:1031:GLY:HA3	1.88	0.55
1:h:152:ILE:HD12	1:I:268:LEU:HB3	1.88	0.55
8:B:891:LYS:O	8:B:918:TYR:HB3	2.07	0.55
8:Z:311:ASN:ND2	8:Z:322:LEU:O	2.39	0.55
3:g:91:ALA:O	3:g:99:ARG:NH2	2.39	0.55
8:a:945:ASN:HD22	8:a:948:ILE:HG12	1.71	0.55
8:Y:49:HIS:O	8:Z:319:HIS:ND1	2.40	0.55
7:S:70:VAL:HG12	8:C:884:GLN:HG3	1.87	0.55
8:a:209:ARG:NH2	8:a:1203:ASP:OD2	2.39	0.55
8:a:1336:LYS:NZ	8:a:1346:THR:OG1	2.40	0.55
8:D:701:GLU:HG2	8:D:714:ARG:HH12	1.72	0.55
8:Z:1191:ASN:ND2	8:Z:1195:ARG:O	2.40	0.55
1:I:35:PRO:HA	1:I:68:MET:HG2	1.88	0.54
8:a:1185:TYR:HA	8:a:1190:ASN:HD22	1.71	0.54
8:a:792:MET:HE3	8:a:1005:VAL:HG22	1.88	0.54
8:D:478:LEU:HD11	8:D:509:VAL:HG13	1.89	0.54
8:Z:681:LEU:HD22	8:Z:783:VAL:HG13	1.89	0.54
4:M:571:HIS:HD2	4:M:576:ARG:HH11	1.53	0.54
8:a:627:ILE:HD11	8:a:882:ALA:HB2	1.90	0.54
8:a:927:PRO:HD2	8:a:952:LEU:HD21	1.89	0.54
8:a:1149:SER:HA	8:a:1152:THR:HG22	1.88	0.54
4:M:322:HIS:O	8:a:737:GLN:NE2	2.41	0.54
8:a:723:LEU:HD13	8:a:768:VAL:HG23	1.89	0.54
8:a:1176:LEU:HD21	8:a:1233:ALA:HB2	1.90	0.54
8:B:712:ASP:O	8:B:782:LYS:NZ	2.38	0.54
3:g:93:ASN:ND2	3:g:170:ASP:O	2.40	0.54
8:a:812:PHE:HE1	8:a:857:LEU:HD11	1.72	0.54
8:D:231:ASN:O	8:D:1369:ASN:ND2	2.41	0.54
1:n:147:ASN:ND2	1:n:284:GLU:OE1	2.41	0.54
7:S:66:ARG:NH1	8:C:751:VAL:O	2.41	0.54
8:B:1196:ALA:HB2	8:B:1223:GLN:HB2	1.89	0.54
8:B:1325:LEU:HB2	8:B:1358:GLU:HB2	1.89	0.54
8:C:263:THR:HG22	8:C:296:VAL:HG12	1.88	0.54
1:n:273:VAL:HG13	3:m:288:GLU:HG3	1.90	0.54
1:o:76:VAL:HG12	1:o:81:ILE:HG23	1.89	0.54
8:D:433:ARG:NH1	8:D:1102:VAL:O	2.41	0.54
8:Z:228:PHE:H	8:Z:232:ARG:HH21	1.55	0.54
8:Z:1289:ALA:HB1	8:Z:1316:ARG:HG2	1.89	0.54
8:B:651:TYR:HA	8:B:654:VAL:HG22	1.90	0.54
8:B:1182:ASP:OD1	8:B:1182:ASP:N	2.40	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Y:225:ALA:O	8:Y:232:ARG:NH1	2.41	0.54
8:Y:662:ALA:HB1	8:Z:605:ASN:HD22	1.73	0.54
8:Z:638:MET:HG2	8:Z:646:VAL:HB	1.90	0.54
6:1:79:GLU:OE1	6:1:83:ARG:NH1	2.41	0.54
8:B:489:GLY:O	8:B:494:ARG:NH2	2.41	0.54
8:B:798:CYS:SG	8:B:799:GLY:N	2.81	0.54
8:C:491:ALA:HA	8:C:494:ARG:HG2	1.88	0.54
8:D:1112:ASP:OD1	8:D:1112:ASP:N	2.41	0.54
8:Y:574:ARG:NH2	8:Y:1010:ALA:O	2.41	0.54
8:a:1334:GLU:O	8:a:1338:LYS:HB2	2.08	0.54
8:B:502:ARG:HH21	8:B:958:ARG:HD2	1.73	0.54
1:o:8:ILE:HB	1:o:83:LEU:HB2	1.89	0.53
8:B:770:ASP:HB3	8:B:772:ARG:HH21	1.72	0.53
8:C:433:ARG:HE	8:D:217:GLN:HG3	1.73	0.53
8:Y:732:VAL:HG12	8:Y:895:VAL:HG12	1.90	0.53
8:a:996:ALA:O	8:Z:686:ARG:NH2	2.41	0.53
8:a:1156:MET:HG2	8:a:1257:LYS:HG2	1.89	0.53
8:Z:249:ALA:HB3	8:Z:1093:ASN:HD21	1.73	0.53
6:1:136:ALA:HB1	6:1:157:VAL:HG21	1.90	0.53
8:a:497:HIS:HA	8:a:500:ARG:HD2	1.89	0.53
8:B:8:GLU:OE1	8:Z:162:ARG:NH1	2.41	0.53
8:Y:87:THR:HG22	8:Y:88:THR:HG23	1.89	0.53
8:Y:273:MET:HE3	8:Y:367:VAL:HG11	1.90	0.53
1:n:37:ARG:NH1	1:n:69:THR:OG1	2.40	0.53
8:a:138:TYR:O	8:a:153:ASN:ND2	2.42	0.53
8:a:625:LEU:HA	8:a:628:ARG:HG3	1.90	0.53
8:Z:182:THR:HG21	8:Z:1083:THR:HG21	1.89	0.53
8:Z:599:THR:O	8:Z:603:SER:OG	2.26	0.53
4:M:316:GLU:OE1	4:M:327:ARG:NH1	2.41	0.53
8:B:295:THR:HA	8:B:355:LEU:O	2.08	0.53
8:C:92:LEU:HD23	8:Z:7:LEU:HD22	1.89	0.53
1:o:71:THR:HG21	1:o:83:LEU:HD13	1.90	0.53
8:a:77:ALA:HB1	8:a:302:TYR:HD1	1.74	0.53
1:n:291:CYS:HG	1:n:301:THR:HG1	1.53	0.53
4:M:172:GLU:OE2	4:M:313:ARG:NH1	2.42	0.53
7:T:75:ARG:NH1	8:D:625:LEU:O	2.41	0.53
8:C:740:ASN:OD1	8:C:740:ASN:N	2.36	0.53
8:Z:694:ASN:ND2	8:Z:704:SER:OG	2.41	0.53
8:B:1027:HIS:HD2	8:C:517:VAL:HG21	1.74	0.53
8:Y:85:LYS:O	8:Y:319:HIS:NE2	2.40	0.53
8:Y:556:ILE:HG21	8:Y:986:TRP:HZ3	1.74	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Y:668:PRO:HB2	8:Z:643:GLN:HG2	1.91	0.53
8:Y:1316:ARG:O	8:Y:1319:GLN:NE2	2.42	0.53
8:C:756:ARG:NH2	8:C:888:GLU:OE1	2.41	0.53
8:Z:681:LEU:HB3	8:Z:780:LEU:HD22	1.90	0.53
8:Z:718:PRO:HD2	8:Z:785:TYR:HB3	1.90	0.53
4:M:531:PHE:O	4:M:542:SER:HA	2.09	0.52
8:a:1234:SER:HG	8:a:1235:GLN:H	1.58	0.52
8:B:495:ILE:HG12	8:B:976:PRO:HG2	1.91	0.52
8:Y:82:ASP:OD1	8:Y:82:ASP:N	2.43	0.52
8:B:413:LYS:HE2	8:B:1335:THR:HG23	1.91	0.52
8:C:1161:ALA:O	8:D:209:ARG:NH1	2.42	0.52
8:C:1268:THR:HA	8:C:1271:ILE:HB	1.91	0.52
3:g:91:ALA:O	3:g:199:ARG:NH2	2.42	0.52
4:M:372:ARG:HD3	4:M:415:MET:HG3	1.92	0.52
8:C:558:ILE:HD11	8:C:1031:GLY:HA3	1.91	0.52
1:n:283:ARG:NH1	1:o:279:ASP:OD2	2.42	0.52
4:M:556:ARG:HH21	4:M:560:GLN:HG3	1.74	0.52
8:C:955:ASP:OD1	8:C:958:ARG:NH2	2.43	0.52
8:Z:138:TYR:O	8:Z:153:ASN:ND2	2.43	0.52
8:Z:1182:ASP:OD1	8:Z:1182:ASP:N	2.40	0.52
8:C:151:ILE:HD12	8:D:332:LEU:HG	1.90	0.52
8:C:578:ILE:HG12	8:C:1028:ILE:HD12	1.91	0.52
8:C:925:THR:HA	8:C:948:ILE:HD12	1.91	0.52
3:m:262:SER:OG	3:m:263:PHE:N	2.43	0.52
8:B:93:PHE:HB3	8:B:95:VAL:HG23	1.92	0.52
8:B:451:HIS:HE2	8:B:1114:PHE:HA	1.75	0.52
8:B:669:GLN:O	8:B:673:HIS:ND1	2.37	0.52
8:D:249:ALA:HB3	8:D:1093:ASN:HD21	1.75	0.52
8:Y:1185:TYR:OH	8:Y:1191:ASN:O	2.25	0.52
1:o:151:LEU:HD21	1:o:281:LEU:HD13	1.91	0.52
4:M:166:ARG:HD3	4:M:350:LEU:HD11	1.92	0.52
4:M:431:ARG:NH2	4:M:527:PRO:O	2.42	0.52
7:R:66:ARG:HG3	7:R:67:MET:HE2	1.92	0.52
8:a:931:ILE:HD12	8:a:952:LEU:HD13	1.92	0.52
8:C:190:TYR:OH	8:C:194:GLN:NE2	2.39	0.52
8:C:487:PRO:O	8:C:494:ARG:NH1	2.43	0.52
8:Y:805:LYS:HB3	8:Y:889:HIS:HE1	1.75	0.52
8:B:620:ASN:ND2	8:B:769:ASP:OD2	2.43	0.52
8:D:382:LYS:NZ	8:D:386:GLU:O	2.43	0.52
1:n:121:ARG:HH21	1:n:123:ASN:HA	1.75	0.51
1:o:62:ARG:NH1	1:o:280:ASP:O	2.43	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:387:PRO:HA	5:N:23:VAL:HG12	1.92	0.51
8:B:609:LEU:HD22	8:B:861:VAL:HG12	1.92	0.51
8:C:1054:CYS:SG	8:C:1055:THR:N	2.83	0.51
8:C:1289:ALA:O	8:C:1316:ARG:NH1	2.43	0.51
1:n:207:VAL:HG23	1:n:271:LEU:HD11	1.91	0.51
4:M:400:TRP:HE3	4:M:403:VAL:HG11	1.75	0.51
7:T:37:HIS:NE2	8:D:818:LEU:O	2.42	0.51
8:B:1162:ALA:O	8:C:209:ARG:NH2	2.39	0.51
8:C:433:ARG:NH2	8:C:1104:THR:O	2.42	0.51
1:I:40:LEU:HD21	8:B:124:PRO:HG2	1.93	0.51
8:a:391:LEU:HB2	8:a:1042:PHE:HE2	1.75	0.51
8:a:1003:HIS:HA	8:a:1006:MET:HG2	1.92	0.51
8:C:341:ASN:HB3	8:C:346:GLN:HE21	1.75	0.51
8:C:524:VAL:HG22	8:C:1227:ALA:HB2	1.92	0.51
8:D:529:LEU:HD21	8:D:1228:THR:HG22	1.91	0.51
8:Y:1223:GLN:NE2	8:Y:1320:GLU:OE2	2.43	0.51
1:o:240:ARG:HD3	3:m:235:ILE:HD11	1.91	0.51
4:M:388:GLN:O	4:M:389:ARG:NH1	2.41	0.51
6:1:29:VAL:HG22	6:1:177:ASN:HA	1.92	0.51
8:Y:1128:ASP:OD1	8:Y:1132:ARG:NH2	2.42	0.51
8:Z:693:LEU:HB3	8:Z:1022:LEU:HD12	1.92	0.51
8:Z:1292:CYS:SG	8:Z:1293:ILE:N	2.83	0.51
5:O:65:LEU:HA	5:O:68:LEU:HG	1.92	0.51
7:S:52:SER:OG	7:S:53:LEU:N	2.44	0.51
7:j:26:LEU:HD13	7:j:64:LEU:HD22	1.93	0.51
1:h:283:ARG:NH2	1:I:279:ASP:OD2	2.44	0.51
1:I:177:PHE:HB3	1:I:180:ALA:HB3	1.93	0.51
1:n:125:LEU:HD13	1:n:132:LEU:HB3	1.93	0.51
6:1:271:LEU:O	6:1:278:TYR:OH	2.29	0.51
8:D:681:LEU:HD21	8:D:788:LEU:HD22	1.92	0.51
1:n:158:LEU:HD11	1:n:197:MET:HE3	1.92	0.51
7:S:72:ARG:NH1	8:C:820:MET:O	2.44	0.51
8:a:237:ASP:OD1	8:a:237:ASP:N	2.41	0.51
8:D:324:ASP:HB2	8:D:343:SER:HB3	1.92	0.51
8:Y:66:PHE:HA	8:Y:176:ILE:HD11	1.93	0.51
8:Z:419:THR:HG22	8:Z:421:ARG:H	1.76	0.51
8:Z:572:GLU:HG2	8:Z:1007:THR:HG21	1.92	0.51
1:h:206:MET:HE2	1:h:210:LEU:HD23	1.93	0.51
7:j:47:TYR:OH	7:j:60:PHE:O	2.25	0.51
8:D:1284:GLU:OE2	8:D:1288:ARG:NH1	2.43	0.51
8:Y:646:VAL:O	8:Y:674:TYR:OH	2.24	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Y:1195:ARG:HG2	8:Y:1234:SER:HB2	1.92	0.51
1:n:149:ARG:HB3	1:n:172:LEU:HD21	1.93	0.51
1:o:104:LYS:NZ	1:o:291:CYS:O	2.44	0.51
4:M:512:ARG:NH2	8:a:546:SER:O	2.42	0.51
8:D:180:LEU:HD23	8:D:384:PRO:HG2	1.93	0.51
8:D:1062:PRO:HA	8:D:1078:THR:O	2.10	0.51
8:a:115:MET:HE3	8:B:36:ARG:HB3	1.92	0.50
8:B:681:LEU:HD22	8:B:783:VAL:HG13	1.93	0.50
8:B:804:LEU:O	8:B:808:LEU:HB2	2.11	0.50
8:B:275:SER:OG	8:B:276:THR:N	2.44	0.50
8:C:93:PHE:HB2	8:C:116:VAL:HG13	1.93	0.50
8:D:740:ASN:OD1	8:D:740:ASN:N	2.45	0.50
8:Z:747:ARG:NH2	8:Z:888:GLU:OE2	2.44	0.50
1:o:29:ALA:O	1:o:95:LEU:N	2.42	0.50
1:o:105:GLY:H	1:o:290:VAL:HG23	1.76	0.50
8:a:507:ARG:NH1	8:a:515:ASP:OD2	2.43	0.50
8:B:38:TYR:OH	8:B:45:ARG:NH1	2.39	0.50
8:B:853:VAL:HG22	8:B:857:LEU:HD13	1.93	0.50
8:C:36:ARG:NH2	8:C:44:GLU:OE1	2.44	0.50
8:D:477:ARG:NH2	8:D:512:MET:SD	2.84	0.50
8:Y:617:VAL:HG11	8:Y:653:LEU:HD21	1.93	0.50
8:Z:719:PHE:HE1	8:Z:917:LEU:HD12	1.77	0.50
1:n:40:LEU:O	8:a:105:GLY:N	2.43	0.50
8:Y:774:THR:OG1	8:Y:777:GLU:OE2	2.24	0.50
1:n:121:ARG:NH2	1:n:122:GLU:O	2.44	0.50
7:R:75:ARG:NH1	8:B:625:LEU:O	2.39	0.50
8:B:487:PRO:O	8:B:494:ARG:NH1	2.44	0.50
8:B:796:ARG:O	8:B:945:ASN:ND2	2.45	0.50
8:B:936:PRO:HB3	8:B:952:LEU:HD12	1.93	0.50
8:C:1284:GLU:OE2	8:C:1288:ARG:NH2	2.45	0.50
8:Z:534:HIS:HD2	8:Z:536:PHE:H	1.58	0.50
8:Z:615:VAL:HG21	8:Z:802:LEU:HD23	1.93	0.50
8:Z:753:ASP:OD2	8:Z:753:ASP:N	2.41	0.50
2:P:2236:ARG:HH22	5:N:68:LEU:HB2	1.76	0.50
8:B:849:GLN:HB2	8:B:873:LEU:HD23	1.94	0.50
8:C:592:GLU:OE1	8:C:595:ARG:NH1	2.45	0.50
1:I:229:MET:HA	1:I:232:VAL:HG22	1.94	0.50
3:g:66:LEU:HD11	3:g:165:LEU:HD21	1.94	0.50
8:a:1313:ASN:HB3	8:a:1316:ARG:HE	1.77	0.50
8:C:216:LEU:HD13	8:C:1200:LEU:HD22	1.93	0.50
8:D:1111:GLN:NE2	8:D:1112:ASP:OD1	2.44	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Y:940:HIS:O	8:Y:944:SER:OG	2.26	0.50
8:Z:36:ARG:NH2	8:Z:44:GLU:OE2	2.45	0.50
1:h:184:ILE:HD12	1:h:185:PRO:HD2	1.93	0.50
8:a:1038:ARG:NH1	8:a:1107:GLY:O	2.45	0.50
8:Y:681:LEU:HD22	8:Y:783:VAL:HG13	1.92	0.50
8:Z:142:THR:OG1	8:Z:149:ASP:OD2	2.26	0.50
3:g:72:THR:HG21	3:g:80:LEU:HD23	1.94	0.50
8:a:83:LEU:HD21	8:a:1082:ASN:HB2	1.94	0.50
8:a:384:PRO:O	8:a:387:ARG:NH2	2.45	0.50
8:C:688:SER:OG	8:C:708:ASN:ND2	2.45	0.50
8:Z:703:LEU:HA	8:Z:706:TYR:HD2	1.77	0.50
1:I:58:TYR:OH	1:I:62:ARG:NH1	2.44	0.49
3:m:258:ASP:OD1	3:m:258:ASP:N	2.43	0.49
4:M:378:VAL:HG21	4:M:543:SER:HB3	1.93	0.49
8:a:452:PRO:HB2	8:a:1120:ASN:HB3	1.94	0.49
8:Z:790:PRO:HA	8:Z:793:THR:HG22	1.93	0.49
8:Z:1157:SER:OG	8:Z:1255:ASN:ND2	2.45	0.49
4:M:454:PRO:HA	4:M:457:LEU:HB2	1.95	0.49
8:Y:618:HIS:NE2	8:Y:886:VAL:O	2.45	0.49
8:Z:594:LEU:HD12	8:Z:792:MET:HE3	1.93	0.49
1:h:189:ILE:HG23	1:h:193:LEU:HD23	1.94	0.49
1:n:10:CYS:HB3	1:n:81:ILE:HB	1.94	0.49
8:B:1091:THR:OG1	8:B:1092:SER:N	2.45	0.49
8:C:225:ALA:O	8:C:232:ARG:NH1	2.42	0.49
8:C:1035:THR:HB	8:C:1176:LEU:HD22	1.93	0.49
8:Y:717:PRO:HB3	8:Y:782:LYS:HA	1.93	0.49
8:Y:775:ASP:N	8:Y:775:ASP:OD1	2.43	0.49
8:Z:1121:VAL:HG12	8:Z:1132:ARG:HH12	1.77	0.49
8:a:610:CYS:O	8:a:614:ASP:HB2	2.12	0.49
8:B:41:ASP:N	8:B:41:ASP:OD1	2.44	0.49
8:B:273:MET:HE2	8:B:1049:TYR:HB2	1.94	0.49
8:D:416:LEU:HD13	8:D:422:ASN:HB3	1.93	0.49
8:Y:1298:ASP:OD1	8:Y:1298:ASP:N	2.41	0.49
1:h:73:MET:HB3	1:h:81:ILE:HD11	1.93	0.49
7:T:73:THR:O	7:T:74:ARG:NE	2.45	0.49
8:B:695:ASN:ND2	8:C:511:GLU:OE2	2.38	0.49
8:B:816:ALA:O	8:B:877:ARG:NH1	2.35	0.49
8:D:624:PHE:HA	8:D:627:ILE:HG22	1.93	0.49
8:D:1247:ARG:HE	8:D:1269:GLU:HG3	1.77	0.49
8:B:404:ASP:OD1	8:B:405:ARG:NH2	2.45	0.49
8:B:484:GLN:O	8:B:981:HIS:NE2	2.44	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:275:SER:OG	8:D:276:THR:N	2.46	0.49
8:Y:311:ASN:ND2	8:Y:322:LEU:O	2.44	0.49
8:Z:420:VAL:HG11	8:Z:576:TRP:HB3	1.94	0.49
8:Z:507:ARG:HE	8:Z:512:MET:HE1	1.78	0.49
7:T:43:MET:HE3	7:T:46:LYS:HG2	1.95	0.49
8:a:478:LEU:HD11	8:a:530:TYR:HE1	1.77	0.49
8:a:953:SER:OG	8:a:954:ASP:N	2.45	0.49
8:B:547:GLU:HG3	8:B:549:VAL:HG13	1.94	0.49
8:C:608:GLU:OE2	8:C:929:THR:OG1	2.30	0.49
8:C:675:ARG:HE	8:D:603:SER:HA	1.77	0.49
8:D:681:LEU:HB3	8:D:780:LEU:HD22	1.94	0.49
8:D:1110:VAL:HA	8:D:1171:ALA:HB3	1.94	0.49
8:Y:629:THR:O	8:Y:633:ARG:NH1	2.46	0.49
8:Z:800:LEU:HD22	8:Z:923:VAL:HB	1.93	0.49
8:B:542:CYS:SG	8:B:543:GLN:N	2.85	0.49
8:C:575:THR:HG22	8:C:1010:ALA:HB3	1.94	0.49
8:D:126:THR:HG22	8:D:128:PRO:HD3	1.94	0.49
8:Z:761:ASP:OD1	8:Z:761:ASP:N	2.43	0.49
8:Z:927:PRO:HB2	8:Z:930:LEU:HB2	1.94	0.49
1:I:159:ASP:OD1	1:I:159:ASP:N	2.43	0.49
8:a:218:SER:OG	8:a:222:LYS:NZ	2.39	0.49
8:B:509:VAL:HG12	8:B:513:LYS:HE3	1.95	0.49
8:C:558:ILE:HB	8:C:1015:ILE:HD11	1.95	0.49
8:C:908:PRO:HG3	8:C:1123:ARG:HH12	1.78	0.49
