



Full wwPDB EM Validation Report (i)

Nov 29, 2022 – 12:03 AM EST

PDB ID : 8EYX
EMDB ID : EMD-28723
Title : Cryo-EM structure of 4 insulins bound full-length mouse IR mutant with physically decoupled alpha CTs (C684S/C685S/C687S; denoted as IR-3CS) Asymmetric conformation 1
Authors : Li, J.; Wu, J.Y.; Hall, C.; Bai, X.C.; Choi, E.
Deposited on : 2022-10-29
Resolution : 4.50 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 (i) 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 \(i\)](#)) were used in the production of this report:

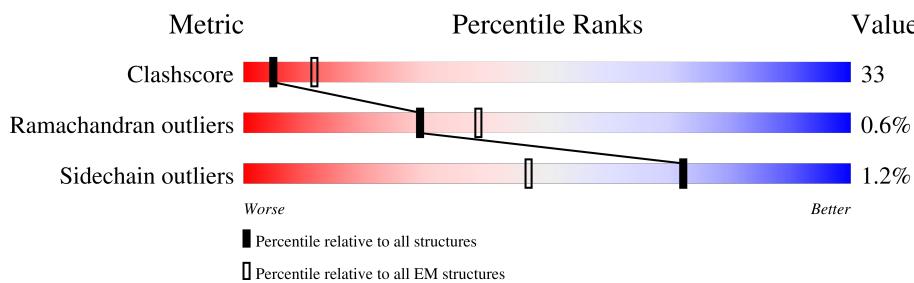
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

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 4.50 Å.

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



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

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



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 14298 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 Insulin receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	815	Total	C	N	O	S	0	0
			6572	4171	1135	1217	49		
1	B	772	Total	C	N	O	S	0	0
			6263	3983	1075	1165	40		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	684	SER	CYS	engineered mutation	UNP P15208
A	685	SER	CYS	engineered mutation	UNP P15208
A	687	SER	CYS	engineered mutation	UNP P15208
B	684	SER	CYS	engineered mutation	UNP P15208
B	685	SER	CYS	engineered mutation	UNP P15208
B	687	SER	CYS	engineered mutation	UNP P15208

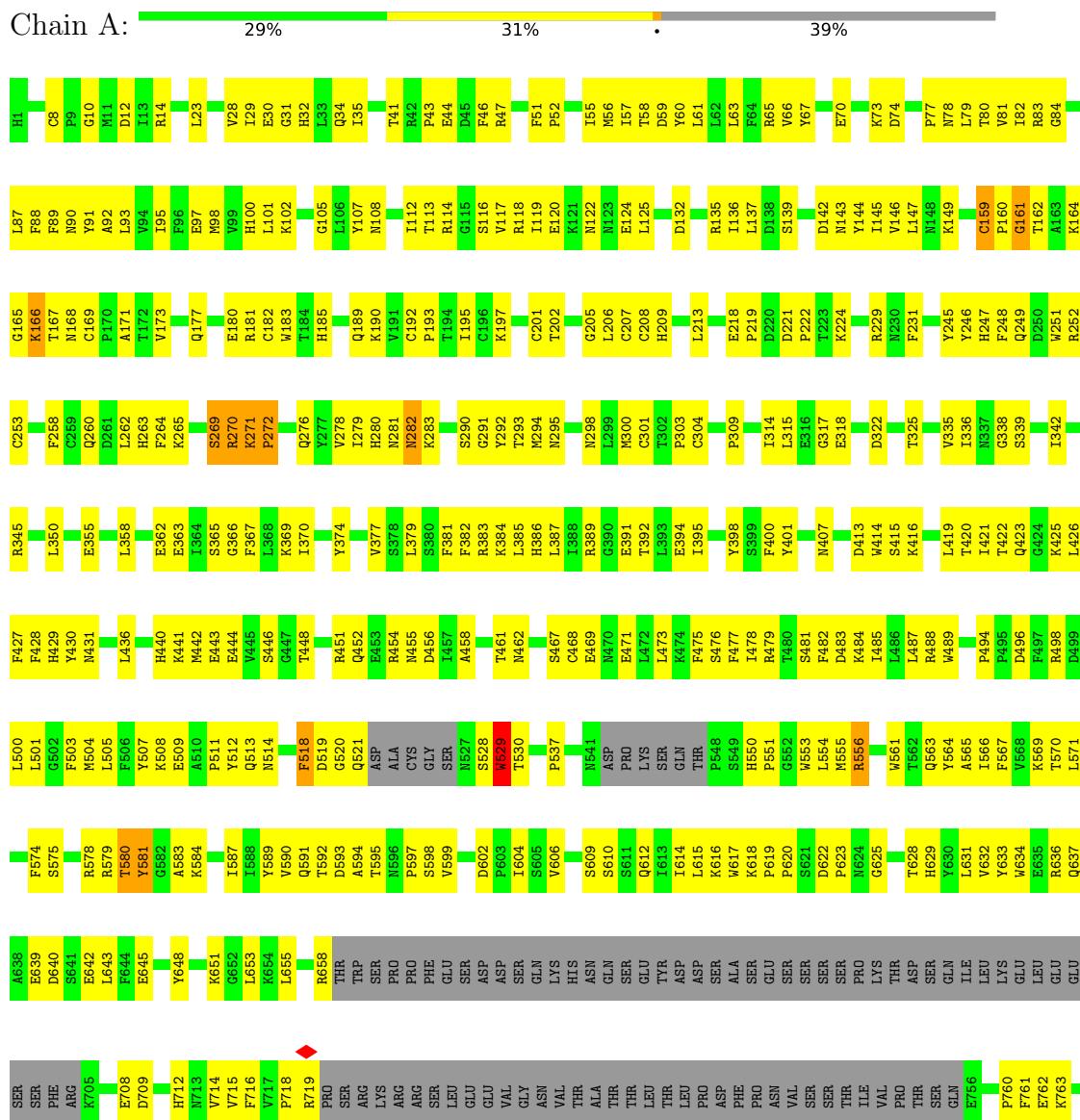
- Molecule 2 is a protein called Insulin.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	44	Total	C	N	O	S	0	0
			347	220	56	65	6		
2	E	48	Total	C	N	O	S	0	0
			376	238	61	71	6		
2	F	47	Total	C	N	O	S	0	0
			370	235	60	69	6		
2	G	47	Total	C	N	O	S	0	0
			370	235	60	69	6		

3 Residue-property plots

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

- Molecule 1: Insulin receptor



I843	K767	T844	I844	T768	V845	S769	L770
R846	W846	I846	S846	T770	V846	S771	T772
Q848	R848	I848	S848	T772	V848	S773	T774
P849	R849	I849	S849	T774	V849	S775	T776

W843	R843	I843	S843	T777	V847	S778	T779
W845	R845	I845	S845	T779	V845	S780	T781
W846	R846	I846	S846	T781	V846	S782	T783

G843	C843	I843	S843	T783	V847	S784	T785
G845	C845	I845	S845	T785	V845	S786	T787
G846	C846	I846	S846	T787	V846	S788	T789

V843	A843	I843	S843	T789	V847	S790	T791
V845	A845	I845	S845	T791	V845	S792	T793
V846	A846	I846	S846	T793	V846	S794	T795

M843	V843	I843	S843	T795	V847	S796	T797
M845	V845	I845	S845	T797	V845	S798	T799
M846	V846	I846	S846	T799	V846	S800	T801

C843	S843	I843	S843	T801	V847	S804	T805
C845	S845	I845	S845	T805	V845	S805	T806
C846	S846	I846	S846	T806	V846	S806	T807

F843	S843	I843	S843	T807	V847	S808	T809
F845	S845	I845	S845	T809	V845	S809	T810
F846	S846	I846	S846	T810	V846	S810	T811

K843	R843	I843	S843	T811	V847	S812	T813
K845	R845	I845	S845	T813	V845	S814	T815
K846	R846	I846	S846	T815	V846	S815	T816

W843	R843	I843	S843	T816	V847	S817	T818
W845	R845	I845	S845	T818	V845	S818	T819
W846	R846	I846	S846	T819	V846	S819	T820

• Molecule 1: Insulin receptor

Chain B: 26% 30% 43%

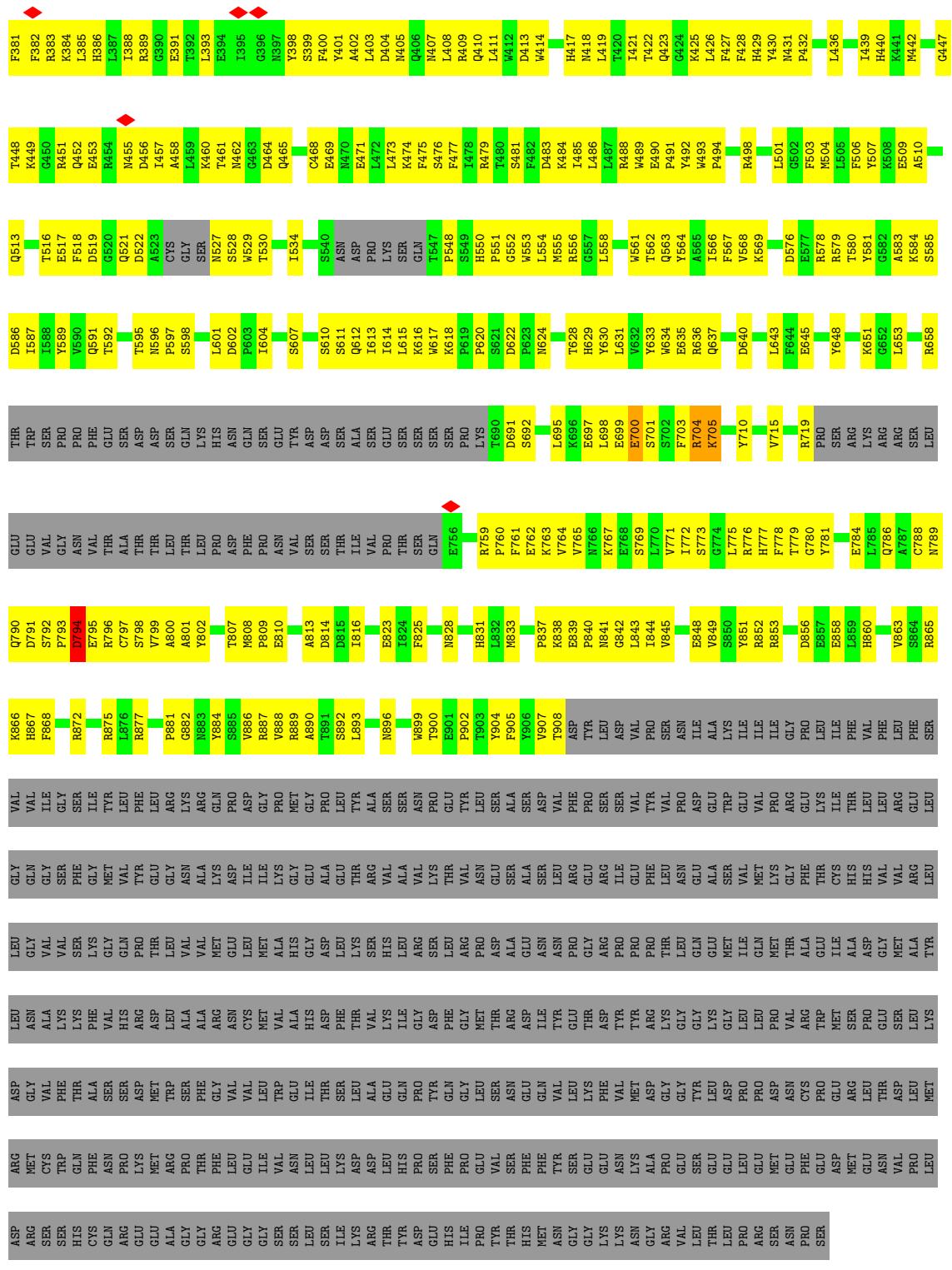
S836	R836	I836	S836	T816	V847	S816	T817
R837	P837	I837	S837	T817	V847	S817	T818
R838	P838	I838	S838	T818	V847	S818	T819

S839	R839	I839	S839	T819	V847	S819	T820
R840	P840	I840	S840	T820	V847	S820	T821
R841	P841	I841	S841	T821	V847	S821	T822

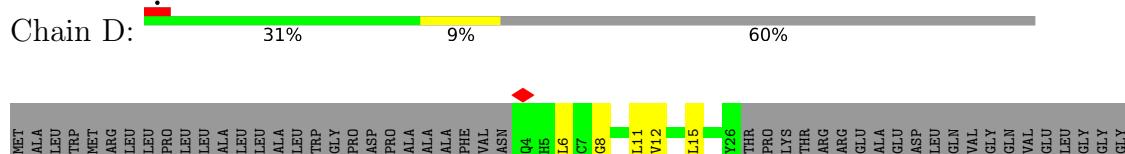
S842	R842	I842	S842	T822	V847	S822	T823
R843	P843	I843	S843	T823	V847	S823	T824
R844	P844	I844	S844	T824	V847	S824	T825

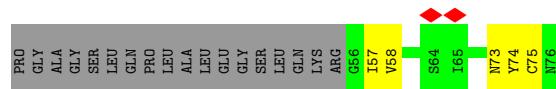
S845	R845	I845	S845	T825	V847	S825	T826
R846	P846	I846	S846	T826	V847	S826	T827
R847	P847	I847	S847	T827	V847	S827	T828

S848	R848	I848	S848	T828	V847	S828	T829
R849	P849	I849	S849	T829	V847	S829	T830
R850	P850	I850	S850	T830	V847	S829	T831



• Molecule 2: Insulin





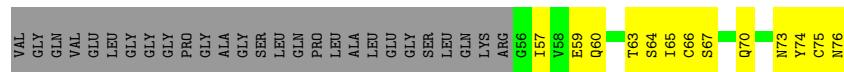
- Molecule 2: Insulin

Chain E:  28% 15% 56%



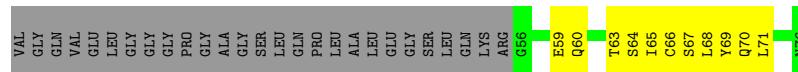
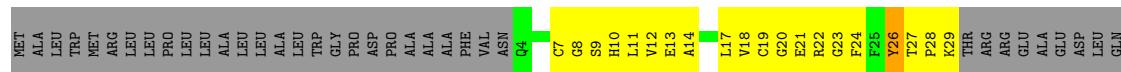
- Molecule 2: Insulin

Chain F:  14% 25% 5% 57%



- Molecule 2: Insulin

Chain G:  15% 27% • 57%



4 Experimental information i

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	101391	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.118	Depositor
Minimum map value	-0.046	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.018	Depositor
Map size (Å)	324.0, 324.0, 324.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality i

5.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.41	1/6736 (0.0%)	0.55	2/9133 (0.0%)
1	B	0.32	0/6415	0.55	6/8693 (0.1%)
2	D	0.25	0/353	0.38	0/475
2	E	0.38	0/383	0.50	0/518
2	F	0.27	0/377	0.46	0/508
2	G	0.33	0/377	0.52	0/508
All	All	0.36	1/14641 (0.0%)	0.54	8/19835 (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
1	A	0	1
1	B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	529	TRP	CB-CG	14.81	1.76	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	548	PRO	CA-N-CD	-8.52	99.58	111.50
1	B	379	LEU	CA-CB-CG	5.32	127.53	115.30
1	B	794	ASP	CB-CG-OD2	5.27	123.04	118.30
1	B	691	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	794	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	522	ASP	CB-CG-OD2	5.22	122.99	118.30
1	A	519	ASP	CB-CG-OD2	5.19	122.97	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	519	ASP	CB-CG-OD2	5.17	122.95	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	580	THR	Peptide
1	B	272	PRO	Peptide

5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6572	0	6387	435	0
1	B	6263	0	6099	440	0
2	D	347	0	317	9	0
2	E	376	0	346	13	0
2	F	370	0	344	37	0
2	G	370	0	344	26	0
All	All	14298	0	13837	932	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 33.

All (932) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:TRP:CB	1:A:529:TRP:CG	1.76	1.61
1:B:506:PHE:HB3	1:B:529:TRP:CD1	1.10	1.59
1:A:260:GLN:HG2	1:A:264:PHE:CE2	1.40	1.54
1:A:260:GLN:CG	1:A:264:PHE:HE2	1.22	1.52
1:B:506:PHE:CB	1:B:529:TRP:CD1	1.93	1.52
1:B:506:PHE:HB3	1:B:529:TRP:NE1	1.22	1.45
1:B:267:ARG:HG2	1:B:276:GLN:NE2	1.35	1.41
1:B:506:PHE:CD2	1:B:529:TRP:NE1	1.88	1.39