8:Y:323:ALA:HB3	8:Y:343:SER:HB2	1.95	0.49
8:Y:1286:LEU:O	8:Y:1290:LYS:NZ	2.46	0.49
8:Z:764:GLU:HG2	8:Z:765:PRO:HD3	1.94	0.49
1:I:229:MET:SD	1:I:229:MET:N	2.85	0.49
8:D:795:ASN:ND2	8:D:969:HIS:O	2.41	0.49
3:m:18:ASN:HB2	3:m:21:VAL:HG23	1.95	0.48
8:C:357:MET:HE3	8:C:358:ASP:H	1.78	0.48
8:Y:41:ASP:OD1	8:Y:41:ASP:N	2.44	0.48
8:Y:54:PHE:HB2	8:Z:91:MET:HG2	1.95	0.48
8:Y:130:GLU:HA	8:Y:1074:THR:HA	1.95	0.48
8:Y:668:PRO:HB3	8:Z:642:ARG:HA	1.94	0.48
8:a:502:ARG:NH1	8:a:962:GLU:OE1	2.46	0.48
8:D:694:ASN:HA	8:D:703:LEU:HD23	1.94	0.48
8:D:1193:ARG:HB3	8:D:1266:PHE:HE1	1.78	0.48
8:Z:176:ILE:HG21	8:Z:375:VAL:HG21	1.95	0.48
1:h:24:LEU:HD21	1:h:81:ILE:HD12	1.95	0.48
6:1:31:LEU:HB3	6:1:38:LEU:HD21	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:a:392:THR:HG22	8:a:1039:THR:HG22	1.94	0.48
8:a:810:ASP:O	8:a:814:ARG:NH1	2.43	0.48
8:Y:780:LEU:HA	8:Y:783:VAL:HG12	1.95	0.48
8:Y:1004:SER:HA	8:Y:1007:THR:HG22	1.95	0.48
8:Y:1054:CYS:SG	8:Y:1055:THR:N	2.86	0.48
8:Z:970:ASP:N	8:Z:970:ASP:OD1	2.45	0.48
1:n:280:ASP:O	3:m:213:GLN:NE2	2.47	0.48
8:B:252:ASP:N	8:B:252:ASP:OD1	2.46	0.48
8:Y:142:THR:OG1	8:Y:153:ASN:ND2	2.37	0.48
8:Y:970:ASP:OD1	8:Y:970:ASP:N	2.47	0.48
1:o:7:ASN:HA	1:o:83:LEU:O	2.13	0.48
1:o:93:THR:HG21	8:C:1071:ILE:HG22	1.95	0.48
3:m:121:GLY:HA3	3:m:128:ARG:HH22	1.78	0.48
8:B:1286:LEU:O	8:B:1290:LYS:NZ	2.45	0.48
8:D:635:ILE:HA	8:D:646:VAL:HG11	1.95	0.48
8:D:709:ALA:HB3	8:D:1012:LEU:HB3	1.96	0.48
3:m:68:ILE:HD12	3:m:131:THR:HG22	1.95	0.48
8:a:1153:PHE:HB2	8:a:1304:VAL:HG11	1.96	0.48
8:B:180:LEU:HD23	8:B:384:PRO:HG2	1.95	0.48
8:B:273:MET:HE3	8:B:367:VAL:HG11	1.95	0.48
8:B:396:PRO:HB2	8:B:399:LEU:HD23	1.96	0.48
8:C:1060:ASN:O	8:C:1079:GLN:NE2	2.45	0.48
1:I:56:ARG:NH2	8:B:1153:PHE:O	2.45	0.48
8:B:126:THR:HG23	8:B:1078:THR:HG22	1.95	0.48
8:B:1183:VAL:HG13	8:B:1187:LYS:HZ1	1.78	0.48
8:D:108:THR:OG1	8:D:109:SER:N	2.47	0.48
8:D:820:MET:HG2	8:D:877:ARG:HE	1.79	0.48
8:Y:503:ARG:HH21	8:Y:505:VAL:HA	1.78	0.48
1:I:23:LYS:HD3	1:I:125:LEU:HA	1.96	0.48
8:a:718:PRO:HD2	8:a:785:TYR:HB3	1.94	0.48
8:B:1064:VAL:HG22	8:B:1077:VAL:HG12	1.95	0.48
8:Y:878:GLU:HA	8:Y:881:LEU:HG	1.96	0.48
1:h:277:GLN:HG3	3:g:290:VAL:HG22	1.94	0.48
3:m:172:TYR:OH	3:m:179:ARG:NH2	2.46	0.48
8:B:388:ASN:HB2	8:B:1311:ILE:HG23	1.95	0.48
8:C:253:SER:HB3	8:C:1054:CYS:HA	1.96	0.48
8:D:1047:LEU:HD23	8:D:1097:ALA:HB2	1.96	0.48
8:D:1147:THR:O	8:D:1151:LEU:N	2.46	0.48
8:Y:229:LEU:HD11	8:Y:238:TYR:HE2	1.78	0.48
8:Y:393:PHE:HD2	8:Y:1038:ARG:HH21	1.62	0.48
1:o:62:ARG:NH2	1:o:284:GLU:OE1	2.47	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:m:61:ALA:HA	3:m:138:VAL:HG11	1.95	0.48
4:M:132:LEU:HD21	4:M:149:LEU:HD23	1.94	0.48
8:a:1285:TYR:HA	8:a:1289:ALA:HB3	1.96	0.48
8:B:478:LEU:HD11	8:B:509:VAL:HG13	1.96	0.48
8:D:246:LEU:O	8:D:1093:ASN:ND2	2.47	0.48
8:D:661:LEU:HD21	8:D:666:LEU:HD21	1.96	0.48
8:D:1106:MET:SD	8:D:1363:GLN:NE2	2.87	0.48
8:Y:189:PRO:HA	8:Y:1094:THR:HB	1.95	0.48
8:Y:651:TYR:HB2	8:Y:784:PHE:CG	2.49	0.48
8:Y:681:LEU:HB3	8:Y:780:LEU:HD22	1.95	0.48
8:Z:396:PRO:HB2	8:Z:399:LEU:HD23	1.96	0.48
1:I:243:ARG:HH11	1:I:247:VAL:HB	1.79	0.47
6:1:129:LEU:HD22	6:1:204:VAL:HG23	1.95	0.47
6:1:253:ILE:HG23	6:1:270:LEU:HD23	1.95	0.47
8:B:427:THR:OG1	8:C:405:ARG:NH1	2.46	0.47
8:D:981:HIS:HB3	8:D:984:HIS:HB2	1.96	0.47
8:D:1294:ARG:HB2	8:D:1303:CYS:HA	1.96	0.47
8:Y:207:LEU:HD13	8:Y:212:ARG:HB3	1.95	0.47
7:T:28:LEU:HD12	7:T:29:PRO:HD2	1.96	0.47
8:a:438:GLN:HE22	8:a:1107:GLY:HA2	1.78	0.47
8:B:895:VAL:HG23	8:B:914:GLN:HB3	1.95	0.47
8:C:120:SER:HB3	8:C:1084:VAL:HG22	1.96	0.47
8:D:605:ASN:O	8:D:642:ARG:NH1	2.47	0.47
8:Z:801:GLY:N	8:Z:935:LEU:O	2.37	0.47
1:o:146:ILE:HD11	1:o:175:ILE:HD13	1.96	0.47
8:B:747:ARG:HH12	8:B:887:GLY:HA2	1.78	0.47
8:C:388:ASN:HB2	8:C:1311:ILE:HG23	1.96	0.47
8:D:450:CYS:O	8:D:1122:TYR:OH	2.29	0.47
8:Z:717:PRO:HD3	8:Z:782:LYS:HG3	1.96	0.47
8:B:1101:ARG:NH2	8:C:218:SER:OG	2.48	0.47
8:B:1290:LYS:HB2	8:B:1310:LEU:HD22	1.95	0.47
8:D:389:VAL:HG13	8:D:1044:VAL:HG21	1.97	0.47
3:g:64:GLY:O	3:g:85:TYR:OH	2.30	0.47
4:M:372:ARG:HA	4:M:375:ILE:HD12	1.97	0.47
7:i:28:LEU:HD12	7:i:29:PRO:HD2	1.96	0.47
8:a:553:THR:HG21	8:a:983:TYR:HB3	1.97	0.47
8:a:801:GLY:HA3	8:a:890:VAL:HG21	1.97	0.47
8:C:520:ASP:HA	8:C:523:LYS:HG3	1.96	0.47
8:C:693:LEU:HG	8:D:515:ASP:HB2	1.95	0.47
8:D:502:ARG:NH1	8:D:962:GLU:OE1	2.43	0.47
1:o:66:ARG:HD3	1:o:285:GLN:HE22	1.80	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:g:69:ARG:HH21	3:g:130:GLU:HG3	1.79	0.47
3:g:233:ARG:HA	3:g:236:THR:HG22	1.96	0.47
8:a:658:ALA:HB2	8:a:674:TYR:HB3	1.95	0.47
8:D:427:THR:OG1	8:D:440:ILE:O	2.33	0.47
8:Y:515:ASP:N	8:Y:515:ASP:OD1	2.47	0.47
8:Z:1248:HIS:CE1	8:Z:1251:ARG:HH22	2.32	0.47
8:Z:1290:LYS:HB2	8:Z:1310:LEU:HD23	1.96	0.47
1:h:105:GLY:H	1:h:290:VAL:HG23	1.80	0.47
1:o:178:ARG:HH22	3:m:79:HIS:CE1	2.31	0.47
3:m:78:ARG:O	3:m:79:HIS:ND1	2.47	0.47
4:M:96:VAL:HG22	4:M:128:VAL:HG12	1.97	0.47
5:O:63:GLN:HA	5:O:66:ARG:HD2	1.97	0.47
6:1:175:ARG:NE	6:1:216:SER:OG	2.43	0.47
8:a:1195:ARG:NH2	8:a:1221:ASP:OD1	2.47	0.47
8:B:127:ILE:HD12	8:B:128:PRO:HD2	1.97	0.47
8:B:413:LYS:HG3	8:B:414:VAL:HG13	1.97	0.47
8:B:610:CYS:HB3	8:B:649:HIS:HE1	1.80	0.47
8:C:399:LEU:HD11	8:C:1180:THR:HG22	1.97	0.47
8:D:182:THR:HG21	8:D:1083:THR:HG21	1.97	0.47
1:o:292:ASP:OD1	1:o:292:ASP:N	2.48	0.47
4:M:378:VAL:HA	4:M:381:ARG:HG2	1.96	0.47
8:a:254:ILE:HG23	8:B:15:ILE:HG21	1.96	0.47
8:B:140:ARG:HG2	8:B:141:GLU:HG2	1.97	0.47
8:B:605:ASN:HD22	8:B:642:ARG:HD3	1.79	0.47
8:C:393:PHE:HZ	8:C:1362:LEU:HD21	1.79	0.47
8:D:420:VAL:HG11	8:D:576:TRP:HB3	1.97	0.47
8:D:1105:ASP:HB2	8:D:1166:HIS:HB3	1.96	0.47
3:g:95:SER:OG	3:g:96:ALA:N	2.48	0.47
3:m:77:PRO:HD3	8:C:1150:MET:HG2	1.96	0.47
7:j:72:ARG:NH2	8:a:820:MET:O	2.48	0.47
8:a:1260:SER:HB3	8:a:1263:ALA:HB2	1.97	0.47
8:B:224:LEU:HD11	8:B:1189:PRO:HG2	1.97	0.47
8:B:941:ARG:NH1	8:B:971:GLY:O	2.48	0.47
8:C:611:TYR:O	8:C:614:ASP:HB3	2.15	0.47
8:D:215:ILE:HG21	8:D:1278:LEU:HD11	1.97	0.47
8:D:387:ARG:NH2	8:D:1310:LEU:O	2.44	0.47
8:Y:798:CYS:SG	8:Y:799:GLY:N	2.87	0.47
8:Z:981:HIS:O	8:Z:985:ASN:N	2.48	0.47
1:h:28:VAL:HG23	1:h:74:ARG:HA	1.96	0.47
1:h:61:LEU:HD12	1:h:64:LEU:HD11	1.97	0.47
3:m:91:ALA:O	3:m:99:ARG:NH2	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:1122:TYR:HB2	8:B:1128:ASP:HB2	1.97	0.47
8:D:631:VAL:HG13	8:D:647:PHE:HE2	1.79	0.47
8:D:861:VAL:HG13	8:D:865:ALA:HB3	1.97	0.47
8:Y:169:ASP:OD2	8:Y:173:ARG:NH2	2.48	0.47
8:Y:263:THR:HB	8:Y:267:ALA:H	1.81	0.47
1:h:142:LEU:HD13	1:h:177:PHE:HB2	1.97	0.46
1:I:15:LYS:NZ	8:B:88:THR:OG1	2.46	0.46
3:m:236:THR:HG23	3:m:237:ARG:HG3	1.96	0.46
8:B:230:LEU:HD12	8:B:1098:TYR:HB2	1.98	0.46
8:C:145:GLY:O	8:C:150:LYS:NZ	2.43	0.46
8:Y:500:ARG:O	8:Y:502:ARG:NH1	2.48	0.46
8:Z:297:SER:HA	8:Z:353:THR:O	2.14	0.46
8:Z:518:VAL:HG22	8:Z:1179:VAL:HG21	1.97	0.46
8:Z:614:ASP:OD1	8:Z:649:HIS:NE2	2.48	0.46
3:m:183:GLN:HG2	3:m:256:ALA:HB2	1.97	0.46
8:B:1122:TYR:HE2	8:B:1131:ILE:HG21	1.81	0.46
8:Y:1182:ASP:OD1	8:Y:1182:ASP:N	2.43	0.46
8:Y:1336:LYS:NZ	8:Y:1343:ALA:O	2.48	0.46
8:Z:537:PHE:O	8:Z:555:ARG:NH1	2.48	0.46
1:o:48:LEU:HD22	1:o:61:LEU:HD21	1.97	0.46
1:o:178:ARG:HD3	3:m:78:ARG:HE	1.80	0.46
6:1:127:ARG:HA	6:1:130:VAL:HG22	1.96	0.46
7:S:62:LEU:HD11	8:C:808:LEU:HB3	1.97	0.46
8:a:1237:GLY:N	8:a:1241:ASP:OD2	2.47	0.46
8:B:82:ASP:OD1	8:B:82:ASP:N	2.49	0.46
8:B:780:LEU:HA	8:B:783:VAL:HG12	1.96	0.46
8:D:785:TYR:O	8:D:943:TYR:OH	2.31	0.46
8:Y:1238:CYS:SG	8:Y:1240:SER:OG	2.69	0.46
1:h:234:CYS:HB2	1:I:206:MET:HE3	1.97	0.46
1:I:292:ASP:OD2	1:I:292:ASP:N	2.48	0.46
3:m:153:TYR:OH	8:Z:1069:ARG:NH1	2.48	0.46
4:M:167:ASP:OD1	4:M:167:ASP:N	2.49	0.46
8:a:707:VAL:HG12	8:a:1019:SER:HA	1.97	0.46
1:n:198:LYS:HE2	1:n:198:LYS:HB2	1.71	0.46
1:n:198:LYS:HD3	1:o:231:LEU:HD13	1.96	0.46
1:n:292:ASP:OD1	1:n:301:THR:OG1	2.34	0.46
3:m:66:LEU:HD12	3:m:84:LEU:HD22	1.98	0.46
8:a:631:VAL:HA	8:a:634:CYS:HB3	1.97	0.46
8:a:1047:LEU:HD22	8:a:1097:ALA:HB2	1.98	0.46
8:Y:416:LEU:HB3	8:Y:422:ASN:HD21	1.79	0.46
8:Y:937:VAL:HG12	8:Y:939:PHE:HB3	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Z:351:SER:OG	8:Z:352:LEU:N	2.48	0.46
8:Z:448:THR:HG23	8:Z:1113:LEU:HG	1.96	0.46
8:Z:594:LEU:HD11	8:Z:788:LEU:HD11	1.98	0.46
4:M:445:ARG:O	4:M:449:ARG:NH2	2.49	0.46
8:B:724:PRO:HA	8:B:773:ALA:HB3	1.97	0.46
8:C:118:LYS:NZ	8:C:1087:GLY:O	2.48	0.46
8:C:1184:ASN:O	8:C:1190:ASN:ND2	2.49	0.46
8:D:576:TRP:HA	8:D:579:MET:HE3	1.97	0.46
8:D:1241:ASP:O	8:D:1248:HIS:ND1	2.49	0.46
8:Y:531:THR:OG1	8:Y:539:PHE:O	2.29	0.46
4:M:518:PRO:HA	4:M:536:PRO:HG2	1.98	0.46
8:a:601:VAL:HG22	8:a:924:VAL:HG11	1.98	0.46
8:a:908:PRO:HG3	8:a:1123:ARG:HH12	1.80	0.46
8:B:604:PRO:HA	8:B:925:THR:HG21	1.98	0.46
8:B:1104:THR:OG1	8:B:1105:ASP:N	2.49	0.46
2:H:2236:ARG:HH12	2:H:2240:LEU:HB2	1.81	0.46
1:n:8:ILE:HB	1:n:83:LEU:HB2	1.97	0.46
8:B:1070:ASP:OD2	8:B:1070:ASP:N	2.48	0.46
8:C:556:ILE:HD12	8:C:899:LEU:HD11	1.97	0.46
8:D:796:ARG:O	8:D:945:ASN:ND2	2.48	0.46
8:Y:1246:THR:HA	8:Y:1249:ARG:HB3	1.97	0.46
8:Z:63:TRP:HH2	8:Z:165:LYS:HB3	1.81	0.46
1:I:196:ASP:OD1	1:I:196:ASP:N	2.49	0.46
1:o:60:ARG:N	1:o:196:ASP:OD2	2.42	0.46
7:j:67:MET:HA	7:j:70:VAL:HG12	1.98	0.46
8:B:447:LYS:HB3	8:B:447:LYS:HE2	1.84	0.46
8:B:1336:LYS:NZ	8:B:1346:THR:OG1	2.39	0.46
8:D:404:ASP:OD1	8:D:404:ASP:N	2.49	0.46
8:Y:180:LEU:HD23	8:Y:384:PRO:HG2	1.98	0.46
8:Z:487:PRO:HG3	8:Z:736:ARG:HE	1.80	0.46
8:Z:715:LEU:HB3	8:Z:782:LYS:HZ3	1.80	0.46
1:o:75:ARG:HB3	1:o:82:LEU:HD12	1.98	0.45
3:m:148:CYS:SG	3:m:149:VAL:N	2.89	0.45
6:1:249:TYR:OH	6:1:274:ASP:OD1	2.28	0.45
7:j:28:LEU:HD13	7:j:32:ILE:HB	1.98	0.45
8:D:268:LYS:O	8:D:366:THR:OG1	2.32	0.45
8:Y:1350:HIS:CD2	8:Y:1351:PHE:H	2.34	0.45
6:1:7:GLY:HA3	6:1:46:LEU:HD21	1.98	0.45
8:B:698:LEU:HD22	8:B:1018:VAL:HG21	1.99	0.45
8:C:712:ASP:O	8:C:782:LYS:NZ	2.47	0.45
8:D:622:ASP:OD1	8:D:622:ASP:N	2.44	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Z:940:HIS:HE1	8:Z:987:LEU:HD12	1.80	0.45
8:a:155:GLU:OE2	8:a:162:ARG:NH1	2.49	0.45
8:a:975:LEU:HB3	8:a:979:PHE:HB2	1.98	0.45
8:C:387:ARG:NH2	8:C:1310:LEU:O	2.40	0.45
8:Y:393:PHE:N	8:Y:1038:ARG:O	2.36	0.45
1:I:59:VAL:HB	1:I:196:ASP:HB2	1.98	0.45
4:M:36:GLU:HA	4:M:153:TRP:HE1	1.81	0.45
7:R:43:MET:HE3	7:R:67:MET:HG3	1.99	0.45
8:B:1129:ARG:HE	8:B:1139:ARG:HH12	1.63	0.45
8:C:8:GLU:OE1	8:C:45:ARG:NH1	2.49	0.45
8:C:388:ASN:HD22	8:C:1043:GLU:HA	1.82	0.45
8:D:1290:LYS:HD2	8:D:1312:GLU:HG3	1.99	0.45
8:Z:1240:SER:O	8:Z:1244:TYR:N	2.47	0.45
1:h:169:VAL:HA	1:h:172:LEU:HB3	1.98	0.45
1:I:34:ILE:HG13	1:I:69:THR:HG23	1.97	0.45
6:1:67:ARG:NH1	6:1:265:ASP:OD1	2.49	0.45
8:a:1158:GLU:O	8:a:1301:TYR:OH	2.32	0.45
8:B:903:GLN:HE22	8:B:1014:LYS:HE2	1.82	0.45
8:B:934:SER:HB2	8:B:952:LEU:HD13	1.99	0.45
8:C:392:THR:HA	8:C:1039:THR:HA	1.99	0.45
8:D:1157:SER:OG	8:D:1158:GLU:N	2.49	0.45
8:Y:940:HIS:HD2	8:Y:942:PHE:H	1.64	0.45
8:Z:21:THR:OG1	8:Z:22:HIS:N	2.49	0.45
8:Z:1023:GLN:HB2	8:Z:1028:ILE:HB	1.98	0.45
1:n:280:ASP:OD1	1:o:283:ARG:NH2	2.49	0.45
1:o:55:THR:HG23	1:o:56:ARG:HE	1.81	0.45
1:o:149:ARG:NH1	1:o:174:THR:O	2.41	0.45
3:g:70:MET:O	3:g:79:HIS:HA	2.15	0.45
8:a:1263:ALA:O	8:a:1267:ASN:ND2	2.49	0.45
8:B:134:ALA:HA	8:B:137:THR:HG22	1.99	0.45
8:B:694:ASN:ND2	8:C:968:ARG:HG3	2.32	0.45
8:D:804:LEU:O	8:D:808:LEU:HB2	2.17	0.45
8:Z:562:PRO:HD2	8:Z:565:LEU:HD12	1.99	0.45
1:n:48:LEU:HB3	1:n:133:VAL:HG13	1.99	0.45
3:g:101:LEU:HD11	3:g:269:LEU:HB3	1.97	0.45
7:T:66:ARG:HG3	8:D:884:GLN:HA	1.99	0.45
8:a:967:HIS:NE2	8:Z:776:ASP:OD2	2.50	0.45
1:h:48:LEU:HB2	1:h:133:VAL:HG23	1.98	0.45
3:m:80:LEU:HD12	3:m:80:LEU:HA	1.88	0.45
3:m:285:ASP:OD1	3:m:285:ASP:N	2.50	0.45
8:a:1189:PRO:HD3	8:a:1359:ILE:HG21	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:798:CYS:SG	8:D:799:GLY:N	2.90	0.45
8:Y:845:SER:OG	8:Y:846:ILE:N	2.49	0.45
8:Z:900:ASP:OD1	8:Z:900:ASP:N	2.49	0.45
1:h:216:MET:HE1	1:I:209:ASN:HA	1.99	0.45
1:I:48:LEU:HD23	1:I:61:LEU:HD21	1.99	0.45