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:386:HIS:CE1	1:B:417:HIS:CE1	2.12	1.37
1:B:506:PHE:CB	1:B:529:TRP:NE1	1.86	1.31
1:B:506:PHE:CG	1:B:529:TRP:NE1	2.00	1.29
1:B:267:ARG:CG	1:B:276:GLN:NE2	1.94	1.28
1:A:508:LYS:HE2	1:A:529:TRP:CB	1.67	1.25
1:A:260:GLN:O	1:A:264:PHE:CD2	1.96	1.19
1:B:516:THR:O	1:B:518:PHE:HD2	1.27	1.17
1:A:508:LYS:HE2	1:A:529:TRP:HB3	1.26	1.14
1:B:267:ARG:CG	1:B:276:GLN:HE22	1.56	1.10
1:B:386:HIS:CE1	1:B:417:HIS:NE2	2.22	1.07
1:B:516:THR:O	1:B:518:PHE:CD2	2.07	1.07
1:A:260:GLN:CG	1:A:264:PHE:CE2	2.12	1.06
1:B:506:PHE:CD2	1:B:529:TRP:HE1	1.02	1.05
1:B:354:LEU:O	1:B:358:LEU:HB3	1.59	1.02
1:B:506:PHE:HB3	1:B:529:TRP:CG	1.93	1.02
1:A:518:PHE:HD1	1:A:521:GLN:NE2	1.56	1.02
1:B:506:PHE:CA	1:B:529:TRP:CD1	2.44	1.00
1:A:508:LYS:HE3	1:A:529:TRP:CE3	1.98	0.99
1:B:266:CYS:HA	1:B:269:SER:OG	1.62	0.99
1:B:507:TYR:CZ	1:B:530:THR:OG1	2.14	0.98
1:B:260:GLN:HG3	1:B:299:LEU:HD11	1.46	0.97
1:A:518:PHE:CD1	1:A:521:GLN:NE2	2.34	0.96
1:B:267:ARG:HG3	1:B:276:GLN:NE2	1.79	0.96
1:A:508:LYS:HE3	1:A:529:TRP:CD2	2.02	0.94
1:A:633:TYR:CD1	1:A:761:PHE:HB3	2.03	0.93
1:A:520:GLY:O	1:A:521:GLN:HG3	1.68	0.93
1:B:484:LYS:HA	1:B:555:MET:O	1.68	0.92
1:B:521:GLN:OE1	1:B:527:ASN:N	2.01	0.92
1:A:508:LYS:HB2	1:A:529:TRP:CG	2.03	0.92
1:A:508:LYS:NZ	1:A:529:TRP:HA	1.85	0.92
1:B:506:PHE:HB3	1:B:529:TRP:CE2	2.05	0.91
1:A:260:GLN:O	1:A:264:PHE:HD2	1.37	0.91
1:A:260:GLN:HG3	1:A:264:PHE:HE2	1.36	0.90
1:A:271:LYS:HB3	1:A:272:PRO:HD2	1.49	0.90
1:B:267:ARG:HG2	1:B:276:GLN:HE22	0.77	0.88
1:B:314:ILE:HG21	1:B:318:GLU:C	1.94	0.88
1:A:91:TYR:HE2	1:A:118:ARG:HD2	1.37	0.88
1:B:792:SER:OG	1:B:793:PRO:HD3	1.74	0.87
1:A:508:LYS:HB2	1:A:529:TRP:CD1	2.10	0.87
1:A:508:LYS:CE	1:A:529:TRP:HA	2.04	0.87
1:A:508:LYS:CB	1:A:529:TRP:CD1	2.57	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:508:LYS:CE	1:A:529:TRP:CB	2.51	0.86
1:B:386:HIS:HE1	1:B:417:HIS:CE1	1.87	0.86
1:A:269:SER:HB3	1:A:271:LYS:HG2	1.56	0.86
1:A:314:ILE:HG22	1:A:315:LEU:O	1.75	0.86
1:B:414:TRP:NE1	1:B:442:MET:SD	2.49	0.85
1:A:260:GLN:HG3	1:A:264:PHE:CE2	2.08	0.85
1:B:247:HIS:HB2	1:B:283:LYS:HG2	1.57	0.85
1:B:501:LEU:HD22	1:B:698:LEU:HD23	1.58	0.84
1:B:354:LEU:O	1:B:358:LEU:CB	2.24	0.84
1:B:886:VAL:O	1:B:902:PRO:HA	1.78	0.84
1:B:386:HIS:ND1	1:B:417:HIS:NE2	2.25	0.83
1:A:374:TYR:CE1	1:B:699:GLU:HG3	2.12	0.83
1:B:506:PHE:HA	1:B:529:TRP:HD1	1.42	0.83
1:B:223:THR:HG22	1:B:236:GLN:HG2	1.59	0.83
1:B:506:PHE:HD2	1:B:529:TRP:HE1	0.88	0.83
1:B:259:CYS:HA	1:B:262:LEU:HD12	1.59	0.83
1:B:469:GLU:OE1	1:B:583:ALA:N	2.12	0.83
1:A:508:LYS:CE	1:A:529:TRP:CG	2.62	0.82
1:B:521:GLN:OE1	1:B:527:ASN:HB2	1.81	0.81
1:A:260:GLN:HG2	1:A:264:PHE:HE2	0.66	0.81
1:A:631:LEU:HD21	1:A:633:TYR:CE2	2.15	0.81
1:A:78:ASN:HA	1:A:108:ASN:HD22	1.45	0.81
1:A:363:GLU:HG3	1:A:387:LEU:HB3	1.63	0.80
1:A:889:ARG:HD2	1:A:896:ASN:HB3	1.62	0.80
1:B:889:ARG:HD2	1:B:896:ASN:HB3	1.62	0.80
1:A:271:LYS:HB3	1:A:272:PRO:CD	2.12	0.80
1:A:508:LYS:HE2	1:A:529:TRP:CG	2.17	0.80
1:B:517:GLU:HG2	1:B:518:PHE:H	1.44	0.79
1:A:213:LEU:HD22	1:A:229:ARG:HA	1.64	0.78
2:G:7:CYS:O	2:G:10:HIS:ND1	2.16	0.78
1:B:844:ILE:HA	1:B:892:SER:HA	1.66	0.78
1:A:849:VAL:HG22	1:A:888:VAL:HG22	1.66	0.78
1:A:422:THR:HG22	1:A:423:GLN:HG3	1.64	0.77
1:B:506:PHE:HA	1:B:529:TRP:CD1	2.17	0.77
1:B:554:LEU:O	1:B:556:ARG:NH1	2.17	0.76
1:B:636:ARG:HH22	1:B:779:THR:HB	1.48	0.76
1:B:409:ARG:HH22	1:B:517:GLU:HG2	1.49	0.76
1:B:719:ARG:NH2	2:E:72:GLU:O	2.18	0.76
1:B:334:THR:HA	1:B:361:ILE:HA	1.66	0.76
1:A:247:HIS:HB2	1:A:283:LYS:HG2	1.69	0.75
1:B:426:LEU:HB3	1:B:428:PHE:HE1	1.49	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:658:ARG:NH2	1:B:841:ASN:O	2.19	0.75
1:A:93:LEU:HB3	1:A:117:VAL:HG22	1.69	0.75
2:G:19:CYS:SG	2:G:22:ARG:NH2	2.61	0.74
1:A:92:ALA:N	1:A:116:SER:O	2.20	0.74
1:B:636:ARG:NH2	1:B:780:GLY:O	2.21	0.74
1:B:279:ILE:CG2	1:B:300:MET:SD	2.76	0.73
1:B:853:ARG:NH1	1:B:881:PRO:O	2.19	0.73
1:A:218:GLU:HB2	1:A:224:LYS:HG3	1.69	0.73
1:A:112:ILE:HG12	1:A:136:ILE:HG22	1.70	0.73
1:A:616:LYS:HE3	1:A:769:SER:HB2	1.69	0.73
1:B:262:LEU:HA	1:B:265:LYS:HE2	1.69	0.73
1:A:91:TYR:CE2	1:A:118:ARG:HD2	2.23	0.73
1:A:598:SER:HB2	1:A:622:ASP:HB2	1.71	0.72
1:B:332:GLY:HA2	1:B:360:LEU:HD12	1.71	0.72
1:A:292:TYR:HB3	1:A:301:CYS:HB3	1.72	0.72
1:A:561:TRP:N	1:A:593:ASP:O	2.22	0.72
1:A:479:ARG:NH2	2:F:17:LEU:O	2.23	0.72
1:B:630:TYR:HB2	1:B:764:VAL:HB	1.72	0.71
1:B:81:VAL:HG22	1:B:111:ASN:HB3	1.72	0.71
1:A:454:ARG:HE	1:A:455:ASN:H	1.38	0.71
1:B:281:ASN:HB3	1:B:283:LYS:HE2	1.73	0.71
1:B:506:PHE:CG	1:B:529:TRP:HE1	1.46	0.71
1:B:506:PHE:HD2	1:B:529:TRP:NE1	1.51	0.71
1:A:631:LEU:HD21	1:A:633:TYR:HE2	1.53	0.71
1:B:9:PRO:HA	1:B:30:GLU:HB3	1.72	0.71
1:A:413:ASP:OD2	1:A:416:LYS:NZ	2.23	0.71
2:F:24:PHE:HA	2:F:76:ASN:H	1.56	0.70
1:B:118:ARG:HG3	1:B:144:TYR:HB3	1.73	0.70
1:B:260:GLN:HG2	1:B:264:PHE:HE2	1.56	0.70
1:A:767:LYS:NZ	1:A:769:SER:O	2.23	0.70
1:A:853:ARG:NH1	1:A:881:PRO:O	2.24	0.70
2:F:22:ARG:NH1	2:F:76:ASN:O	2.25	0.70
1:B:448:THR:O	1:B:452:GLN:NE2	2.23	0.70
1:A:640:ASP:HB2	1:A:643:LEU:HD13	1.72	0.70
1:B:790:GLN:NE2	1:B:794:ASP:O	2.24	0.70
1:A:844:ILE:HA	1:A:892:SER:HA	1.73	0.69
1:A:77:PRO:O	1:A:108:ASN:ND2	2.26	0.69
1:B:269:SER:OG	1:B:274:CYS:SG	2.50	0.69
1:A:520:GLY:O	1:A:521:GLN:CG	2.40	0.69
1:A:95:ILE:HG22	1:A:122:ASN:HD21	1.58	0.69
1:A:508:LYS:HE3	1:A:529:TRP:CG	2.26	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:7:CYS:HA	2:G:11:LEU:HD23	1.74	0.69
1:A:508:LYS:CB	1:A:529:TRP:CG	2.76	0.69
1:A:84:GLY:O	1:A:114:ARG:NH1	2.25	0.68
1:A:881:PRO:HA	1:A:907:VAL:HG23	1.75	0.68
1:B:513:GLN:HA	1:B:589:TYR:HE2	1.58	0.68
1:A:778:PHE:O	1:A:806:ARG:NH1	2.26	0.68
1:B:853:ARG:HD2	1:B:882:GLY:HA3	1.76	0.68
1:B:388:ILE:HG22	1:B:421:ILE:HA	1.74	0.68
1:A:79:LEU:HD21	1:A:82:ILE:HD11	1.75	0.68
1:A:477:PHE:HB3	1:A:488:ARG:HB2	1.76	0.68
1:A:537:PRO:HG3	1:A:551:PRO:HG3	1.76	0.68
1:B:507:TYR:CE1	1:B:530:THR:OG1	2.46	0.68
1:B:566:ILE:O	1:B:587:ILE:HA	1.94	0.67
1:B:776:ARG:NH2	1:B:839:GLU:OE1	2.27	0.67
1:A:782:ARG:HH12	1:A:784:GLU:HB2	1.59	0.67
1:B:221:ASP:HB3	1:B:224:LYS:HB2	1.75	0.67
1:B:32:HIS:HD2	1:B:86:ARG:HH21	1.40	0.67
2:G:24:PHE:CE2	2:G:26:TYR:HB3	2.30	0.67
1:A:508:LYS:CE	1:A:529:TRP:CA	2.72	0.67
1:B:385:LEU:O	1:B:417:HIS:NE2	2.23	0.67
1:B:517:GLU:HG2	1:B:518:PHE:N	2.09	0.67
1:A:192:CYS:SG	1:A:201:CYS:N	2.66	0.67
1:A:575:SER:HB2	1:A:580:THR:HA	1.77	0.66
1:B:14:ARG:HD3	1:B:37:LEU:HD12	1.75	0.66
1:B:517:GLU:CD	1:B:567:PHE:CZ	2.68	0.66
2:G:24:PHE:HE2	2:G:26:TYR:HB3	1.60	0.66
1:B:828:ASN:ND2	1:B:908:THR:O	2.28	0.66
1:B:849:VAL:HG22	1:B:888:VAL:HG22	1.77	0.66
2:G:26:TYR:HD1	2:G:28:PRO:HD3	1.60	0.66
1:A:473:LEU:HD11	1:A:570:THR:HG23	1.77	0.66
1:B:633:TYR:HD1	1:B:759:ARG:HB2	1.60	0.66
1:A:73:LYS:HB3	1:A:105:GLY:HA3	1.77	0.66
1:A:828:ASN:ND2	1:A:908:THR:O	2.29	0.66
1:A:824:ILE:HG12	1:A:830:VAL:HG22	1.76	0.66
1:B:658:ARG:HH21	1:B:893:LEU:HB2	1.61	0.66
1:A:853:ARG:HA	1:A:884:TYR:HA	1.78	0.65
1:B:510:ALA:O	1:B:563:GLN:NE2	2.24	0.65
1:A:458:ALA:O	1:A:462:ASN:ND2	2.30	0.65
1:B:521:GLN:OE1	1:B:527:ASN:CA	2.44	0.65
1:B:331:ARG:NH1	1:B:357:ASN:OD1	2.30	0.65
1:A:87:LEU:HD23	1:A:90:ASN:HA	1.79	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:VAL:N	1:A:143:ASN:OD1	2.23	0.65
1:B:263:HIS:CE1	1:B:276:GLN:HB3	2.32	0.65
1:B:363:GLU:OE1	1:B:389:ARG:NH2	2.30	0.65
1:B:476:SER:H	1:B:489:TRP:HA	1.61	0.65
1:A:160:PRO:HD3	1:A:185:HIS:HA	1.78	0.65
1:A:293:THR:OG1	1:A:304:CYS:SG	2.53	0.65
1:A:787:ALA:H	1:A:798:SER:HB3	1.62	0.65
1:A:858:GLU:OE2	1:A:860:HIS:NE2	2.30	0.65
1:B:233:LEU:HD13	1:B:253:CYS:HB2	1.79	0.65
1:A:89:PHE:HB2	1:B:710:TYR:CE2	2.31	0.65
1:B:275:HIS:HB3	1:B:286:PRO:HB3	1.79	0.65
1:A:776:ARG:NH2	1:A:839:GLU:OE1	2.30	0.64
1:B:436:LEU:O	1:B:440:HIS:ND1	2.31	0.64
1:A:137:LEU:HG	1:A:139:SER:H	1.62	0.64
1:A:159:CYS:O	1:A:162:THR:HG22	1.97	0.64
1:B:310:LYS:NZ	1:B:331:ARG:O	2.26	0.64
1:B:56:MET:HE1	1:B:83:ARG:H	1.62	0.64
1:B:358:LEU:HD21	1:B:382:PHE:CD1	2.32	0.64
1:B:124:GLU:HA	1:B:149:LYS:HD2	1.80	0.64
1:B:260:GLN:HG2	1:B:264:PHE:CE2	2.33	0.64
1:A:886:VAL:HB	1:A:903:THR:HB	1.80	0.63
1:A:183:TRP:CZ3	1:A:189:GLN:HA	2.34	0.63
1:A:367:PHE:HD2	1:A:392:THR:O	1.82	0.63
1:A:369:LYS:HG3	1:A:401:TYR:HB3	1.81	0.63
1:B:267:ARG:CG	1:B:276:GLN:HE21	2.09	0.63
1:B:521:GLN:OE1	1:B:527:ASN:CB	2.45	0.63
1:A:508:LYS:HB3	1:A:529:TRP:CD1	2.33	0.63
1:A:529:TRP:CG	1:A:529:TRP:CA	2.79	0.63
1:A:389:ARG:HB3	1:A:391:GLU:HG3	1.79	0.63
1:B:503:PHE:HB2	1:B:534:ILE:HB	1.80	0.63
1:B:790:GLN:HB3	1:B:796:ARG:HB2	1.80	0.63
1:A:455:ASN:OD1	1:B:455:ASN:ND2	2.32	0.62
2:F:7:CYS:HA	2:F:11:LEU:HD23	1.80	0.62
1:A:190:LYS:NZ	1:A:201:CYS:SG	2.70	0.62
1:A:508:LYS:HE2	1:A:529:TRP:CA	2.28	0.62
1:B:401:TYR:HA	1:B:427:PHE:HB3	1.80	0.62
2:F:7:CYS:O	2:F:10:HIS:ND1	2.32	0.62
1:A:708:GLU:O	1:A:712:HIS:ND1	2.31	0.62
1:A:469:GLU:HB2	1:A:584:LYS:HB2	1.82	0.62
2:F:15:LEU:HD21	2:F:26:TYR:HA	1.82	0.62
1:A:471:GLU:HB2	1:A:583:ALA:HA	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:471:GLU:HB2	1:B:583:ALA:HB2	1.81	0.62
1:A:853:ARG:HD2	1:A:882:GLY:HA3	1.82	0.62
1:B:218:GLU:OE1	1:B:224:LYS:NZ	2.33	0.62
1:B:881:PRO:HA	1:B:907:VAL:HG23	1.81	0.62
1:B:321:ILE:HD12	1:B:342:ILE:HG13	1.82	0.61
1:A:83:ARG:O	1:A:113:THR:HB	2.00	0.61
1:B:563:GLN:HA	1:B:591:GLN:HA	1.83	0.61
1:B:719:ARG:NE	2:E:75:CYS:O	2.27	0.61
1:B:80:THR:HG22	1:B:81:VAL:HG23	1.82	0.61
1:B:367:PHE:HA	1:B:388:ILE:HD11	1.82	0.61
1:A:14:ARG:NH2	1:B:715:VAL:O	2.25	0.61
1:B:279:ILE:HG22	1:B:300:MET:SD	2.40	0.61
1:A:269:SER:CB	1:A:271:LYS:HE2	2.30	0.61
1:A:501:LEU:HB2	1:A:571:LEU:HG	1.81	0.60
1:A:95:ILE:HB	1:A:119:ILE:HD13	1.82	0.60
1:A:260:GLN:HG2	1:A:264:PHE:CD2	2.25	0.60
1:A:358:LEU:HD13	1:A:382:PHE:HE1	1.66	0.60
1:A:787:ALA:O	1:A:798:SER:N	2.29	0.60
1:B:425:LYS:HD2	1:B:452:GLN:HA	1.83	0.60
1:B:33:LEU:HD23	1:B:61:LEU:HD13	1.83	0.60
2:F:19:CYS:HB2	2:F:24:PHE:HB3	1.83	0.60
2:F:24:PHE:HA	2:F:75:CYS:HA	1.83	0.60
1:A:58:THR:O	1:A:84:GLY:N	2.34	0.60
1:B:384:LYS:O	1:B:386:HIS:CD2	2.54	0.60
1:A:454:ARG:HE	1:A:455:ASN:N	1.99	0.60
1:A:633:TYR:CE1	1:A:761:PHE:HB3	2.37	0.60
1:B:377:VAL:HB	1:B:407:ASN:ND2	2.16	0.60
1:B:507:TYR:CE2	1:B:530:THR:OG1	2.47	0.60
1:A:512:TYR:CE2	1:A:514:ASN:OD1	2.54	0.60
1:B:453:GLU:N	1:B:456:ASP:OD2	2.26	0.60
1:B:596:ASN:ND2	1:B:797:CYS:O	2.35	0.60
2:F:60:GLN:HA	2:F:64:SER:HB3	1.83	0.60
1:A:808:MET:SD	1:A:808:MET:N	2.70	0.60
1:B:314:ILE:HG21	1:B:319:LYS:N	2.16	0.60
1:B:386:HIS:CE1	1:B:417:HIS:CD2	2.90	0.60
1:B:426:LEU:HB3	1:B:428:PHE:CE1	2.34	0.60
2:F:20:GLY:H	2:F:23:GLY:H	1.50	0.60
1:B:55:ILE:HB	1:B:227:ALA:HB3	1.84	0.59
1:B:267:ARG:O	1:B:270:ARG:HG3	2.02	0.59
1:B:355:GLU:OE1	1:B:383:ARG:NH2	2.31	0.59