1:n:13:ASP:OD1	1:n:13:ASP:N	2.50	0.45
8:B:1124:HIS:CE1	8:B:1126:GLU:HB3	2.52	0.45
8:C:207:LEU:HD12	8:Z:29:GLU:HG2	1.98	0.45
8:C:1165:VAL:HG13	8:C:1166:HIS:HD2	1.82	0.45
8:C:1183:VAL:HA	8:C:1187:LYS:HE2	1.99	0.45
8:Y:1032:PHE:HA	8:Y:1178:PRO:HD3	1.98	0.45
1:I:75:ARG:NH2	1:I:77:GLU:OE2	2.50	0.45
3:m:245:THR:HG23	3:m:290:VAL:HG22	1.98	0.45
4:M:479:ARG:HA	4:M:520:VAL:HG12	1.98	0.45
7:i:33:SER:OG	7:i:34:GLU:N	2.50	0.45
8:a:1222:ALA:HB1	8:Z:1165:VAL:HG22	2.00	0.45
8:B:555:ARG:NH1	8:B:560:ASN:O	2.49	0.45
8:B:1106:MET:HE2	8:B:1106:MET:HB3	1.87	0.45
8:D:1246:THR:HA	8:D:1249:ARG:HB2	1.99	0.45
8:Y:854:GLY:O	8:Y:858:THR:OG1	2.32	0.45
8:Y:1176:LEU:HD13	8:Y:1176:LEU:HA	1.81	0.45
8:Y:1360:ILE:HG13	8:Y:1362:LEU:HD22	1.99	0.45
8:Z:1:MET:SD	8:Z:1:MET:N	2.82	0.45
8:Z:392:THR:HA	8:Z:1039:THR:HA	1.99	0.45
8:Z:1172:CYS:HB2	8:Z:1261:PRO:HG2	1.98	0.45
4:M:433:SER:OG	4:M:434:ARG:N	2.50	0.44
5:N:25:ARG:HH11	5:O:5:HIS:HB2	1.82	0.44
5:N:41:THR:HG23	5:N:42:MET:HE2	1.98	0.44
8:a:867:ASP:HB2	8:a:870:THR:HG22	1.98	0.44
8:a:942:PHE:HE2	8:a:987:LEU:HD22	1.81	0.44
8:a:1366:MET:HE3	8:a:1366:MET:HB3	1.92	0.44
8:D:288:SER:HA	8:D:291:ILE:HG12	1.99	0.44
8:D:682:ARG:HA	8:D:682:ARG:HD3	1.77	0.44
8:Y:310:GLU:HA	8:Y:313:VAL:HG12	1.98	0.44
3:m:82:ILE:HG23	3:m:86:LEU:HD22	1.99	0.44
3:m:154:LEU:O	3:m:163:PHE:N	2.49	0.44
6:l:175:ARG:HE	6:l:216:SER:HG	1.65	0.44
8:a:120:SER:OG	8:a:1083:THR:O	2.34	0.44
8:a:426:THR:HG23	8:a:427:THR:HG23	1.99	0.44
8:B:1285:TYR:OH	8:B:1312:GLU:OE1	2.27	0.44
8:D:553:THR:HG21	8:D:983:TYR:HB3	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Y:228:PHE:H	8:Y:232:ARG:HH21	1.65	0.44
8:Y:534:HIS:HD2	8:Y:536:PHE:H	1.65	0.44
8:Z:1193:ARG:NH2	8:Z:1234:SER:O	2.48	0.44
1:h:13:ASP:OD1	1:h:13:ASP:N	2.49	0.44
1:o:91:LEU:HD22	3:m:46:LEU:HD22	1.99	0.44
3:g:168:PRO:HB3	3:g:271:LEU:HD21	2.00	0.44
6:1:11:ARG:NH1	6:1:12:ASP:OD1	2.50	0.44
8:B:424:LEU:HD12	8:B:424:LEU:HA	1.88	0.44
8:C:741:PRO:HB2	8:C:743:ASN:H	1.81	0.44
8:D:220:LYS:HZ2	8:D:1318:THR:HG1	1.59	0.44
8:Y:421:ARG:NH2	8:Y:1027:HIS:O	2.49	0.44
8:Y:690:LEU:HB3	8:Y:693:LEU:HD13	1.98	0.44
8:Y:1191:ASN:ND2	8:Y:1319:GLN:O	2.51	0.44
8:Z:1021:VAL:HG12	8:Z:1025:LYS:HE2	1.98	0.44
8:Z:1105:ASP:OD1	8:Z:1105:ASP:N	2.51	0.44
4:M:54:SER:OG	4:M:55:THR:N	2.50	0.44
8:C:53:ILE:HG23	8:D:92:LEU:HD13	1.99	0.44
8:C:1109:ARG:HH11	8:C:1169:LYS:HB3	1.83	0.44
8:C:1303:CYS:SG	8:C:1304:VAL:N	2.89	0.44
8:D:433:ARG:HH22	8:D:1101:ARG:HH21	1.66	0.44
8:Y:1034:LEU:HD12	8:Y:1175:ILE:HA	2.00	0.44
8:Y:1235:GLN:HB2	8:Y:1238:CYS:HB3	1.99	0.44
1:h:194:LEU:HA	1:h:197:MET:HE3	2.00	0.44
3:m:264:LEU:O	3:m:270:LYS:HA	2.18	0.44
8:B:393:PHE:HB3	8:B:1324:ILE:HB	1.99	0.44
8:B:1280:LYS:HE2	8:B:1280:LYS:HB3	1.83	0.44
8:C:496:PRO:O	8:C:500:ARG:HB2	2.17	0.44
8:C:1322:LEU:HD12	8:C:1359:ILE:HG21	1.99	0.44
8:Z:430:LEU:HD12	8:Z:1108:VAL:HG12	1.99	0.44
8:Z:866:THR:OG1	8:Z:870:THR:O	2.34	0.44
1:I:71:THR:OG1	1:I:72:LEU:N	2.50	0.44
8:B:332:LEU:O	8:B:336:GLN:HB2	2.16	0.44
8:B:723:LEU:HD13	8:B:768:VAL:HG21	2.00	0.44
8:B:1290:LYS:HE2	8:B:1312:GLU:HG2	2.00	0.44
8:C:122:LYS:HB3	8:C:1082:ASN:HB3	1.99	0.44
8:C:611:TYR:O	8:C:614:ASP:CB	2.66	0.44
8:Y:1110:VAL:HA	8:Y:1171:ALA:HB3	1.99	0.44
8:Z:237:ASP:OD1	8:Z:241:LYS:NZ	2.45	0.44
8:Z:469:PRO:HB3	8:Z:541:HIS:CE1	2.53	0.44
1:n:221:LYS:HB3	1:o:158:LEU:HD22	1.98	0.44
1:o:236:GLU:OE2	5:O:9:ARG:N	2.49	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:a:968:ARG:HH11	8:Z:695:ASN:HB3	1.82	0.44
8:B:16:PRO:HD3	8:Z:60:ARG:HD2	1.98	0.44
8:B:495:ILE:HG21	8:B:938:PRO:HD2	2.00	0.44
8:B:719:PHE:HD1	8:B:917:LEU:HD22	1.82	0.44
8:B:1285:TYR:HA	8:B:1289:ALA:HB3	1.99	0.44
8:B:1296:ASP:OD1	8:B:1296:ASP:N	2.49	0.44
8:D:608:GLU:OE2	8:D:928:LYS:N	2.51	0.44
8:Y:1265:TYR:OH	8:Y:1320:GLU:O	2.33	0.44
4:M:164:LEU:HG	4:M:166:ARG:H	1.83	0.44
7:R:33:SER:H	7:R:36:THR:HG1	1.66	0.44
7:S:46:LYS:HA	7:S:49:ARG:HH21	1.81	0.44
8:C:892:VAL:HG11	8:C:979:PHE:HE1	1.82	0.44
8:C:1189:PRO:HB3	8:C:1322:LEU:HD13	2.00	0.44
8:D:522:TYR:OH	8:D:1177:THR:OG1	2.29	0.44
8:Y:127:ILE:HB	8:Z:101:ALA:HA	1.99	0.44
8:Z:1224:THR:HG22	8:Z:1226:ALA:H	1.82	0.44
3:g:189:ILE:HG22	3:g:202:ILE:HG13	2.00	0.44
5:N:53:MET:HB3	5:N:57:ARG:HH12	1.83	0.44
6:1:175:ARG:NH1	6:1:212:ASN:HB3	2.33	0.44
8:D:1155:SER:OG	8:D:1255:ASN:OD1	2.26	0.44
8:D:1215:TYR:OH	8:D:1268:THR:OG1	2.28	0.44
8:Y:125:ILE:HG22	8:Z:103:GLY:HA2	1.99	0.44
8:Y:508:THR:HG23	8:Y:511:GLU:H	1.81	0.44
8:Y:945:ASN:HB2	8:Y:969:HIS:HD2	1.82	0.44
8:a:67:LEU:HA	8:a:72:ALA:HB2	2.00	0.43
8:a:1234:SER:HG	8:a:1235:GLN:N	2.15	0.43
8:a:1290:LYS:HA	8:a:1316:ARG:HH22	1.82	0.43
8:B:235:ASP:OD2	8:B:238:TYR:N	2.48	0.43
8:C:203:ALA:O	8:Z:25:THR:OG1	2.36	0.43
8:C:709:ALA:HB3	8:C:1012:LEU:HD12	2.00	0.43
8:D:1328:THR:HB	8:D:1353:ASN:HB3	2.00	0.43
8:Y:617:VAL:HG13	8:Y:619:GLY:H	1.82	0.43
1:o:303:ILE:HD11	3:m:151:ARG:HD2	2.00	0.43
5:N:29:ARG:O	5:N:33:ARG:NE	2.50	0.43
8:B:182:THR:HG21	8:B:1083:THR:HG21	2.00	0.43
8:C:1122:TYR:HB2	8:C:1128:ASP:HB2	2.01	0.43
8:C:1330:LEU:HD13	8:D:1183:VAL:HG11	2.00	0.43
8:C:1348:GLU:H	8:C:1355:VAL:HG23	1.83	0.43
8:D:1045:ASP:HB2	8:D:1098:TYR:HB3	1.99	0.43
8:Y:1101:ARG:HD2	8:Z:214:ASN:HB3	2.00	0.43
8:Z:297:SER:O	8:Z:297:SER:OG	2.36	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Z:1277:THR:O	8:Z:1281:THR:N	2.49	0.43
8:a:1132:ARG:HH12	8:a:1140:PRO:HB3	1.84	0.43
8:C:427:THR:OG1	8:C:428:ALA:N	2.51	0.43
8:C:534:HIS:HD2	8:C:536:PHE:H	1.66	0.43
8:C:806:THR:HA	8:C:809:VAL:HG12	2.00	0.43
8:D:182:THR:HG22	8:D:186:LYS:HE2	2.00	0.43
8:Y:600:THR:HG23	8:Y:601:VAL:HG23	2.00	0.43
8:Z:508:THR:HG23	8:Z:511:GLU:H	1.83	0.43
8:Z:583:ARG:HE	8:Z:583:ARG:HB3	1.69	0.43
8:Z:1242:VAL:HA	8:Z:1248:HIS:CD2	2.54	0.43
1:o:206:MET:HG2	1:o:274:MET:HG3	2.00	0.43
7:T:13:LYS:HB3	7:T:14:ARG:H	1.67	0.43
8:a:518:VAL:HB	8:a:1179:VAL:HG11	2.01	0.43
8:a:717:PRO:HA	8:a:718:PRO:HD3	1.88	0.43
8:B:205:GLN:NE2	8:B:206:ALA:O	2.45	0.43
8:C:235:ASP:HB3	8:C:238:TYR:HB3	1.99	0.43
8:C:1327:THR:OG1	8:C:1329:THR:O	2.34	0.43
8:Z:272:VAL:HG23	8:Z:368:ILE:HB	2.00	0.43
6:l:101:LYS:HA	6:l:101:LYS:HD3	1.86	0.43
7:i:72:ARG:NE	8:Z:820:MET:O	2.45	0.43
8:a:214:ASN:OD1	8:Z:433:ARG:NH2	2.49	0.43
8:a:792:MET:HE1	8:a:1000:ASN:HA	1.99	0.43
8:C:59:ASN:HB2	8:D:95:VAL:HG13	2.01	0.43
8:D:449:LEU:HD11	8:D:1034:LEU:HD21	2.01	0.43
8:Y:682:ARG:NH1	8:Y:776:ASP:OD2	2.50	0.43
1:h:91:LEU:HA	1:h:303:ILE:HA	1.99	0.43
1:I:263:ASP:OD1	1:I:263:ASP:N	2.50	0.43
2:H:2240:LEU:HD12	5:N:62:ARG:HG3	2.01	0.43
4:M:479:ARG:HE	4:M:479:ARG:HB2	1.70	0.43
8:a:253:SER:OG	8:a:254:ILE:N	2.51	0.43
8:B:1176:LEU:HD12	8:B:1177:THR:H	1.83	0.43
8:C:459:PRO:HB2	8:C:1242:VAL:HG21	2.01	0.43
8:C:624:PHE:HA	8:C:627:ILE:HG22	2.00	0.43
8:C:1164:THR:OG1	8:C:1166:HIS:O	2.36	0.43
8:C:1240:SER:O	8:C:1244:TYR:HB2	2.19	0.43
8:C:1277:THR:O	8:C:1281:THR:OG1	2.35	0.43
8:C:1358:GLU:OE2	8:C:1363:GLN:N	2.50	0.43
8:D:263:THR:HG22	8:D:296:VAL:HG12	2.01	0.43
8:D:393:PHE:O	8:D:1038:ARG:N	2.47	0.43
8:Z:71:LEU:HD22	8:Z:372:LEU:HD11	1.99	0.43
8:Z:999:PRO:O	8:Z:1004:SER:OG	2.31	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:h:100:VAL:HG21	1:h:138:VAL:HG22	2.01	0.43
1:h:267:ARG:HH21	3:g:234:ARG:HH22	1.65	0.43
1:o:41:ILE:HD11	1:o:45:GLN:HB2	2.00	0.43
4:M:68:ALA:HB3	4:M:547:LEU:HB3	2.00	0.43
6:1:72:ASP:N	6:1:72:ASP:OD1	2.48	0.43
6:1:167:ILE:HD11	6:1:186:LEU:HD21	2.00	0.43
8:a:297:SER:HB2	8:a:352:LEU:HD23	2.01	0.43
8:a:417:ASN:OD1	8:a:422:ASN:ND2	2.42	0.43
8:a:743:ASN:OD1	8:a:743:ASN:N	2.51	0.43
8:B:373:ARG:HH21	8:B:377:LYS:HA	1.84	0.43
8:B:440:ILE:HB	8:B:1108:VAL:HB	2.01	0.43
8:C:6:ALA:HA	8:D:316:ILE:HG22	2.00	0.43
8:D:216:LEU:HD13	8:D:1200:LEU:HD12	2.00	0.43
8:Z:629:THR:OG1	8:Z:878:GLU:OE2	2.34	0.43
8:Z:1334:GLU:HA	8:Z:1337:LEU:HB2	2.01	0.43
1:o:190:ASP:O	1:o:192:HIS:ND1	2.45	0.43
4:M:428:LEU:HD13	4:M:431:ARG:HD2	2.00	0.43
8:a:936:PRO:HD3	8:a:952:LEU:HB3	2.00	0.43
8:B:194:GLN:O	8:B:198:GLU:HB2	2.19	0.43
8:C:820:MET:HE3	8:C:877:ARG:HH11	1.84	0.43
8:C:853:VAL:HG11	8:C:872:LEU:HD22	2.01	0.43
8:C:1217:HIS:CE1	8:C:1235:GLN:HG2	2.53	0.43
8:Y:186:LYS:HE3	8:Y:1085:ASP:HB2	1.99	0.43
8:Y:424:LEU:HB2	8:Y:573:LEU:HD21	2.00	0.43
8:Z:209:ARG:HA	8:Z:212:ARG:HG2	2.01	0.43
1:n:161:SER:HG	1:n:164:GLU:H	1.67	0.43
1:n:273:VAL:HG21	3:m:243:LEU:HD12	2.00	0.43
3:g:234:ARG:HH12	3:g:241:ILE:HD13	1.83	0.43
3:g:253:TRP:O	3:g:280:SER:OG	2.31	0.43
6:1:134:ILE:HD12	6:1:144:LEU:HD22	2.01	0.43
8:B:575:THR:HG22	8:B:1010:ALA:HB3	2.01	0.43
8:B:1343:ALA:H	8:B:1364:GLN:HE22	1.66	0.43
8:Y:1336:LYS:NZ	8:Y:1346:THR:OG1	2.50	0.43
8:Z:388:ASN:ND2	8:Z:1043:GLU:OE2	2.50	0.43
8:Z:585:ARG:HD2	8:Z:585:ARG:HA	1.85	0.43
8:Z:936:PRO:HB3	8:Z:952:LEU:HD12	2.01	0.43
8:Z:1366:MET:HE3	8:Z:1366:MET:HB3	1.87	0.43
1:I:48:LEU:H	1:I:133:VAL:HG13	1.84	0.43
4:M:24:HIS:HA	4:M:131:THR:HG22	2.00	0.43
6:1:266:THR:HA	6:1:269:GLU:HG3	2.00	0.43
8:a:1327:THR:HG22	8:a:1333:MET:HE2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:878:GLU:HA	8:B:881:LEU:HG	2.00	0.43
3:g:175:TRP:CE2	3:g:222:LYS:HG2	2.54	0.42
4:M:362:ALA:HA	5:N:49:GLU:HG3	2.01	0.42
8:a:650:SER:HB3	8:a:653:LEU:HB2	2.00	0.42
8:B:562:PRO:HD2	8:B:565:LEU:HD13	2.01	0.42
8:C:625:LEU:HD12	8:C:628:ARG:HD2	2.00	0.42
8:C:671:LEU:HD12	8:C:671:LEU:HA	1.86	0.42
8:C:1167:GLY:HA2	8:D:210:ILE:HD11	2.01	0.42
8:Z:812:PHE:HZ	8:Z:879:LEU:HG	1.84	0.42
3:g:259:ILE:HA	3:g:275:ARG:O	2.20	0.42
4:M:311:VAL:HG23	4:M:330:TRP:H	1.83	0.42
4:M:367:LEU:HG	4:M:424:ILE:HD12	2.01	0.42
6:1:79:GLU:HA	6:1:82:VAL:HG12	2.01	0.42
6:1:123:GLU:HB3	6:1:127:ARG:HH21	1.84	0.42
8:a:81:HIS:HE1	8:a:304:ASN:HD21	1.66	0.42
8:a:1200:LEU:HD21	8:a:1281:THR:HG21	2.00	0.42
8:a:1234:SER:OG	8:a:1235:GLN:OE1	2.36	0.42
8:B:255:LEU:HD23	8:B:255:LEU:HA	1.86	0.42
8:B:710:LEU:HG	8:B:1012:LEU:HD12	2.00	0.42
8:C:128:PRO:HB3	8:C:1076:HIS:CE1	2.54	0.42
8:C:293:LYS:HZ1	8:C:356:SER:HB2	1.84	0.42
8:Y:672:PHE:HA	8:Y:675:ARG:HG2	2.01	0.42
8:Z:184:LEU:HD13	8:Z:387:ARG:HH21	1.84	0.42
8:Z:507:ARG:NH1	8:Z:511:GLU:OE1	2.53	0.42
7:j:57:LYS:H	7:j:57:LYS:HG2	1.61	0.42
8:a:84:ASN:OD1	8:a:84:ASN:N	2.52	0.42
8:a:106:LEU:HD11	8:Z:1307:THR:HA	2.01	0.42
8:a:710:LEU:HD23	8:a:710:LEU:HA	1.92	0.42
8:B:12:LYS:HG3	8:Z:58:CYS:HB2	2.01	0.42
8:B:216:LEU:HD23	8:B:219:PHE:HD2	1.85	0.42
8:C:234:ARG:HA	8:C:234:ARG:HD3	1.81	0.42
8:C:533:LEU:HD23	8:C:539:PHE:HE2	1.84	0.42
8:D:77:ALA:HB1	8:D:302:TYR:CE1	2.53	0.42
8:Y:139:LEU:HD22	8:Y:160:VAL:HG21	2.01	0.42
8:Y:1228:THR:HG22	8:Y:1230:ASN:H	1.83	0.42
8:Z:420:VAL:HA	8:Z:423:ALA:HB3	2.00	0.42
8:Z:704:SER:HA	8:Z:707:VAL:HG12	2.01	0.42
2:P:2239:TYR:HE2	5:N:64:GLU:HG3	1.84	0.42
4:M:475:ALA:HA	4:M:523:LEU:O	2.19	0.42
8:B:78:ILE:HA	8:B:303:GLY:H	1.83	0.42
8:C:66:PHE:HD1	8:C:176:ILE:HG12	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:724:PRO:HA	8:C:773:ALA:HB3	2.02	0.42
8:D:472:GLU:HB2	8:D:475:MET:HG2	2.00	0.42
8:Z:744:ILE:HD12	8:Z:744:ILE:HA	1.93	0.42
1:I:270:ALA:HA	1:I:273:VAL:HG12	2.02	0.42
2:P:2236:ARG:HE	2:P:2236:ARG:HB2	1.55	0.42
1:n:231:LEU:O	1:n:235:GLN:HB2	2.20	0.42
3:m:19:GLU:OE2	8:C:1075:TYR:OH	2.32	0.42
4:M:585:SER:OG	4:M:586:GLY:N	2.52	0.42
7:R:67:MET:HA	7:R:70:VAL:HG12	2.01	0.42
8:a:1191:ASN:ND2	8:a:1195:ARG:O	2.43	0.42
8:B:148:LEU:HA	8:B:151:ILE:HG12	2.01	0.42
8:C:1366:MET:HE3	8:C:1366:MET:HB2	1.82	0.42
8:D:435:ARG:NH2	8:D:1364:GLN:O	2.53	0.42
8:D:993:ARG:HA	8:D:993:ARG:HD2	1.93	0.42
8:D:1182:ASP:OD1	8:D:1182:ASP:N	2.52	0.42
8:Z:1142:LEU:HD12	8:Z:1142:LEU:HA	1.89	0.42
6:1:174:VAL:HG13	6:1:175:ARG:NH1	2.32	0.42
8:a:941:ARG:NE	8:a:987:LEU:O	2.43	0.42
8:B:645:LEU:HD12	8:B:674:TYR:CZ	2.55	0.42
8:C:888:GLU:H	8:C:919:ASN:HD22	1.67	0.42
8:D:1336:LYS:NZ	8:D:1346:THR:O	2.45	0.42
8:Y:591:GLU:O	8:Y:595:ARG:HB2	2.20	0.42
8:Z:192:VAL:HA	8:Z:219:PHE:HE1	1.84	0.42
1:I:142:LEU:HD12	1:I:177:PHE:CG	2.55	0.42
1:I:244:GLU:HA	1:I:247:VAL:HG12	2.02	0.42
3:g:216:VAL:HG12	3:g:248:ILE:HG13	2.02	0.42
4:M:539:PHE:HZ	5:O:4:LEU:HD22	1.85	0.42
6:1:34:HIS:HB3	6:1:37:ILE:HD12	2.02	0.42
8:a:273:MET:HA	8:a:1048:LEU:O	2.19	0.42
8:a:424:LEU:HD13	8:a:573:LEU:HD23	2.02	0.42
8:a:1212:LYS:HE3	8:a:1212:LYS:HB2	1.85	0.42
8:B:520:ASP:HA	8:B:523:LYS:HE2	2.01	0.42
8:B:534:HIS:CD2	8:B:536:PHE:H	2.31	0.42
8:C:624:PHE:HZ	8:C:657:ILE:HD13	1.84	0.42
8:D:420:VAL:HA	8:D:423:ALA:HB3	2.01	0.42
8:D:733:VAL:HG23	8:D:894:GLU:HB3	2.01	0.42
8:D:968:ARG:HD3	8:D:969:HIS:H	1.85	0.42
8:Y:127:ILE:HD12	8:Y:128:PRO:HD2	2.02	0.42
8:Y:273:MET:HE2	8:Y:273:MET:HB3	1.85	0.42
1:I:274:MET:HE1	8:B:1148:ILE:HD13	2.01	0.42
4:M:44:TYR:HB2	4:M:150:ARG:HB3	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:a:472:GLU:HB3	8:a:475:MET:HE3	2.01	0.42
8:C:847:ALA:HA	8:C:850:ARG:HG2	2.01	0.42
8:D:273:MET:HE3	8:D:273:MET:HB2	1.92	0.42
8:Y:1210:ALA:HB1	8:Y:1272:ILE:HD12	2.01	0.42
8:Z:1290:LYS:HG2	8:Z:1312:GLU:HA	2.02	0.42
1:h:263:ASP:OD2	3:g:239:ARG:NH1	2.53	0.42
1:o:169:VAL:O	1:o:173:GLN:HB2	2.19	0.42
4:M:19:GLU:H	4:M:135:ARG:NH2	2.18	0.42
6:1:194:THR:HB	6:1:197:VAL:HG23	2.02	0.42
6:1:244:SER:N	6:1:247:SER:OG	2.51	0.42
7:T:72:ARG:NE	8:D:820:MET:O	2.42	0.42
8:a:184:LEU:HD11	8:a:385:LEU:HD23	2.02	0.42
8:a:233:THR:OG1	8:a:235:ASP:OD1	2.37	0.42
8:Y:314:THR:O	8:Y:319:HIS:N	2.38	0.42
8:Z:414:VAL:HG21	8:Z:1331:ALA:HB1	2.01	0.42
4:M:378:VAL:HG22	4:M:381:ARG:HE	1.85	0.42
7:i:73:THR:OG1	7:i:74:ARG:N	2.52	0.42
8:a:359:VAL:HG12	8:a:368:ILE:HD13	2.02	0.42
8:B:1195:ARG:NH1	8:B:1227:ALA:O	2.53	0.42
8:C:940:HIS:HD2	8:C:942:PHE:H	1.68	0.42
8:Y:622:ASP:OD1	8:Y:622:ASP:N	2.53	0.42
8:Y:970:ASP:HB2	8:Y:993:ARG:HG3	2.02	0.42
8:Z:726:ASN:HB2	8:Z:728:GLU:HG2	2.01	0.42
4:M:505:ARG:HD3	4:M:509:GLY:HA2	2.02	0.41
7:R:63:ASP:HA	7:R:66:ARG:HG2	2.01	0.41
8:a:424:LEU:HD12	8:a:425:PRO:HD2	2.01	0.41
8:a:428:ALA:HB3	8:a:440:ILE:HG23	2.02	0.41
8:a:632:ALA:HA	8:a:666:LEU:HD21	2.02	0.41
8:D:1324:ILE:HA	8:D:1358:GLU:HB3	2.01	0.41
8:Z:311:ASN:O	8:Z:314:THR:OG1	2.28	0.41
8:Z:1009:ALA:HA	8:Z:1012:LEU:HD12	2.02	0.41
8:a:647:PHE:HD2	8:a:653:LEU:HB3	1.85	0.41
8:a:1245:ASN:O	8:a:1249:ARG:N	2.51	0.41
8:B:651:TYR:HB2	8:B:784:PHE:CG	2.55	0.41
8:B:651:TYR:N	8:B:785:TYR:OH	2.54	0.41
8:C:1049:TYR:O	8:C:1092:SER:HA	2.20	0.41
8:D:597:PHE:HA	8:D:600:THR:HG22	2.03	0.41
8:D:1196:ALA:HB3	8:D:1222:ALA:HB3	2.02	0.41
8:Y:297:SER:HB3	8:Y:352:LEU:HD22	2.02	0.41
8:Y:472:GLU:OE1	8:Y:1218:ARG:NE	2.53	0.41
8:Y:600:THR:HG21	8:Y:645:LEU:HG	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Z:670:LEU:HD23	8:Z:670:LEU:HA	1.88	0.41
7:T:67:MET:HA	7:T:70:VAL:HG12	2.02	0.41
8:B:73:ALA:HA	8:B:261:TYR:CZ	2.55	0.41
8:B:164:LEU:HD12	8:B:332:LEU:HD13	2.02	0.41
8:C:163:ALA:O	8:C:167:THR:OG1	2.29	0.41
8:C:618:HIS:O	8:C:721:THR:OG1	2.37	0.41
8:C:733:VAL:HG11	8:C:738:PRO:HA	2.02	0.41
8:C:913:ARG:HH21	8:C:984:HIS:CG	2.38	0.41
8:D:1044:VAL:HG13	8:D:1096:VAL:HG13	2.02	0.41
8:Y:83:LEU:HD11	8:Y:1082:ASN:HD22	1.85	0.41
8:Y:905:GLN:HA	8:Y:1123:ARG:HE	1.85	0.41
8:Y:1176:LEU:HD13	8:Y:1232:TRP:HB2	2.01	0.41
8:Z:544:GLU:HG2	8:Z:549:VAL:HG12	2.01	0.41
8:Z:814:ARG:NH2	8:Z:851:GLN:O	2.52	0.41
1:I:10:CYS:O	1:I:80:GLN:HA	2.20	0.41
2:H:2237:PHE:HB2	8:a:755:PRO:HB2	2.01	0.41
1:n:49:HIS:CD2	1:n:131:GLU:H	2.38	0.41
8:a:517:VAL:HG21	8:Z:1027:HIS:CD2	2.56	0.41
8:a:1280:LYS:HB3	8:a:1280:LYS:HE2	1.89	0.41
8:B:611:TYR:CZ	8:B:923:VAL:HG13	2.56	0.41
8:B:1286:LEU:HD23	8:B:1286:LEU:HA	1.94	0.41
8:D:1144:ASP:OD1	8:D:1144:ASP:N	2.53	0.41
8:Y:1183:VAL:HA	8:Y:1187:LYS:HE3	2.03	0.41
8:Z:292:THR:HG22	8:Z:294:GLU:HG3	2.02	0.41
8:Z:1132:ARG:HA	8:Z:1132:ARG:HD3	1.86	0.41
8:Z:1143:LEU:O	8:Z:1147:THR:OG1	2.34	0.41
1:h:48:LEU:HA	1:h:51:PHE:HD2	1.84	0.41
1:n:33:PRO:HA	1:n:69:THR:O	2.20	0.41
1:o:106:ASP:HA	3:m:69:ARG:HH21	1.85	0.41
3:m:42:ASP:O	3:m:159:LYS:NZ	2.38	0.41
4:M:171:GLU:HG3	4:M:315:ARG:NE	2.35	0.41
7:j:46:LYS:HA	7:j:49:ARG:HD2	2.02	0.41
8:a:192:VAL:O	8:a:195:THR:OG1	2.36	0.41
8:a:1148:ILE:O	8:a:1152:THR:N	2.44	0.41
8:a:1286:LEU:HD12	8:a:1286:LEU:HA	1.95	0.41
8:B:41:ASP:OD2	8:Z:132:SER:N	2.53	0.41
8:B:747:ARG:HD3	8:B:749:HIS:HE1	1.84	0.41
8:B:1061:ASN:HA	8:B:1062:PRO:HD3	1.91	0.41
8:B:1072:SER:OG	8:B:1073:THR:N	2.54	0.41
8:C:718:PRO:HG2	8:C:943:TYR:HE2	1.84	0.41
8:Y:359:VAL:HG12	8:Y:368:ILE:HD13	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Y:912:SER:OG	8:Y:914:GLN:NE2	2.53	0.41
8:Z:399:LEU:HD22	8:Z:1033:ALA:HB1	2.03	0.41
8:Z:775:ASP:OD1	8:Z:775:ASP:N	2.52	0.41
8:Z:780:LEU:HA	8:Z:783:VAL:HG12	2.01	0.41
1:n:275:LEU:HD23	1:n:275:LEU:HA	1.86	0.41
8:a:209:ARG:HH12	8:Z:1160:ASN:HD22	1.69	0.41
8:a:1242:VAL:HA	8:a:1248:HIS:HD2	1.85	0.41
8:B:122:LYS:HG2	8:B:124:PRO:HD3	2.01	0.41
8:C:212:ARG:NH2	8:C:1202:VAL:O	2.53	0.41
8:C:677:LEU:HD23	8:C:677:LEU:HA	1.92	0.41
8:D:1150:MET:O	8:D:1154:GLY:N	2.50	0.41
8:Y:209:ARG:HA	8:Y:212:ARG:HG2	2.03	0.41
8:Y:391:LEU:HD13	8:Y:1042:PHE:HE2	1.85	0.41
8:Z:608:GLU:H	8:Z:608:GLU:HG2	1.70	0.41
1:h:161:SER:OG	1:h:162:TYR:N	2.53	0.41
3:g:234:ARG:NH1	3:g:240:GLN:O	2.53	0.41
3:m:17:ASP:N	3:m:17:ASP:OD1	2.54	0.41
7:i:19:ARG:HA	7:i:22:VAL:HG12	2.02	0.41
8:a:297:SER:HA	8:a:353:THR:O	2.21	0.41
8:a:612:LEU:HD21	8:a:860:LEU:HD21	2.01	0.41
8:a:814:ARG:NE	8:a:853:VAL:O	2.53	0.41
8:B:275:SER:HB3	8:B:280:MET:HE2	2.02	0.41
8:B:1297:THR:OG1	8:B:1299:THR:O	2.31	0.41
8:C:241:LYS:HG3	8:C:245:ARG:HH12	1.85	0.41
8:C:1038:ARG:NH1	8:C:1107:GLY:O	2.54	0.41
8:C:1160:ASN:OD1	8:C:1160:ASN:N	2.54	0.41
8:D:1098:TYR:OH	8:D:1370:SER:OXT	2.35	0.41
8:Y:957:LYS:HE2	8:Y:957:LYS:HB3	1.86	0.41
8:Z:717:PRO:HB3	8:Z:782:LYS:HA	2.03	0.41
3:g:64:GLY:HA3	3:g:166:MET:HG2	2.02	0.41
3:g:170:ASP:N	3:g:170:ASP:OD1	2.52	0.41
7:T:37:HIS:CE1	8:D:818:LEU:HB3	2.56	0.41
8:a:392:THR:HA	8:a:1038:ARG:O	2.21	0.41
8:a:569:PRO:HA	8:a:572:GLU:HG2	2.03	0.41
8:C:311:ASN:HD22	8:C:311:ASN:HA	1.72	0.41
8:C:499:TYR:OH	8:C:974:PRO:O	2.33	0.41
8:D:431:LEU:HD23	8:D:435:ARG:HA	2.03	0.41
8:D:469:PRO:HA	8:D:470:PRO:HD3	1.94	0.41
8:Y:734:ALA:HB2	8:Y:893:LEU:HD13	2.02	0.41
8:Z:91:MET:HE2	8:Z:91:MET:HB3	1.96	0.41
8:Z:416:LEU:HD13	8:Z:422:ASN:HB3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:h:294:SER:HA	1:h:295:PRO:HD3	1.92	0.41
1:o:33:PRO:HD2	1:o:47:GLY:HA2	2.02	0.41
1:o:34:ILE:HD11	1:o:46:LEU:HD12	2.03	0.41
1:o:61:LEU:HD22	1:o:112:PRO:HG3	2.03	0.41
3:g:126:HIS:HA	3:g:129:LEU:HB2	2.03	0.41
4:M:398:MET:HE1	5:O:24:LEU:HD23	2.03	0.41
6:1:40:LYS:HE3	6:1:40:LYS:HB2	1.88	0.41
8:a:175:LEU:HD13	8:a:1081:ILE:HD13	2.03	0.41
8:a:420:VAL:HG11	8:a:577:GLU:HA	2.03	0.41
8:a:682:ARG:HD3	8:a:682:ARG:HA	1.92	0.41
8:a:1144:ASP:HB3	8:a:1148:ILE:HG23	2.03	0.41
8:a:1310:LEU:HD23	8:a:1310:LEU:HA	1.97	0.41
8:B:457:PRO:HG3	8:B:537:PHE:CG	2.56	0.41
8:B:995:SER:HA	8:B:998:CYS:HB3	2.03	0.41
8:B:1281:THR:HA	8:B:1284:GLU:HG3	2.03	0.41
8:C:9:LEU:HD23	8:C:9:LEU:HA	1.93	0.41
8:C:646:VAL:O	8:C:674:TYR:OH	2.38	0.41
8:C:999:PRO:HG2	8:C:1004:SER:HB2	2.02	0.41
8:D:534:HIS:HD2	8:D:536:PHE:H	1.68	0.41
8:D:536:PHE:HD1	8:D:1015:ILE:HD12	1.86	0.41
8:Y:534:HIS:H	8:Y:539:PHE:HE2	1.69	0.41
8:Y:653:LEU:HD23	8:Y:653:LEU:HA	1.84	0.41
8:a:310:GLU:HA	8:a:313:VAL:HG22	2.03	0.41
8:a:967:HIS:O	8:a:967:HIS:ND1	2.53	0.41
8:B:636:VAL:O	8:B:640:HIS:HB2	2.20	0.41
8:B:785:TYR:O	8:B:943:TYR:OH	2.30	0.41
8:D:1264:GLN:HE22	8:D:1315:CYS:HB2	1.85	0.41
8:D:1350:HIS:CD2	8:D:1351:PHE:H	2.39	0.41
8:Y:588:PRO:HD2	8:Y:683:LEU:HD11	2.03	0.41
1:I:162:TYR:HB2	1:I:165:VAL:HG12	2.03	0.40
2:P:2221:LEU:HB3	2:P:2222:ARG:H	1.77	0.40
6:1:194:THR:HG22	6:1:196:LEU:H	1.86	0.40
8:a:638:MET:SD	8:a:642:ARG:NH1	2.94	0.40
8:B:273:MET:HA	8:B:1048:LEU:O	2.21	0.40
8:C:534:HIS:CE1	8:C:1239:LEU:HD12	2.56	0.40
8:D:209:ARG:HA	8:D:212:ARG:HE	1.85	0.40
8:D:814:ARG:NH2	8:D:855:GLU:OE1	2.53	0.40
8:Y:314:THR:O	8:Y:318:TYR:N	2.54	0.40
8:Y:332:LEU:HD23	8:Y:332:LEU:HA	1.91	0.40
8:Z:42:ASP:OD1	8:Z:42:ASP:N	2.53	0.40
1:h:278:LEU:HG	1:I:275:LEU:HD22	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:m:234:ARG:HA	3:m:234:ARG:HD2	1.85	0.40
3:m:265:VAL:HG22	3:m:270:LYS:HG2	2.03	0.40
4:M:49:ASP:OD1	4:M:49:ASP:N	2.51	0.40
8:a:563:ASP:N	8:a:563:ASP:OD1	2.53	0.40
8:B:276:THR:OG1	8:B:277:ALA:N	2.54	0.40
8:B:615:VAL:HG11	8:B:802:LEU:HD12	2.03	0.40
8:B:915:HIS:NE2	8:B:978:ALA:O	2.54	0.40
8:B:946:PRO:HA	8:B:949:CYS:HB2	2.03	0.40
8:D:222:LYS:O	8:D:226:THR:OG1	2.34	0.40
8:D:429:TYR:HD2	8:D:1327:THR:HG23	1.86	0.40
8:D:572:GLU:OE2	8:D:994:TYR:OH	2.38	0.40
8:D:1055:THR:OG1	8:D:1056:SER:N	2.54	0.40
8:D:1132:ARG:HD2	8:D:1139:ARG:HB3	2.03	0.40
8:Z:705:ALA:HB1	8:Z:712:ASP:HB3	2.03	0.40
1:h:153:MET:O	1:h:157:SER:HB3	2.22	0.40
1:h:268:LEU:HD13	1:h:271:LEU:HD23	2.03	0.40
1:o:127:LEU:HB2	1:o:130:TRP:HB3	2.03	0.40
4:M:478:VAL:HG23	4:M:485:VAL:HG22	2.04	0.40
7:R:58:CYS:HA	7:R:61:LYS:HE3	2.03	0.40
8:a:635:ILE:HG21	8:a:666:LEU:HD13	2.04	0.40
8:a:759:ALA:HB1	8:a:762:ALA:HB3	2.03	0.40
8:a:786:LEU:HD23	8:a:786:LEU:HA	1.88	0.40
8:a:1276:LYS:HD3	8:a:1280:LYS:HE2	2.01	0.40
8:B:675:ARG:HH12	8:C:602:THR:HG23	1.85	0.40
8:C:114:ILE:HG22	8:Z:37:ILE:HG23	2.03	0.40
8:C:134:ALA:HA	8:C:137:THR:HG22	2.03	0.40
8:C:251:THR:HG21	8:Z:19:PHE:HA	2.03	0.40
8:D:454:LEU:HD12	8:D:1239:LEU:HD11	2.02	0.40
8:D:789:MET:HE2	8:D:789:MET:HB2	1.96	0.40
8:Z:369:MET:HE2	8:Z:369:MET:HB3	1.92	0.40
8:Z:796:ARG:HA	8:Z:945:ASN:HD22	1.86	0.40
1:n:268:LEU:HG	1:o:152:ILE:HD11	2.03	0.40
3:g:90:ARG:HG3	3:g:118:LEU:HD22	2.03	0.40
3:g:220:ARG:O	3:g:227:ARG:NH1	2.54	0.40
6:1:244:SER:H	6:1:247:SER:HG	1.67	0.40
7:T:37:HIS:HE1	8:D:818:LEU:HB3	1.86	0.40
8:C:811:LEU:HD12	8:C:857:LEU:HD13	2.03	0.40
8:D:222:LYS:HD3	8:D:222:LYS:HA	1.96	0.40
8:D:341:ASN:ND2	8:D:345:SER:OG	2.54	0.40
8:D:976:PRO:HB2	8:D:979:PHE:HD1	1.86	0.40
8:Z:321:ILE:HD13	8:Z:321:ILE:HA	1.94	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:h:273:VAL:HA	1:h:276:ARG:HE	1.87	0.40
1:I:113:PRO:HD3	1:I:135:PRO:HA	2.04	0.40
3:g:211:HIS:NE2	3:g:213:GLN:HB3	2.37	0.40
8:a:811:LEU:HD12	8:a:811:LEU:HA	1.91	0.40
8:a:1173:GLU:O	8:a:1244:TYR:OH	2.31	0.40
8:C:177:HIS:ND1	8:C:376:TYR:OH	2.43	0.40
8:C:250:ALA:HB2	8:C:1093:ASN:HD21	1.87	0.40
8:C:283:ILE:HG23	8:C:287:LEU:HD12	2.02	0.40
8:D:463:THR:HG21	8:D:1237:GLY:HA3	2.03	0.40
8:D:475:MET:HG2	8:D:475:MET:H	1.75	0.40
8:Y:796:ARG:HD3	8:Y:796:ARG:HA	1.88	0.40
8:Y:808:LEU:HA	8:Y:811:LEU:HB3	2.02	0.40
8:Y:983:TYR:HA	8:Y:988:ARG:HE	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	279/306 (91%)	264 (95%)	15 (5%)	0	100	100
1	h	281/306 (92%)	262 (93%)	19 (7%)	0	100	100
1	n	289/306 (94%)	267 (92%)	22 (8%)	0	100	100
1	o	276/306 (90%)	263 (95%)	13 (5%)	0	100	100
2	H	18/2241 (1%)	17 (94%)	1 (6%)	0	100	100
2	P	18/2241 (1%)	17 (94%)	1 (6%)	0	100	100
3	g	233/290 (80%)	214 (92%)	19 (8%)	0	100	100
3	m	288/290 (99%)	273 (95%)	15 (5%)	0	100	100
4	M	462/594 (78%)	432 (94%)	30 (6%)	0	100	100
5	N	63/642 (10%)	61 (97%)	2 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	O	65/642 (10%)	64 (98%)	1 (2%)	0	100	100
6	l	283/1048 (27%)	270 (95%)	13 (5%)	0	100	100
7	R	61/75 (81%)	57 (93%)	4 (7%)	0	100	100
7	S	61/75 (81%)	58 (95%)	3 (5%)	0	100	100
7	T	61/75 (81%)	60 (98%)	1 (2%)	0	100	100
7	i	61/75 (81%)	59 (97%)	2 (3%)	0	100	100
7	j	61/75 (81%)	60 (98%)	1 (2%)	0	100	100
8	B	1324/1370 (97%)	1245 (94%)	79 (6%)	0	100	100
8	C	1322/1370 (96%)	1244 (94%)	78 (6%)	0	100	100
8	D	1293/1370 (94%)	1228 (95%)	65 (5%)	0	100	100
8	Y	1343/1370 (98%)	1254 (93%)	89 (7%)	0	100	100
8	Z	1331/1370 (97%)	1252 (94%)	79 (6%)	0	100	100
8	a	1280/1370 (93%)	1192 (93%)	88 (7%)	0	100	100
All	All	10753/17807 (60%)	10113 (94%)	640 (6%)	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	I	257/273 (94%)	257 (100%)	0	100	100
1	h	256/273 (94%)	254 (99%)	2 (1%)	73	77
1	n	262/273 (96%)	262 (100%)	0	100	100
1	o	254/273 (93%)	254 (100%)	0	100	100
2	H	19/1941 (1%)	19 (100%)	0	100	100
2	P	19/1941 (1%)	19 (100%)	0	100	100
3	g	207/252 (82%)	207 (100%)	0	100	100
3	m	252/252 (100%)	250 (99%)	2 (1%)	73	77