1:A:429:HIS:HB3	1:A:430:TYR:HD1	1.68	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:GLU:HG2	1:B:384:LYS:HB3	1.83	0.59
1:B:578:ARG:HH12	1:B:580:THR:HA	1.67	0.59
1:A:436:LEU:O	1:A:440:HIS:ND1	2.35	0.59
1:B:266:CYS:CA	1:B:269:SER:OG	2.45	0.59
1:B:853:ARG:HA	1:B:884:TYR:HA	1.85	0.59
1:B:778:PHE:HB2	1:B:809:PRO:HA	1.84	0.59
1:A:448:THR:HG22	1:A:451:ARG:HH21	1.68	0.59
1:B:314:ILE:CG2	1:B:318:GLU:C	2.68	0.59
1:B:494:PRO:HB3	1:B:580:THR:HG21	1.84	0.59
1:B:602:ASP:HB3	1:B:618:LYS:HD3	1.83	0.59
1:A:314:ILE:HG13	1:A:336:ILE:HD11	1.84	0.59
1:A:249:GLN:HB2	1:A:251:TRP:CD1	2.39	0.58
1:A:579:ARG:HD3	1:A:581:TYR:HA	1.86	0.58
2:F:19:CYS:HB2	2:F:24:PHE:CD2	2.38	0.58
1:A:473:LEU:N	1:A:584:LYS:O	2.34	0.58
1:B:506:PHE:CA	1:B:529:TRP:HD1	1.97	0.58
1:A:355:GLU:OE2	1:A:383:ARG:NH2	2.36	0.58
1:A:425:LYS:HA	1:A:452:GLN:HE22	1.69	0.58
1:B:245:TYR:HB3	1:B:253:CYS:HB3	1.86	0.58
1:B:789:ASN:HD21	1:B:796:ARG:HH12	1.50	0.58
1:A:89:PHE:N	1:A:325:THR:OG1	2.37	0.58
1:A:816:ILE:HA	1:A:837:PRO:HG3	1.86	0.58
2:G:68:LEU:HA	2:G:71:LEU:HD12	1.86	0.58
1:A:631:LEU:CD2	1:A:633:TYR:HE2	2.17	0.57
1:B:386:HIS:HE1	1:B:417:HIS:ND1	2.02	0.57
1:B:513:GLN:HA	1:B:589:TYR:CE2	2.38	0.57
1:B:816:ILE:HA	1:B:837:PRO:HG3	1.86	0.57
1:A:59:ASP:O	1:A:84:GLY:HA2	2.04	0.57
1:A:639:GLU:OE2	1:A:658:ARG:NH1	2.37	0.57
1:A:52:PRO:O	1:A:78:ASN:ND2	2.34	0.57
1:A:263:HIS:ND1	1:A:276:GLN:HG2	2.19	0.57
1:A:507:TYR:O	1:A:529:TRP:HB3	2.03	0.57
1:A:606:VAL:HB	1:A:614:ILE:HG13	1.85	0.57
1:A:41:THR:OG1	1:A:67:TYR:O	2.21	0.57
1:B:852:ARG:HB2	1:B:858:GLU:HA	1.87	0.57
1:A:91:TYR:OH	1:A:118:ARG:NH1	2.38	0.57
1:A:260:GLN:C	1:A:264:PHE:CD2	2.75	0.57
1:A:529:TRP:CE3	1:A:529:TRP:N	2.73	0.57
1:B:506:PHE:HB3	1:B:529:TRP:CD2	2.37	0.57
1:A:504:MET:SD	1:A:569:LYS:HB3	2.45	0.57
1:B:840:PRO:HG2	1:B:843:LEU:HA	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:506:PHE:CB	1:B:529:TRP:CE2	2.77	0.57
1:A:628:THR:H	1:A:789:ASN:HA	1.69	0.56
1:B:436:LEU:HA	1:B:439:ILE:HG12	1.87	0.56
1:B:613:ILE:HG22	1:B:772:ILE:HG22	1.86	0.56
1:A:35:ILE:HB	1:A:63:LEU:HD13	1.86	0.56
1:A:43:PRO:HA	1:A:46:PHE:HD2	1.70	0.56
1:A:209:HIS:HB2	1:A:221:ASP:N	2.20	0.56
1:A:563:GLN:HA	1:A:591:GLN:HA	1.87	0.56
1:B:321:ILE:HG22	1:B:344:ILE:HD11	1.87	0.56
1:A:338:GLY:N	1:A:365:SER:OG	2.39	0.56
1:A:615:LEU:HD21	1:A:770:LEU:HB3	1.87	0.56
1:A:629:HIS:HE1	1:A:791:ASP:HB3	1.70	0.56
1:A:631:LEU:CD2	1:A:633:TYR:CE2	2.89	0.56
1:A:394:GLU:HB3	1:A:398:TYR:HB2	1.88	0.56
1:A:335:VAL:HG22	1:A:363:GLU:HB2	1.87	0.56
1:A:398:TYR:OH	1:A:456:ASP:OD1	2.23	0.56
1:B:875:ARG:O	1:B:877:ARG:NH2	2.33	0.56
1:A:70:GLU:HA	1:A:101:LEU:HA	1.89	0.55
1:A:518:PHE:CE1	1:A:521:GLN:HG2	2.41	0.55
1:B:477:PHE:CE2	1:B:479:ARG:HB2	2.41	0.55
1:A:314:ILE:HG22	1:A:315:LEU:N	2.21	0.55
1:A:400:PHE:HB3	1:A:426:LEU:HD13	1.88	0.55
1:B:418:ASN:OD1	1:B:419:LEU:N	2.39	0.55
2:F:59:GLU:OE1	2:F:59:GLU:N	2.39	0.55
1:A:712:HIS:HD2	1:A:716:PHE:HE2	1.54	0.55
1:B:409:ARG:HH22	1:B:517:GLU:CG	2.19	0.55
1:A:55:ILE:O	1:A:80:THR:N	2.38	0.55
1:B:212:CYS:N	1:B:225:CYS:SG	2.79	0.55
1:B:513:GLN:HG2	1:B:589:TYR:HD2	1.71	0.55
1:A:719:ARG:N	2:D:73:ASN:O	2.40	0.55
1:B:586:ASP:OD1	1:B:587:ILE:N	2.37	0.55
1:B:469:GLU:HB2	1:B:584:LYS:HE2	1.88	0.55
1:A:56:MET:SD	1:A:83:ARG:HG3	2.47	0.55
1:A:561:TRP:HB2	1:A:594:ALA:HB2	1.89	0.55
1:B:658:ARG:HE	1:B:893:LEU:HB3	1.72	0.55
1:B:762:GLU:OE2	1:B:763:LYS:N	2.40	0.55
1:A:484:LYS:HA	1:A:555:MET:O	2.06	0.55
1:B:336:ILE:HB	1:B:364:ILE:HG12	1.88	0.55
1:B:414:TRP:CZ2	1:B:442:MET:HA	2.42	0.55
2:F:67:SER:OG	2:F:70:GLN:OE1	2.21	0.55
1:A:485:ILE:HG22	1:A:555:MET:HB3	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:LEU:O	1:A:149:LYS:HB3	2.07	0.54
1:A:565:ALA:HB1	1:A:587:ILE:HD11	1.87	0.54
1:A:655:LEU:HD21	1:A:893:LEU:HA	1.88	0.54
1:B:432:PRO:HB2	1:B:465:GLN:HB2	1.88	0.54
1:B:485:ILE:HB	1:B:555:MET:HB2	1.89	0.54
1:B:825:PHE:HE1	1:B:831:HIS:HB2	1.71	0.54
1:B:888:VAL:N	1:B:900:THR:OG1	2.38	0.54
1:A:610:SER:HA	1:A:807:THR:HB	1.88	0.54
1:A:789:ASN:OD1	1:A:796:ARG:NH1	2.41	0.54
1:B:776:ARG:O	1:B:779:THR:OG1	2.24	0.54
1:A:201:CYS:HB2	1:A:205:GLY:HA2	1.87	0.54
1:A:553:TRP:HZ2	1:A:556:ARG:HH12	1.55	0.54
1:A:778:PHE:HE2	1:A:893:LEU:HB3	1.73	0.54
1:B:266:CYS:SG	1:B:274:CYS:O	2.66	0.54
1:A:171:ALA:HA	1:A:180:GLU:HA	1.89	0.54
1:B:7:VAL:HG13	1:B:251:TRP:HZ2	1.73	0.54
1:B:260:GLN:O	1:B:264:PHE:HD2	1.90	0.54
1:B:464:ASP:OD1	1:B:465:GLN:N	2.40	0.54
1:A:770:LEU:HG	1:A:771:VAL:N	2.22	0.54
1:A:567:PHE:HB3	1:A:587:ILE:HA	1.90	0.54
1:A:598:SER:HB3	1:A:620:PRO:HB2	1.88	0.54
1:A:718:PRO:HB3	2:D:74:TYR:CZ	2.42	0.54
1:A:778:PHE:HB2	1:A:809:PRO:HA	1.90	0.54
1:B:78:ASN:HA	1:B:108:ASN:HD22	1.72	0.54
1:B:598:SER:HB3	1:B:620:PRO:HB2	1.90	0.54
1:A:508:LYS:HZ3	1:A:529:TRP:HA	1.69	0.54
1:B:506:PHE:CD2	1:B:529:TRP:CE2	2.89	0.54
1:B:601:LEU:O	1:B:618:LYS:N	2.37	0.54
1:A:161:GLY:O	1:A:162:THR:C	2.46	0.53
1:A:478:ILE:HG23	1:A:485:ILE:HD11	1.90	0.53
1:A:504:MET:SD	1:A:504:MET:N	2.81	0.53
1:B:368:LEU:HB3	1:B:400:PHE:CD1	2.43	0.53
1:A:95:ILE:HB	1:A:119:ILE:CD1	2.38	0.53
1:A:777:HIS:HD2	1:A:841:ASN:HA	1.73	0.53
1:B:636:ARG:NH2	1:B:779:THR:HB	2.21	0.53
1:A:342:ILE:HD11	1:A:370:ILE:HG12	1.90	0.53
1:B:484:LYS:NZ	2:G:10:HIS:O	2.41	0.53
1:B:853:ARG:NE	1:B:856:ASP:OD2	2.40	0.53
2:F:20:GLY:N	2:F:23:GLY:H	2.06	0.53
1:A:31:GLY:O	1:A:58:THR:OG1	2.26	0.53
1:A:107:TYR:HA	1:A:183:TRP:CD2	2.43	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:VAL:HG13	1:A:147:LEU:HG	1.91	0.53
1:A:509:GLU:HA	1:A:564:TYR:HA	1.90	0.53
1:B:401:TYR:CE1	1:B:403:LEU:HB2	2.44	0.53
1:B:386:HIS:HA	1:B:419:LEU:HD13	1.90	0.53
1:B:479:ARG:HH22	2:G:21:GLU:HG2	1.73	0.53
1:B:521:GLN:OE1	1:B:528:SER:N	2.41	0.53
1:A:512:TYR:CD2	1:A:514:ASN:OD1	2.61	0.53
1:A:615:LEU:C	1:A:616:LYS:HD2	2.29	0.53
1:B:322:ASP:HA	1:B:344:ILE:HG13	1.91	0.53
1:B:402:ALA:HB3	1:B:428:PHE:HA	1.91	0.53
1:B:578:ARG:NH1	1:B:580:THR:HA	2.24	0.53
1:A:314:ILE:HG22	1:A:315:LEU:C	2.29	0.53
1:A:520:GLY:C	1:A:521:GLN:HG3	2.29	0.53
1:A:712:HIS:CE1	2:D:8:GLY:HA2	2.44	0.53
1:B:323:SER:O	1:B:326:SER:OG	2.22	0.53
1:B:615:LEU:O	1:B:769:SER:HA	2.09	0.53
1:B:635:GLU:HB2	1:B:759:ARG:HD2	1.90	0.53
1:A:202:THR:HG22	1:A:206:LEU:H	1.74	0.53
1:A:636:ARG:NH2	1:A:781:TYR:OH	2.30	0.53
1:B:209:HIS:HB2	1:B:221:ASP:N	2.23	0.53
2:G:20:GLY:H	2:G:23:GLY:H	1.56	0.53
1:B:597:PRO:HA	1:B:624:ASN:HD22	1.74	0.52
1:A:852:ARG:HB2	1:A:858:GLU:HA	1.90	0.52
1:B:338:GLY:N	1:B:365:SER:OG	2.42	0.52
1:B:887:ARG:HE	1:B:899:TRP:HB3	1.74	0.52
1:B:426:LEU:H	1:B:452:GLN:HG3	1.73	0.52
1:B:598:SER:HB2	1:B:622:ASP:HB2	1.90	0.52
1:B:637:GLN:HG2	1:B:781:TYR:HA	1.92	0.52
2:F:16:TYR:HA	2:F:24:PHE:HE2	1.74	0.52
2:G:20:GLY:N	2:G:23:GLY:H	2.07	0.52
1:A:448:THR:HB	1:A:451:ARG:HE	1.75	0.52
1:B:279:ILE:HG21	1:B:300:MET:SD	2.49	0.52
1:B:310:LYS:HG3	1:B:312:CYS:SG	2.49	0.52
2:F:15:LEU:HG	2:F:24:PHE:CD2	2.44	0.52
1:A:12:ASP:OD1	1:A:34:GLN:NE2	2.41	0.52
1:A:835:GLN:NE2	1:A:836:GLU:O	2.42	0.52
1:B:28:VAL:HG22	1:B:56:MET:HB3	1.90	0.52
1:B:858:GLU:OE2	1:B:860:HIS:NE2	2.42	0.52
1:A:28:VAL:HG13	1:A:56:MET:O	2.09	0.52
1:A:483:ASP:C	1:A:484:LYS:HD3	2.30	0.52
1:B:587:ILE:HG22	1:B:589:TYR:HE1	1.75	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:13:GLU:O	2:F:17:LEU:HG	2.09	0.52
1:A:32:HIS:HB3	1:A:59:ASP:HB2	1.92	0.52
1:A:358:LEU:HD13	1:A:382:PHE:CE1	2.44	0.52
1:A:518:PHE:CE1	1:A:521:GLN:CG	2.93	0.52
1:B:386:HIS:ND1	1:B:417:HIS:CD2	2.78	0.52
1:B:428:PHE:HB2	1:B:457:ILE:HG12	1.91	0.52
1:A:182:CYS:HA	1:A:189:GLN:N	2.25	0.52
1:B:481:SER:OG	2:G:17:LEU:HD11	2.10	0.52
1:A:88:PHE:CE1	1:B:710:TYR:HE2	2.28	0.51
1:A:269:SER:HB3	1:A:271:LYS:HE2	1.90	0.51
1:B:52:PRO:O	1:B:78:ASN:ND2	2.42	0.51
1:B:601:LEU:HB2	1:B:618:LYS:HB2	1.91	0.51
2:E:56:GLY:N	2:E:59:GLU:OE2	2.43	0.51
2:F:64:SER:OG	2:F:65:ILE:N	2.43	0.51
1:A:508:LYS:HB2	1:A:529:TRP:CB	2.39	0.51
1:A:617:TRP:CE2	1:A:768:GLU:HA	2.45	0.51
1:A:719:ARG:NE	2:D:75:CYS:O	2.43	0.51
1:B:208:CYS:HA	1:B:219:PRO:HA	1.91	0.51
1:B:331:ARG:HG3	1:B:357:ASN:HA	1.92	0.51
1:B:579:ARG:HH12	1:B:581:TYR:HA	1.76	0.51
1:A:78:ASN:HA	1:A:108:ASN:ND2	2.19	0.51
1:A:314:ILE:CG2	1:A:315:LEU:N	2.73	0.51
1:A:790:GLN:OE1	1:A:796:ARG:NH2	2.43	0.51
1:A:161:GLY:CA	1:A:169:CYS:H	2.24	0.51
1:A:181:ARG:HB3	1:A:189:GLN:HB3	1.92	0.51
1:A:618:LYS:HD2	1:A:619:PRO:O	2.09	0.51
1:A:798:SER:OG	1:A:799:VAL:N	2.43	0.51
1:B:248:PHE:HD2	1:B:252:ARG:HE	1.58	0.51
1:B:614:ILE:HB	1:B:616:LYS:HZ2	1.75	0.51
1:B:784:GLU:HB2	1:B:802:TYR:CE1	2.46	0.51
1:B:269:SER:HB2	1:B:271:LYS:HG3	1.93	0.51
2:F:25:PHE:HE1	2:F:74:TYR:HD2	1.58	0.51
1:B:379:LEU:HD23	1:B:379:LEU:O	2.11	0.51
1:B:631:LEU:HG	1:B:786:GLN:HB2	1.93	0.51
2:G:24:PHE:HD2	2:G:26:TYR:N	2.08	0.51
1:A:295:ASN:HB2	1:A:298:ASN:OD1	2.10	0.51
1:B:218:GLU:OE1	1:B:224:LYS:HG3	2.11	0.51
1:B:798:SER:OG	1:B:799:VAL:N	2.44	0.51
1:B:868:PHE:O	1:B:872:ARG:N	2.44	0.51
1:A:574:PHE:HA	1:A:580:THR:HG23	1.93	0.51
1:A:869:ALA:O	1:A:872:ARG:NH1	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:602:ASP:O	1:B:617:TRP:HA	2.11	0.51
1:B:248:PHE:HD1	1:B:284:CYS:HB3	1.76	0.51
1:B:401:TYR:HE1	1:B:403:LEU:HB2	1.76	0.51
1:B:648:TYR:O	1:B:653:LEU:HB3	2.11	0.51
1:A:166:LYS:O	1:A:167:THR:OG1	2.25	0.50
1:A:270:ARG:O	1:A:271:LYS:C	2.48	0.50
1:B:576:ASP:OD1	1:B:576:ASP:N	2.42	0.50
1:B:700:GLU:HG2	1:B:701:SER:N	2.25	0.50
1:A:476:SER:N	1:A:488:ARG:O	2.34	0.50
1:A:634:TRP:NE1	1:A:760:PRO:HB2	2.27	0.50
1:A:791:ASP:N	1:A:791:ASP:OD1	2.44	0.50
1:B:29:ILE:HD13	1:B:33:LEU:HB2	1.93	0.50
1:B:814:ASP:OD2	1:B:841:ASN:ND2	2.42	0.50
1:A:429:HIS:HB3	1:A:430:TYR:CD1	2.46	0.50
1:A:853:ARG:NE	1:A:856:ASP:OD2	2.43	0.50
1:B:611:SER:HA	1:B:775:LEU:HB2	1.94	0.50
2:E:64:SER:OG	2:E:65:ILE:N	2.43	0.50
2:F:24:PHE:HA	2:F:76:ASN:N	2.24	0.50
2:G:14:ALA:O	2:G:17:LEU:HB2	2.10	0.50
1:A:61:LEU:HB3	1:A:93:LEU:HD13	1.92	0.50
1:A:260:GLN:C	1:A:264:PHE:HD2	2.06	0.50
1:A:781:TYR:O	1:A:804:SER:HA	2.12	0.50
1:B:280:HIS:HB3	1:B:285:ILE:HD11	1.92	0.50
1:A:386:HIS:O	1:A:419:LEU:HD12	2.12	0.50
2:D:6:LEU:HB3	2:D:11:LEU:HA	1.93	0.50
1:A:249:GLN:HB2	1:A:251:TRP:HD1	1.75	0.50
1:A:362:GLU:HG3	1:A:384:LYS:O	2.11	0.50
1:A:570:THR:HG21	1:A:583:ALA:HB3	1.94	0.50
1:A:788:CYS:HA	1:A:797:CYS:HA	1.93	0.50
1:B:314:ILE:HG23	1:B:319:LYS:HB2	1.94	0.50
1:B:341:ILE:HG12	1:B:369:LYS:HB3	1.92	0.50
2:F:25:PHE:CE1	2:F:74:TYR:HD2	2.29	0.50
1:A:30:GLU:HA	1:A:58:THR:HG21	1.94	0.50
2:F:14:ALA:O	2:F:18:VAL:HG23	2.10	0.50
1:A:369:LYS:HE3	1:A:401:TYR:CD1	2.47	0.49
1:A:709:ASP:HA	2:D:58:VAL:HG11	1.94	0.49
1:B:386:HIS:NE2	1:B:417:HIS:CE1	2.73	0.49
1:B:640:ASP:HB2	1:B:643:LEU:HG	1.94	0.49
1:B:791:ASP:HA	1:B:795:GLU:HA	1.93	0.49
1:A:414:TRP:CH2	1:A:442:MET:HG2	2.47	0.49