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	M	395/500 (79%)	394 (100%)	1 (0%)	86	84
5	N	58/526 (11%)	58 (100%)	0	100	100
5	O	64/526 (12%)	63 (98%)	1 (2%)	55	69
6	1	256/883 (29%)	255 (100%)	1 (0%)	84	82
7	R	59/68 (87%)	59 (100%)	0	100	100
7	S	59/68 (87%)	58 (98%)	1 (2%)	53	67
7	T	59/68 (87%)	59 (100%)	0	100	100
7	i	59/68 (87%)	59 (100%)	0	100	100
7	j	59/68 (87%)	57 (97%)	2 (3%)	32	55
8	B	1162/1192 (98%)	1156 (100%)	6 (0%)	81	81
8	C	1158/1192 (97%)	1154 (100%)	4 (0%)	86	84
8	D	1130/1192 (95%)	1126 (100%)	4 (0%)	84	82
8	Y	1174/1192 (98%)	1166 (99%)	8 (1%)	76	78
8	Z	1163/1192 (98%)	1161 (100%)	2 (0%)	87	85
8	a	1120/1192 (94%)	1114 (100%)	6 (0%)	81	81
All	All	9501/15405 (62%)	9461 (100%)	40 (0%)	81	82

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	h	71	THR
1	h	259	VAL
3	m	185	VAL
3	m	281	VAL
4	M	584	VAL
5	O	4	LEU
6	1	6	ILE
7	S	44	LEU
7	j	40	LEU
7	j	44	LEU
8	a	479	LEU
8	a	861	VAL
8	a	1001	VAL
8	a	1096	VAL
8	a	1179	VAL
8	a	1304	VAL
8	B	518	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	B	677	LEU
8	B	937	VAL
8	B	1084	VAL
8	B	1228	THR
8	B	1303	CYS
8	C	116	VAL
8	C	740	ASN
8	C	861	VAL
8	C	937	VAL
8	D	740	ASN
8	D	916	VAL
8	D	1179	VAL
8	D	1297	THR
8	Y	82	ASP
8	Y	418	ASP
8	Y	644	LEU
8	Y	864	VAL
8	Y	870	THR
8	Y	1112	ASP
8	Y	1176	LEU
8	Y	1239	LEU
8	Z	446	LEU
8	Z	937	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (179) such sidechains are listed below:

Mol	Chain	Res	Type
1	h	116	HIS
1	h	129	GLN
1	h	257	GLN
1	I	209	ASN
2	H	2226	GLN
2	H	2229	GLN
2	P	2226	GLN
1	n	39	HIS
1	n	79	ASN
1	n	84	HIS
1	n	173	GLN
1	n	209	ASN
1	n	258	HIS
1	n	277	GLN
1	n	297	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	o	147	ASN
1	o	170	GLN
1	o	297	ASN
3	g	183	GLN
3	g	232	ASN
3	m	31	ASN
3	m	213	GLN
3	m	240	GLN
3	m	249	GLN
3	m	266	HIS
4	M	47	ASN
4	M	471	GLN
4	M	571	HIS
5	N	63	GLN
5	O	63	GLN
6	1	170	ASN
6	1	177	ASN
6	1	252	ASN
7	R	37	HIS
7	S	18	HIS
7	T	55	ASN
8	a	81	HIS
8	a	208	ASN
8	a	217	GLN
8	a	438	GLN
8	a	484	GLN
8	a	534	HIS
8	a	643	GLN
8	a	660	HIS
8	a	694	ASN
8	a	919	ASN
8	a	940	HIS
8	a	945	ASN
8	a	1003	HIS
8	a	1061	ASN
8	a	1082	ASN
8	a	1111	GLN
8	a	1264	GLN
8	a	1275	ASN
8	a	1350	HIS
8	a	1363	GLN
8	a	1364	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	B	158	HIS
8	B	181	GLN
8	B	208	ASN
8	B	438	GLN
8	B	514	GLN
8	B	534	HIS
8	B	543	GLN
8	B	571	HIS
8	B	618	HIS
8	B	620	ASN
8	B	749	HIS
8	B	945	ASN
8	B	1000	ASN
8	B	1027	HIS
8	B	1079	GLN
8	B	1093	ASN
8	B	1100	ASN
8	B	1124	HIS
8	B	1191	ASN
8	B	1264	GLN
8	B	1309	GLN
8	B	1319	GLN
8	B	1350	HIS
8	C	153	ASN
8	C	194	GLN
8	C	211	GLN
8	C	231	ASN
8	C	338	HIS
8	C	346	GLN
8	C	422	ASN
8	C	514	GLN
8	C	534	HIS
8	C	618	HIS
8	C	849	GLN
8	C	884	GLN
8	C	903	GLN
8	C	919	ASN
8	C	940	HIS
8	C	985	ASN
8	C	1061	ASN
8	C	1363	GLN
8	C	1364	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	D	76	HIS
8	D	111	GLN
8	D	194	GLN
8	D	205	GLN
8	D	208	ASN
8	D	214	ASN
8	D	331	HIS
8	D	341	ASN
8	D	484	GLN
8	D	534	HIS
8	D	543	GLN
8	D	637	ASN
8	D	660	HIS
8	D	676	ASN
8	D	722	HIS
8	D	737	GLN
8	D	945	ASN
8	D	1000	ASN
8	D	1076	HIS
8	D	1080	ASN
8	D	1093	ASN
8	D	1100	ASN
8	D	1124	HIS
8	D	1223	GLN
8	D	1264	GLN
8	D	1313	ASN
8	D	1350	HIS
8	D	1363	GLN
8	Y	3	ASN
8	Y	47	ASN
8	Y	153	ASN
8	Y	158	HIS
8	Y	194	GLN
8	Y	199	ASN
8	Y	331	HIS
8	Y	422	ASN
8	Y	476	GLN
8	Y	484	GLN
8	Y	534	HIS
8	Y	695	ASN
8	Y	748	HIS
8	Y	889	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	Y	914	GLN
8	Y	940	HIS
8	Y	1000	ASN
8	Y	1003	HIS
8	Y	1100	ASN
8	Y	1120	ASN
8	Y	1190	ASN
8	Y	1191	ASN
8	Y	1313	ASN
8	Y	1350	HIS
8	Z	47	ASN
8	Z	76	HIS
8	Z	81	HIS
8	Z	111	GLN
8	Z	153	ASN
8	Z	181	GLN
8	Z	214	ASN
8	Z	217	GLN
8	Z	257	ASN
8	Z	534	HIS
8	Z	620	ASN
8	Z	637	ASN
8	Z	640	HIS
8	Z	676	ASN
8	Z	849	GLN
8	Z	919	ASN
8	Z	969	HIS
8	Z	1027	HIS
8	Z	1029	HIS
8	Z	1061	ASN
8	Z	1079	GLN
8	Z	1080	ASN
8	Z	1093	ASN
8	Z	1223	GLN
8	Z	1248	HIS
8	Z	1350	HIS
8	Z	1353	ASN
8	Z	1364	GLN

5.3.3 RNA ⓘ

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](#)

There are no ligands in this entry.

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.

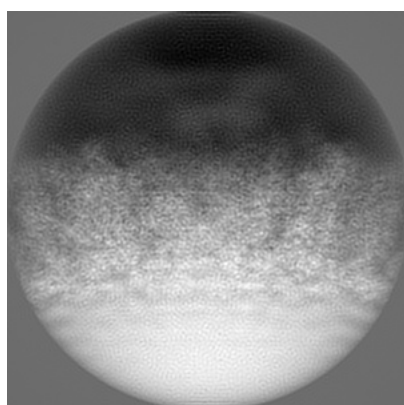
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31297. These allow visual inspection of the internal detail of the map and identification of artifacts.

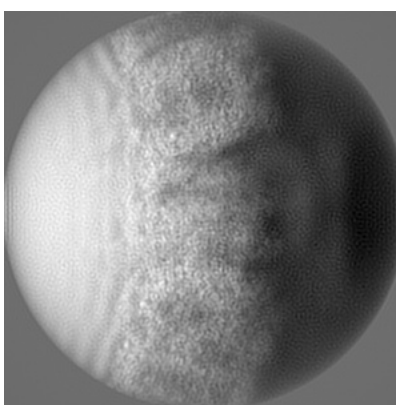
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

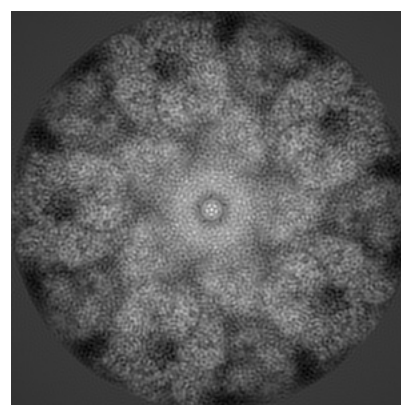
6.1.1 Primary map



X



Y

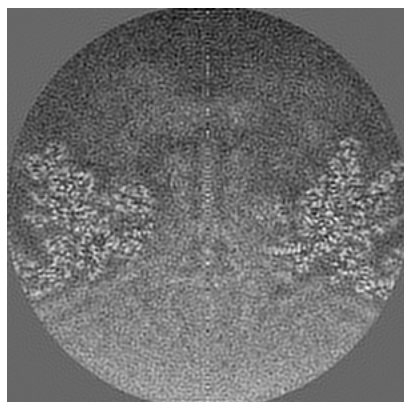


Z

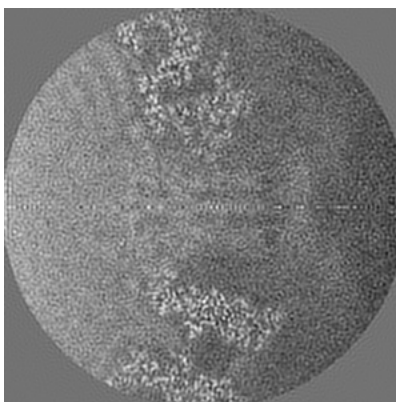
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

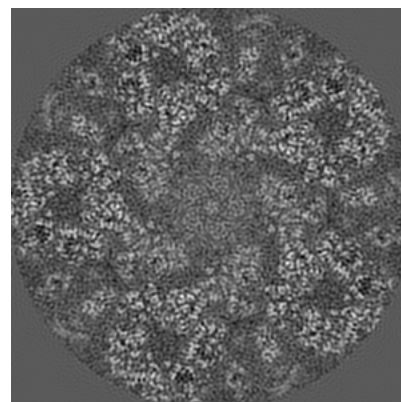
6.2.1 Primary map



X Index: 128



Y Index: 128

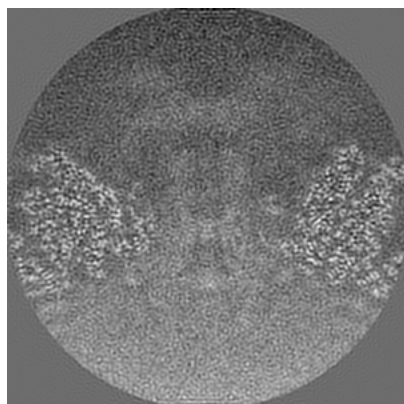


Z Index: 128

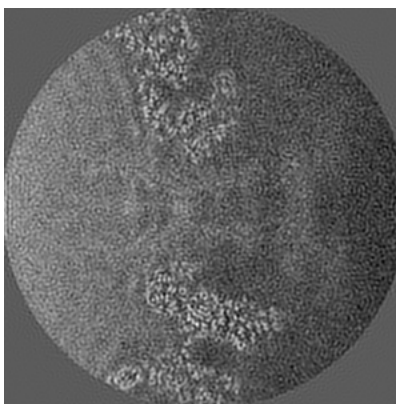
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

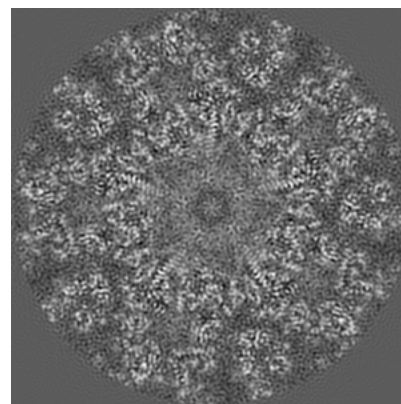
6.3.1 Primary map



X Index: 123



Y Index: 123

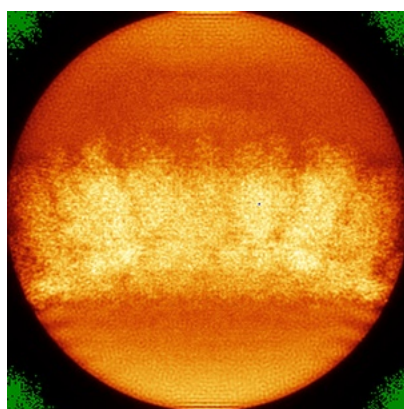


Z Index: 101

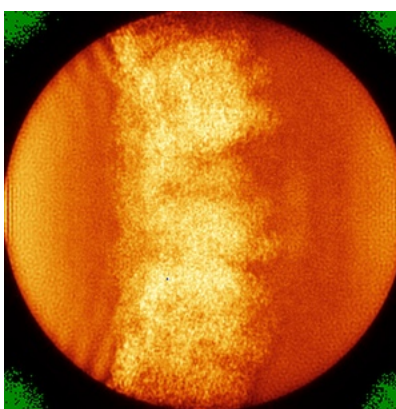
The images above show the largest variance slices of the map in three orthogonal directions.

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

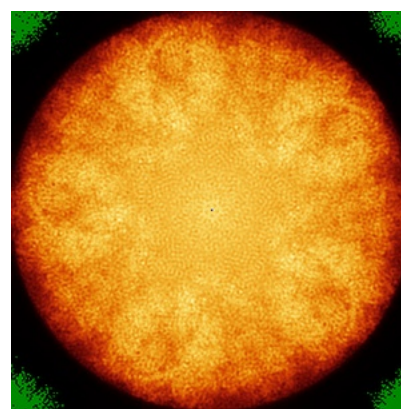
6.4.1 Primary map



X



Y

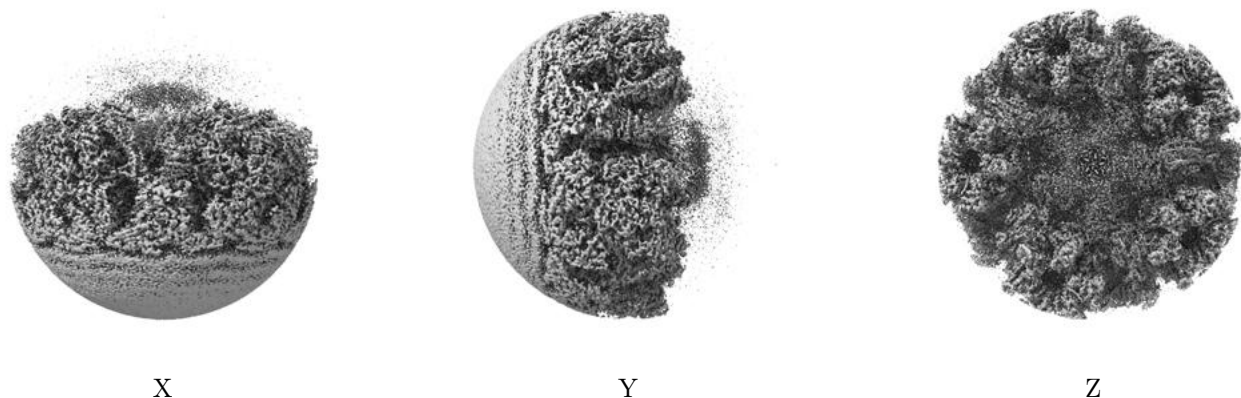


Z

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

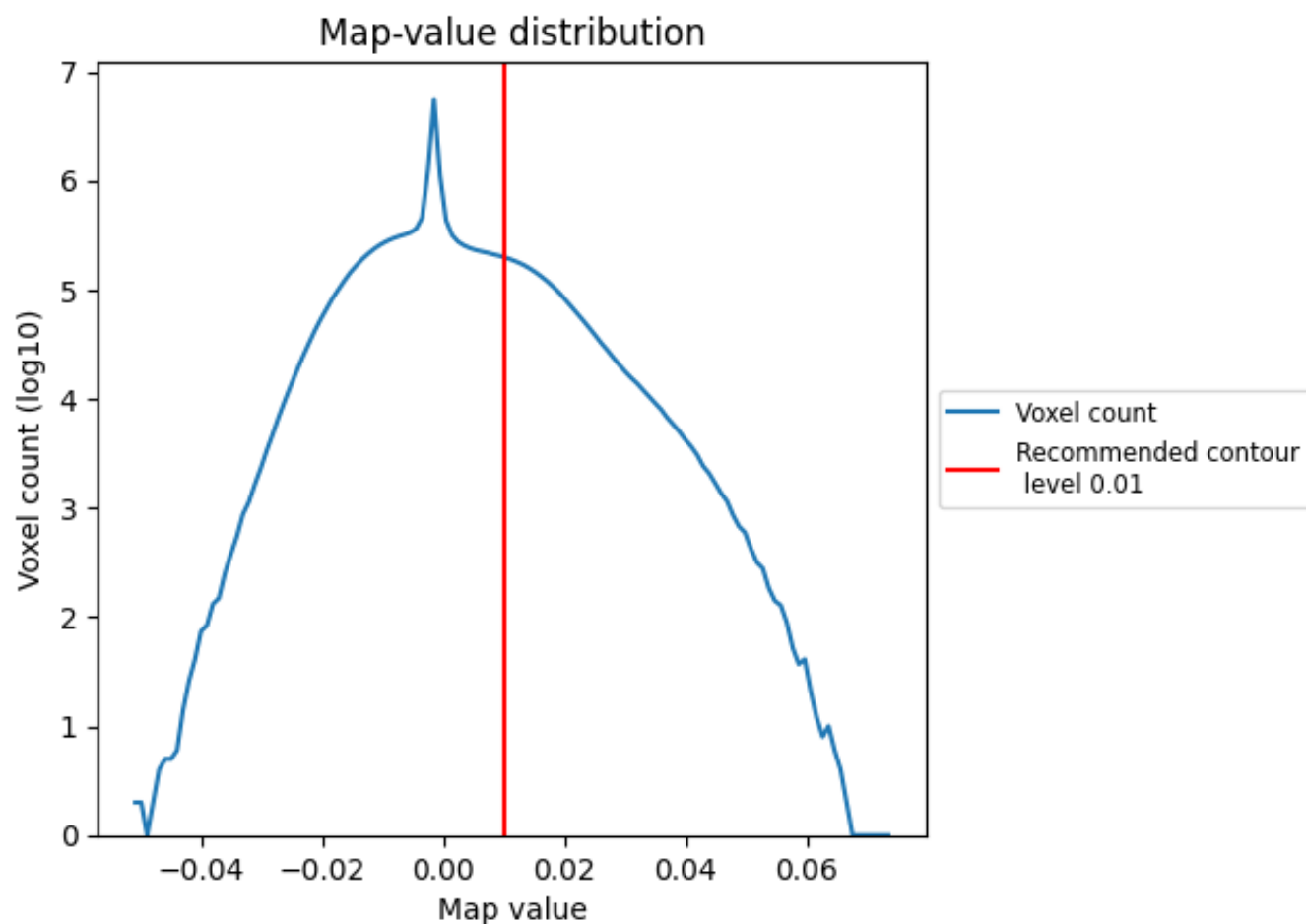
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

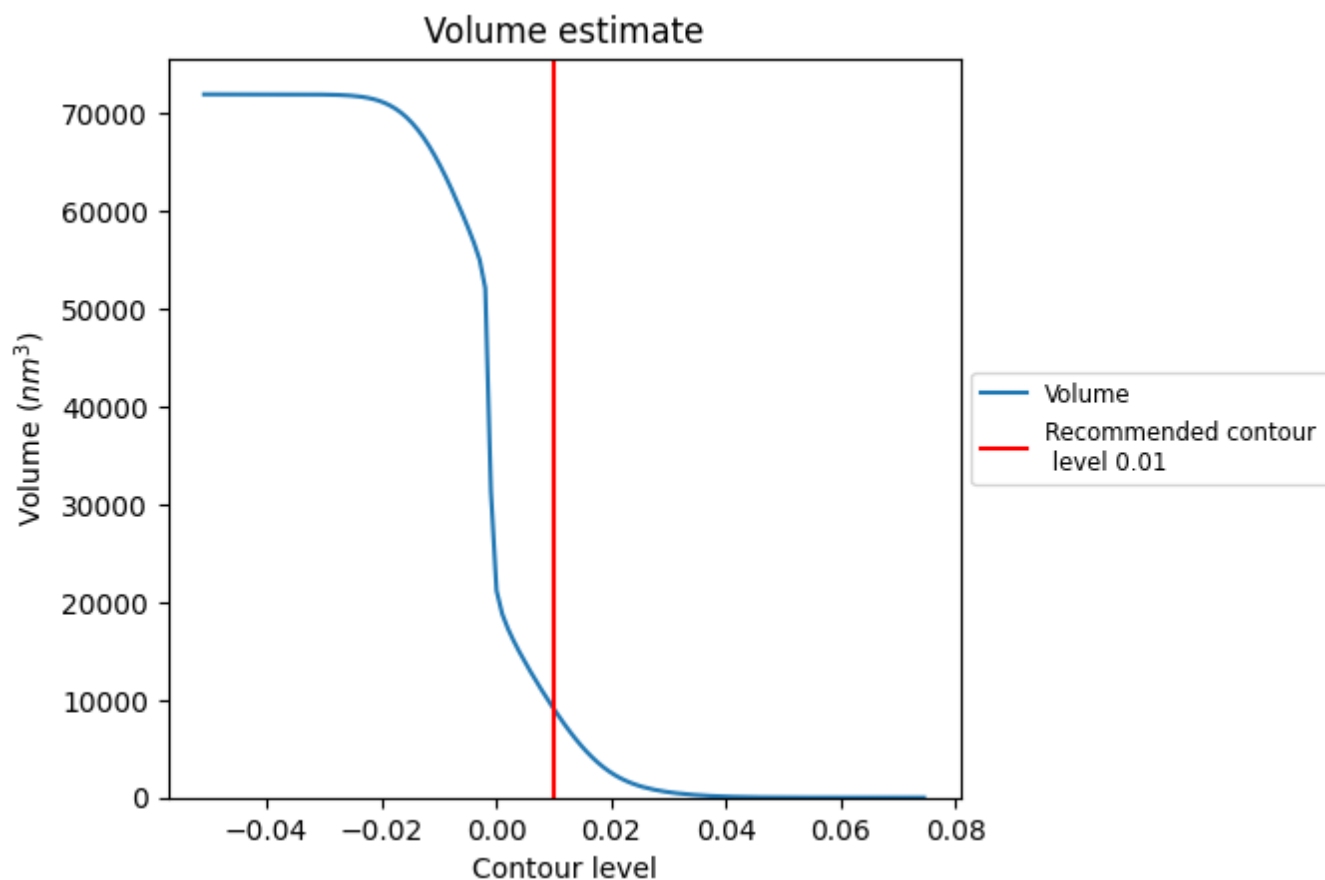
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