1:B:260:GLN:O	1:B:264:PHE:CD2	2.64	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:GLU:CG	1:B:384:LYS:HB3	2.42	0.49
2:G:59:GLU:OE1	2:G:59:GLU:N	2.39	0.49
1:A:139:SER:OG	1:A:142:ASP:OD2	2.26	0.49
1:A:160:PRO:O	1:A:161:GLY:C	2.49	0.49
1:A:599:VAL:HG22	1:A:799:VAL:HG22	1.94	0.49
1:B:336:ILE:HD11	1:B:361:ILE:HD13	1.94	0.49
1:B:612:GLN:NE2	1:B:773:SER:OG	2.39	0.49
1:A:836:GLU:OE1	1:A:847:TYR:OH	2.31	0.49
1:B:628:THR:H	1:B:789:ASN:HA	1.77	0.49
1:A:98:MET:HB3	1:A:101:LEU:HB2	1.93	0.49
1:A:278:VAL:HG12	1:A:294:MET:HG3	1.94	0.49
1:A:292:TYR:CD1	1:A:303:PRO:HA	2.47	0.49
1:A:874:CYS:SG	1:A:875:ARG:N	2.85	0.49
1:B:517:GLU:OE1	1:B:567:PHE:CZ	2.66	0.49
1:B:778:PHE:HB2	1:B:809:PRO:CA	2.42	0.49
2:E:21:GLU:HG2	2:E:22:ARG:HG3	1.93	0.49
1:B:636:ARG:HE	1:B:637:GLN:N	2.09	0.49
1:B:788:CYS:HA	1:B:797:CYS:HA	1.94	0.49
1:A:606:VAL:O	1:A:614:ILE:N	2.44	0.49
1:A:629:HIS:CE1	1:A:791:ASP:HB3	2.48	0.49
1:B:294:MET:CE	1:B:295:ASN:H	2.25	0.49
1:B:636:ARG:HH12	1:B:779:THR:HB	1.76	0.49
1:A:887:ARG:HE	1:A:899:TRP:HB3	1.77	0.49
1:B:597:PRO:HG2	1:B:798:SER:HB2	1.95	0.49
1:A:159:CYS:O	1:A:160:PRO:C	2.49	0.49
1:A:209:HIS:HB2	1:A:221:ASP:H	1.78	0.49
1:A:209:HIS:CD2	1:A:222:PRO:HD3	2.47	0.49
1:A:246:TYR:HA	1:A:282:ASN:ND2	2.28	0.49
1:A:314:ILE:CG1	1:A:336:ILE:HD11	2.43	0.49
1:A:512:TYR:HE2	1:A:514:ASN:OD1	1.95	0.49
1:B:23:LEU:HA	1:B:26:CYS:SG	2.53	0.49
1:B:765:VAL:H	1:B:767:LYS:NZ	2.11	0.49
1:A:269:SER:HB3	1:A:271:LYS:CG	2.35	0.48
1:A:528:SER:C	1:A:529:TRP:HE3	2.16	0.48
1:B:488:ARG:NH1	1:B:550:HIS:O	2.46	0.48
1:B:517:GLU:OE2	1:B:567:PHE:CZ	2.66	0.48
1:A:44:GLU:HA	1:A:47:ARG:CZ	2.42	0.48
1:A:60:TYR:CD2	1:A:88:PHE:HB2	2.47	0.48
1:A:118:ARG:NE	1:A:120:GLU:OE1	2.37	0.48
1:A:422:THR:O	1:A:451:ARG:NH1	2.45	0.48
1:B:393:LEU:HD11	1:B:423:GLN:OE1	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:613:ILE:O	1:B:771:VAL:HA	2.13	0.48
1:A:23:LEU:HD23	1:A:23:LEU:O	2.14	0.48
1:A:144:TYR:HE2	1:A:146:VAL:HG11	1.77	0.48
1:B:491:PRO:HD3	1:B:550:HIS:CE1	2.48	0.48
1:B:578:ARG:NH1	1:B:579:ARG:O	2.46	0.48
1:B:889:ARG:HB2	1:B:899:TRP:CD2	2.48	0.48
1:A:208:CYS:HA	1:A:219:PRO:HA	1.96	0.48
1:A:494:PRO:HG2	1:A:496:ASP:O	2.14	0.48
1:A:513:GLN:O	1:A:589:TYR:OH	2.19	0.48
1:B:429:HIS:CE1	1:B:458:ALA:HB2	2.48	0.48
1:B:610:SER:HA	1:B:807:THR:HB	1.95	0.48
1:A:421:ILE:HB	1:A:448:THR:HG21	1.95	0.48
1:B:561:TRP:N	1:B:592:THR:OG1	2.46	0.48
1:B:29:ILE:HD12	1:B:57:ILE:HG12	1.94	0.48
1:B:853:ARG:HB2	1:B:884:TYR:CE2	2.49	0.48
1:A:414:TRP:CD1	1:A:441:LYS:HD2	2.49	0.48
1:B:59:ASP:O	1:B:84:GLY:HA2	2.14	0.48
1:B:414:TRP:HZ2	1:B:442:MET:HG3	1.79	0.48
1:B:705:LYS:HB3	1:B:705:LYS:HE2	1.54	0.48
2:F:24:PHE:CA	2:F:75:CYS:HA	2.44	0.48
1:A:436:LEU:HB3	1:A:440:HIS:HE1	1.79	0.48
1:B:379:LEU:HB3	1:B:411:LEU:O	2.14	0.48
1:B:430:TYR:H	1:B:461:THR:HB	1.79	0.48
1:A:32:HIS:HB2	1:A:60:TYR:CE1	2.49	0.48
1:A:107:TYR:HA	1:A:183:TRP:CE3	2.49	0.48
1:A:218:GLU:H	1:A:224:LYS:HB3	1.78	0.48
1:A:248:PHE:HE2	1:A:252:ARG:HH21	1.62	0.48
1:A:604:ILE:HD11	1:A:616:LYS:HB2	1.96	0.48
1:B:338:GLY:O	1:B:364:ILE:HG23	2.14	0.48
1:B:601:LEU:HG	1:B:620:PRO:HA	1.96	0.48
2:G:9:SER:HA	2:G:12:VAL:HG22	1.95	0.48
1:A:505:LEU:HD11	1:A:566:ILE:HG23	1.94	0.47
1:B:378:SER:HA	1:B:410:GLN:O	2.14	0.47
1:B:490:GLU:HA	1:B:550:HIS:CE1	2.49	0.47
1:A:632:VAL:HB	1:A:762:GLU:HG2	1.96	0.47
1:B:700:GLU:HB2	1:B:704:ARG:HH22	1.78	0.47
1:A:56:MET:HG2	1:A:81:VAL:O	2.14	0.47
1:B:475:PHE:HA	1:B:489:TRP:HA	1.97	0.47
1:B:553:TRP:HZ3	2:G:67:SER:HA	1.78	0.47
1:A:173:VAL:HA	1:A:177:GLN:O	2.14	0.47
1:A:290:SER:HB3	1:A:309:PRO:HA	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:GLU:N	1:A:398:TYR:O	2.33	0.47
1:B:34:GLN:HB3	1:B:36:LEU:HD22	1.95	0.47
1:B:372:ARG:HA	1:B:404:ASP:O	2.14	0.47
1:B:431:ASN:O	1:B:462:ASN:HA	2.13	0.47
1:B:695:LEU:O	1:B:699:GLU:HG2	2.14	0.47
1:A:618:LYS:HG2	1:A:619:PRO:HD2	1.97	0.47
1:B:355:GLU:O	1:B:359:GLY:N	2.29	0.47
1:A:35:ILE:HG22	1:A:66:VAL:HG21	1.97	0.47
1:A:119:ILE:HB	1:A:145:ILE:HG12	1.97	0.47
1:A:271:LYS:CB	1:A:272:PRO:CD	2.88	0.47
1:A:461:THR:OG1	1:A:462:ASN:OD1	2.33	0.47
1:A:481:SER:HB3	1:A:484:LYS:HB2	1.97	0.47
1:A:485:ILE:O	1:A:554:LEU:HD12	2.15	0.47
1:A:504:MET:CE	1:A:571:LEU:HB2	2.45	0.47
1:A:507:TYR:HA	1:A:565:ALA:O	2.14	0.47
1:B:326:SER:HA	1:B:329:GLU:OE2	2.15	0.47
1:B:484:LYS:HZ1	2:G:13:GLU:HB3	1.80	0.47
2:F:24:PHE:CB	2:F:75:CYS:HA	2.45	0.47
2:G:8:GLY:O	2:G:11:LEU:HG	2.15	0.47
2:G:64:SER:OG	2:G:65:ILE:N	2.47	0.47
1:A:181:ARG:HB3	1:A:189:GLN:OE1	2.15	0.47
1:A:482:PHE:HA	1:A:593:ASP:OD1	2.14	0.47
1:A:595:THR:O	1:A:789:ASN:ND2	2.38	0.47
2:F:27:THR:HG21	2:F:57:ILE:HD13	1.97	0.47
2:F:60:GLN:HG3	2:F:66:CYS:SG	2.55	0.47
1:A:93:LEU:O	1:A:117:VAL:HA	2.15	0.47
1:A:762:GLU:OE2	1:A:770:LEU:HD22	2.14	0.47
1:B:506:PHE:CG	1:B:529:TRP:CE2	2.96	0.47
1:B:648:TYR:HD1	1:B:653:LEU:HA	1.80	0.47
1:A:251:TRP:NE1	1:A:252:ARG:HG2	2.30	0.47
1:A:441:LYS:O	1:A:444:GLU:HG2	2.15	0.47
1:A:602:ASP:O	1:A:617:TRP:HA	2.15	0.47
1:A:612:GLN:HA	1:A:772:ILE:O	2.15	0.47
1:B:786:GLN:HE21	1:B:800:ALA:N	2.13	0.47
1:A:339:SER:OG	1:A:366:GLY:HA3	2.15	0.46
1:B:501:LEU:CD2	1:B:698:LEU:HD23	2.36	0.46
1:B:765:VAL:O	1:B:767:LYS:NZ	2.42	0.46
1:A:561:TRP:CE2	1:A:625:GLY:HA2	2.50	0.46
1:B:365:SER:O	1:B:389:ARG:HB2	2.15	0.46
1:B:597:PRO:HA	1:B:624:ASN:ND2	2.29	0.46
1:A:578:ARG:HG3	1:A:579:ARG:O	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:ASN:ND2	1:B:300:MET:HG3	2.31	0.46