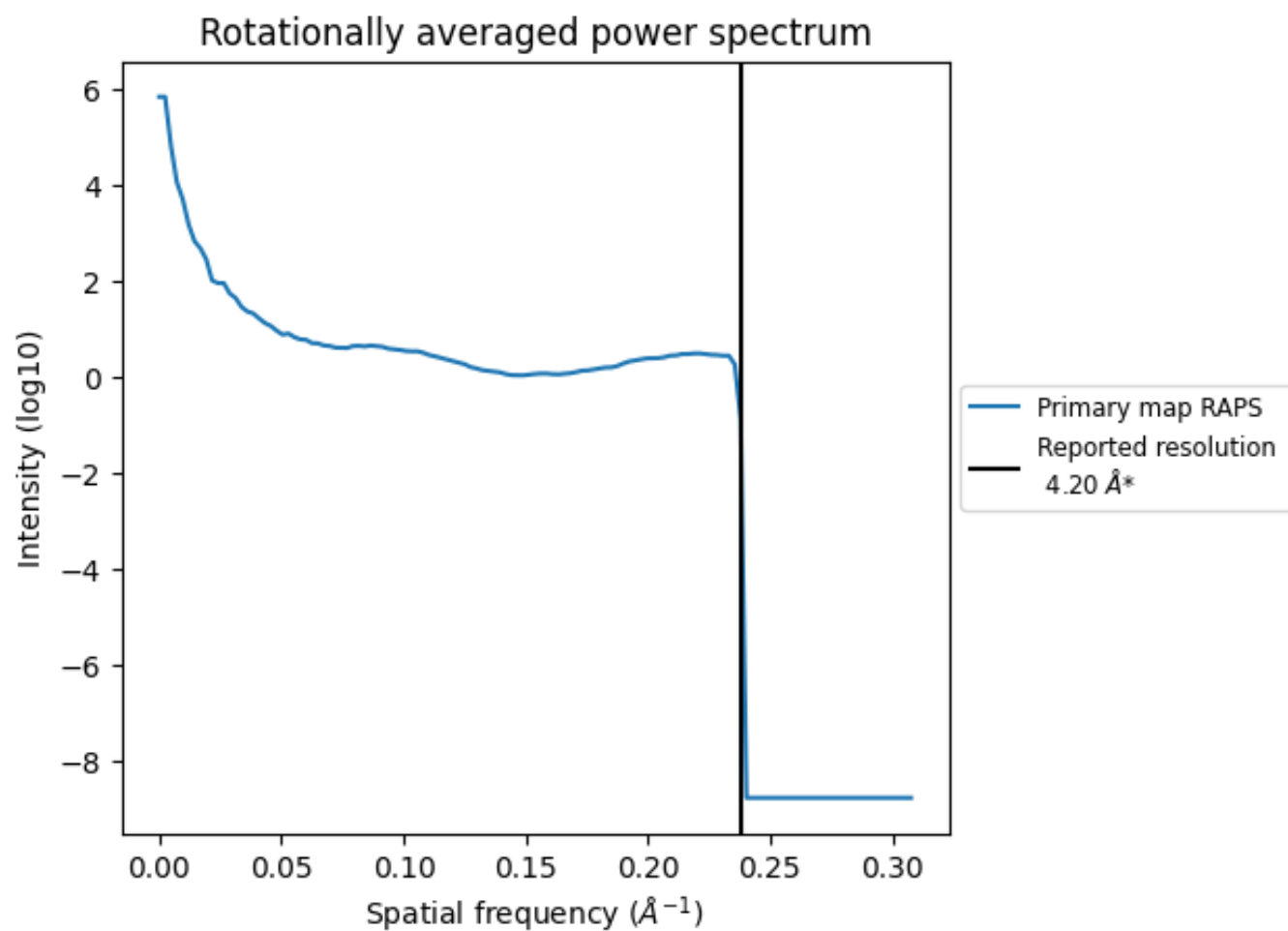
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 9110 nm³; this corresponds to an approximate mass of 8230 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

8 Fourier-Shell correlation ⓘ

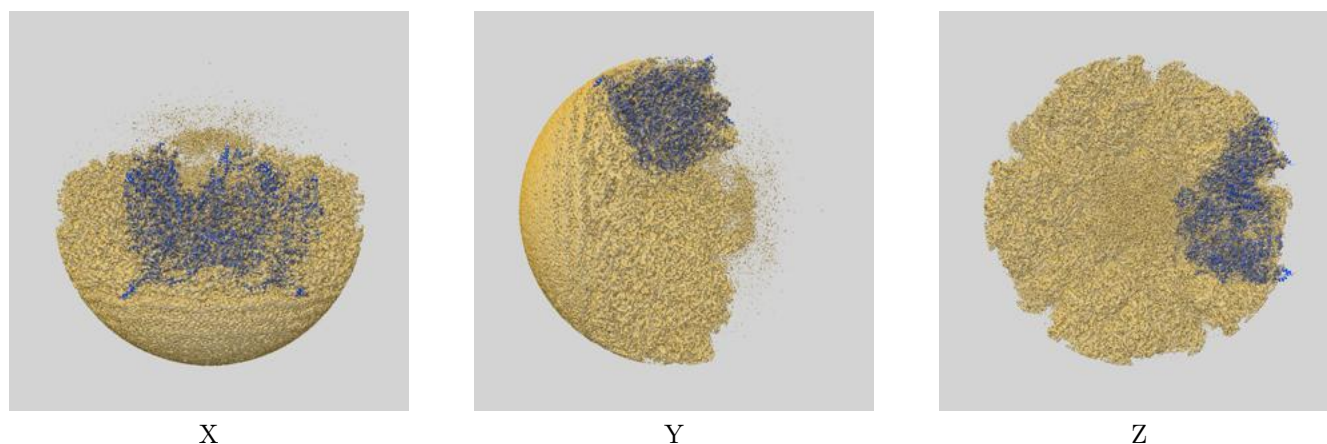
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

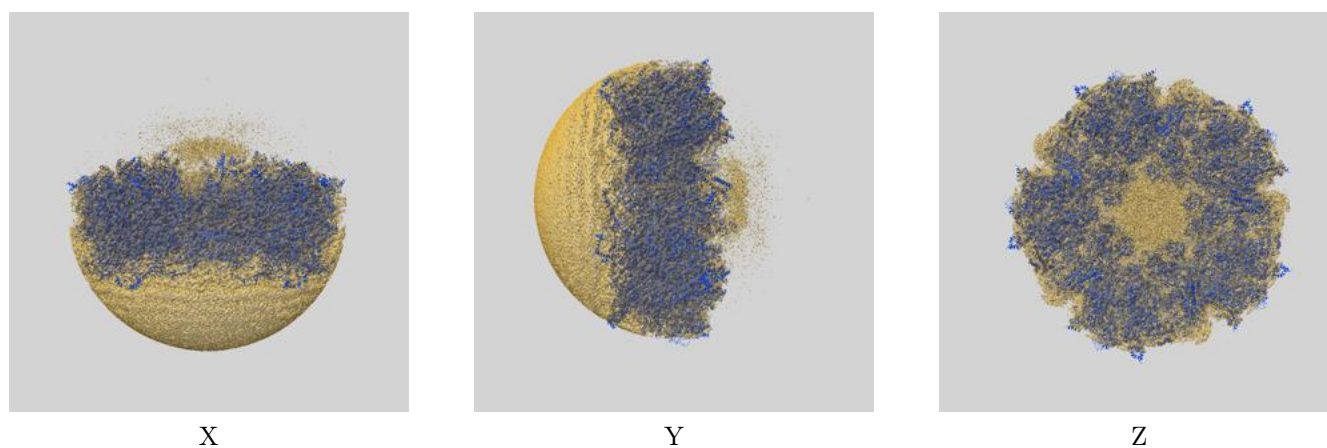
This section contains information regarding the fit between EMDB map EMD-31297 and PDB model 7ET3. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

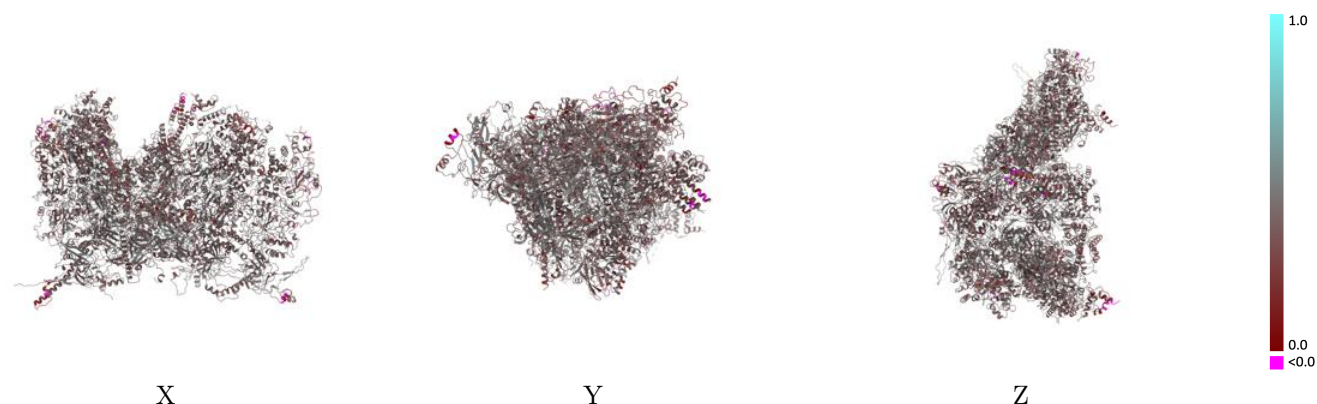


9.1.2 Map-model assembly overlay [i](#)



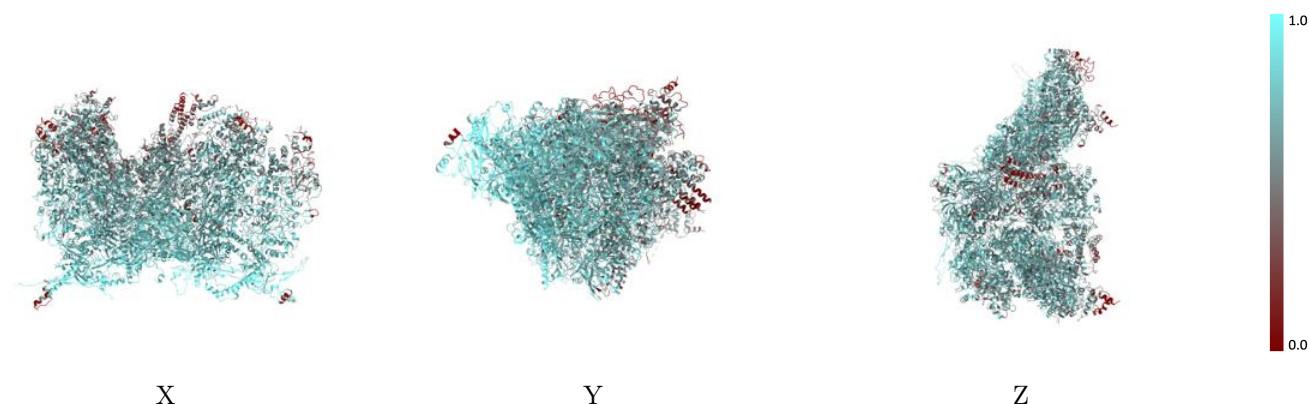
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



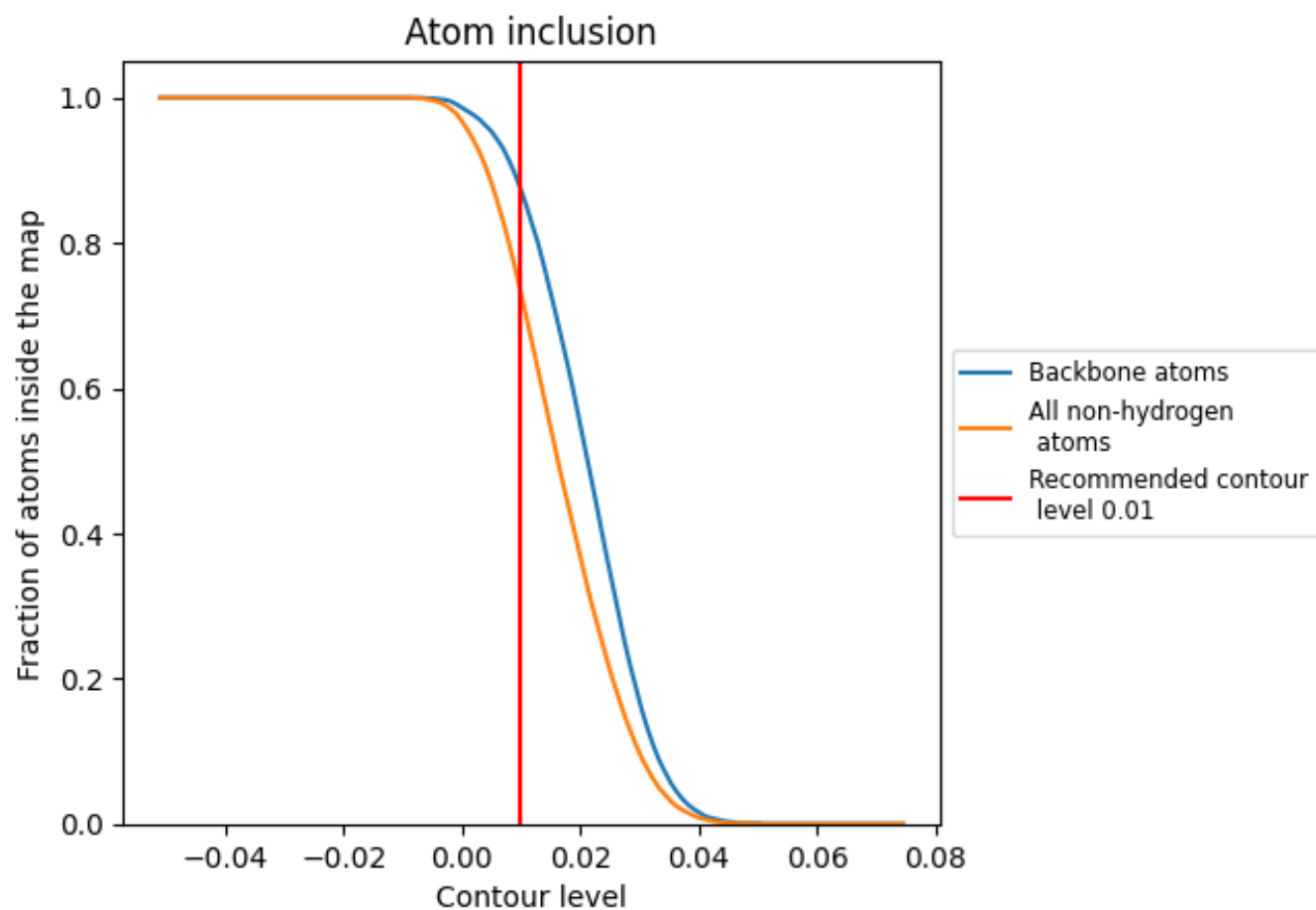
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

9.4 Atom inclusion ⓘ



At the recommended contour level, 87% of all backbone atoms, 73% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7310	 0.3980
1	 0.5500	 0.3720
B	 0.7680	 0.4060
C	 0.7790	 0.4130
D	 0.7550	 0.4000
H	 0.2870	 0.3060
I	 0.7260	 0.3830
M	 0.6010	 0.3910
N	 0.4520	 0.3440
O	 0.3990	 0.3210
P	 0.2640	 0.2900
R	 0.4780	 0.3630
S	 0.5200	 0.3800
T	 0.2790	 0.2660
Y	 0.7390	 0.3930
Z	 0.7650	 0.4070
a	 0.7750	 0.4090
g	 0.6770	 0.3630
h	 0.7020	 0.3750
i	 0.3590	 0.3420
j	 0.4900	 0.3610
m	 0.8030	 0.4100
n	 0.7570	 0.4000
o	 0.7730	 0.4000