1:B:429:HIS:NE2	1:B:455:ASN:O	2.49	0.46
1:A:279:ILE:O	1:A:300:MET:HA	2.15	0.46
1:A:413:ASP:OD1	1:A:415:SER:OG	2.28	0.46
1:B:231:PHE:HA	1:B:251:TRP:O	2.16	0.46
2:F:67:SER:H	2:F:70:GLN:HE22	1.64	0.46
1:A:365:SER:HA	1:A:389:ARG:HD2	1.98	0.46
1:B:263:HIS:ND1	1:B:277:TYR:O	2.48	0.46
1:B:376:LEU:O	1:B:407:ASN:HB3	2.15	0.46
1:B:447:GLY:HA2	1:B:449:LYS:NZ	2.31	0.46
1:B:553:TRP:CG	1:B:554:LEU:N	2.84	0.46
1:B:629:HIS:CD2	1:B:763:LYS:HD2	2.51	0.46
1:B:468:CYS:HB2	1:B:581:TYR:CD1	2.50	0.46
1:A:159:CYS:HA	1:A:182:CYS:SG	2.56	0.46
1:B:371:ARG:HG3	1:B:403:LEU:HD23	1.98	0.46
1:A:164:LYS:O	1:A:165:GLY:C	2.52	0.46
1:A:634:TRP:O	1:A:760:PRO:HG2	2.16	0.46
1:A:853:ARG:HB2	1:A:884:TYR:CE2	2.51	0.46
1:A:889:ARG:HB2	1:A:899:TRP:CD2	2.51	0.46
1:B:295:ASN:O	1:B:299:LEU:N	2.48	0.46
2:E:58:VAL:HG23	2:E:62:CYS:HB3	1.97	0.46
1:A:57:ILE:HG22	1:A:82:ILE:HA	1.98	0.46
1:A:262:LEU:HA	1:A:265:LYS:HZ2	1.79	0.46
1:A:479:ARG:O	1:A:485:ILE:HD12	2.16	0.46
1:A:636:ARG:NH2	1:A:776:ARG:HB2	2.31	0.46
1:B:342:ILE:HD13	1:B:370:ILE:HD13	1.97	0.46
1:B:359:GLY:O	1:B:383:ARG:HB3	2.16	0.46
1:B:428:PHE:HB2	1:B:457:ILE:HG23	1.97	0.46
1:B:506:PHE:CE1	1:B:569:LYS:HE2	2.50	0.46
1:B:631:LEU:HD23	1:B:797:CYS:SG	2.56	0.46
2:G:59:GLU:O	2:G:63:THR:HB	2.16	0.46
1:A:633:TYR:CE1	1:A:761:PHE:CB	2.99	0.46
1:A:888:VAL:O	1:A:900:THR:N	2.43	0.46
1:B:432:PRO:HA	1:B:464:ASP:OD1	2.15	0.46
1:B:498:ARG:HH21	2:E:8:GLY:CA	2.29	0.46
1:B:504:MET:N	1:B:569:LYS:O	2.36	0.46
2:D:15:LEU:HD11	2:D:57:ILE:HD11	1.98	0.46
1:A:580:THR:O	1:A:581:TYR:CG	2.69	0.45
1:B:265:LYS:HE3	1:B:265:LYS:HB2	1.31	0.45
1:B:551:PRO:HA	2:G:69:TYR:OH	2.16	0.45
1:B:614:ILE:HG22	1:B:771:VAL:HB	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:776:ARG:HD3	1:B:779:THR:HG21	1.98	0.45
1:B:843:LEU:HG	1:B:893:LEU:HD12	1.97	0.45
2:E:6:LEU:O	2:E:11:LEU:HD12	2.17	0.45
1:A:90:ASN:HD22	1:A:350:LEU:HD21	1.81	0.45
1:A:386:HIS:O	1:A:420:THR:N	2.43	0.45
1:A:642:GLU:HA	1:A:645:GLU:OE2	2.16	0.45
1:B:56:MET:HE1	1:B:83:ARG:HG3	1.97	0.45
1:B:604:ILE:O	1:B:615:LEU:HD12	2.17	0.45
1:A:10:GLY:HA3	1:A:31:GLY:HA3	1.99	0.45
1:A:322:ASP:N	1:A:322:ASP:OD1	2.49	0.45
1:A:469:GLU:HB3	1:A:583:ALA:N	2.31	0.45
1:B:92:ALA:HB2	1:B:115:GLY:HA3	1.99	0.45
1:B:379:LEU:HG	1:B:382:PHE:CD2	2.51	0.45
1:B:784:GLU:HA	1:B:801:ALA:O	2.17	0.45
1:A:481:SER:OG	1:A:482:PHE:N	2.50	0.45
1:A:816:ILE:HG12	1:A:837:PRO:HD3	1.99	0.45
1:A:509:GLU:OE1	1:A:511:PRO:HD3	2.17	0.45
1:A:246:TYR:HD1	1:A:282:ASN:HA	1.81	0.45
1:B:792:SER:OG	1:B:793:PRO:CD	2.57	0.45
1:B:863:VAL:HG13	1:B:867:HIS:ND1	2.32	0.45
2:E:21:GLU:OE1	2:E:21:GLU:N	2.36	0.45
2:F:67:SER:H	2:F:70:GLN:NE2	2.14	0.45
1:B:27:SER:OG	1:B:227:ALA:HA	2.16	0.45
1:B:634:TRP:NE1	1:B:760:PRO:HB2	2.31	0.45
2:F:29:LYS:HB2	2:F:29:LYS:HE2	1.32	0.45
1:A:260:GLN:O	1:A:264:PHE:CE2	2.62	0.45
2:F:24:PHE:HD1	2:F:24:PHE:O	2.00	0.45
1:A:8:CYS:O	1:A:29:ILE:HG23	2.17	0.44
1:A:87:LEU:HD12	1:A:87:LEU:HA	1.70	0.44
1:A:428:PHE:O	1:A:429:HIS:ND1	2.50	0.44
1:A:714:VAL:HG11	1:B:88:PHE:HE1	1.82	0.44
1:B:427:PHE:CE1	1:B:429:HIS:HB2	2.52	0.44
1:B:697:GLU:HA	1:B:700:GLU:CD	2.38	0.44
1:A:118:ARG:HH12	1:B:703:PHE:HZ	1.61	0.44
1:A:167:THR:O	1:A:168:ASN:C	2.55	0.44
1:A:508:LYS:HG2	1:A:529:TRP:CD2	2.52	0.44
1:B:405:ASN:O	1:B:432:PRO:HD2	2.16	0.44
1:B:509:GLU:HA	1:B:564:TYR:HA	1.98	0.44
1:B:776:ARG:HB3	1:B:779:THR:HG21	1.99	0.44
1:B:810:GLU:HB2	1:B:813:ALA:HB2	1.99	0.44
1:A:29:ILE:HB	1:A:57:ILE:HD12	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:PRO:O	1:B:309:PRO:HD3	2.18	0.44
1:A:102:LYS:C	1:A:125:LEU:HD12	2.37	0.44
1:A:314:ILE:HB	1:A:317:GLY:HA2	1.99	0.44
1:A:98:MET:HG3	1:A:101:LEU:HD22	2.00	0.44
1:B:579:ARG:NH1	1:B:581:TYR:HA	2.31	0.44
1:A:80:THR:HA	1:A:108:ASN:O	2.17	0.44
1:A:280:HIS:CE1	1:A:281:ASN:HB2	2.52	0.44
1:A:614:ILE:HB	1:A:616:LYS:NZ	2.33	0.44
1:A:651:LYS:HA	1:B:651:LYS:HE3	2.00	0.44
1:B:312:CYS:HB3	1:B:330:LEU:HD12	2.00	0.44
2:F:27:THR:HG21	2:F:57:ILE:CD1	2.47	0.44
1:A:181:ARG:CB	1:A:189:GLN:HB3	2.48	0.44
1:A:553:TRP:NE1	1:A:554:LEU:O	2.51	0.44
1:A:790:GLN:NE2	1:A:796:ARG:HB2	2.33	0.44
1:B:93:LEU:HB3	1:B:117:VAL:HG22	1.99	0.44
1:B:307:PRO:HG2	1:B:309:PRO:HG3	2.00	0.44
1:B:628:THR:HG1	1:B:629:HIS:CE1	2.35	0.44
2:G:14:ALA:O	2:G:18:VAL:HG23	2.17	0.44
1:A:65:ARG:NE	1:A:97:GLU:OE1	2.51	0.44
1:A:377:VAL:HA	1:A:407:ASN:O	2.18	0.44
1:A:500:LEU:HD21	1:A:503:PHE:CZ	2.53	0.44
1:B:567:PHE:HB3	1:B:587:ILE:HG12	1.99	0.44
1:B:7:VAL:HG11	1:B:252:ARG:CZ	2.47	0.44
1:B:11:MET:SD	1:B:11:MET:N	2.91	0.44
1:B:81:VAL:HA	1:B:111:ASN:O	2.18	0.44
1:B:506:PHE:CD2	1:B:529:TRP:CD1	2.90	0.44
1:B:633:TYR:CE1	1:B:761:PHE:HB3	2.52	0.44
2:G:66:CYS:HA	2:G:70:GLN:OE1	2.17	0.44
1:A:100:HIS:H	1:A:124:GLU:HG3	1.83	0.43
1:A:358:LEU:HD23	1:A:358:LEU:HA	1.79	0.43
1:A:715:VAL:HA	1:B:14:ARG:HH22	1.83	0.43
1:B:96:PHE:CD1	1:B:120:GLU:HB3	2.53	0.43
1:B:460:LYS:O	1:B:464:ASP:HB3	2.17	0.43
1:B:784:GLU:HG3	1:B:800:ALA:HB1	2.00	0.43
2:F:25:PHE:CE1	2:F:27:THR:HG22	2.53	0.43
1:A:401:TYR:HA	1:A:427:PHE:HB3	2.00	0.43
1:A:633:TYR:CD1	1:A:761:PHE:CB	2.88	0.43
1:A:637:GLN:HB2	1:A:780:GLY:C	2.39	0.43
1:A:793:PRO:O	1:A:794:ASP:HB2	2.19	0.43
1:B:614:ILE:HB	1:B:616:LYS:NZ	2.33	0.43
1:B:844:ILE:HD13	1:B:890:ALA:HB1	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:GLY:HA2	1:A:169:CYS:H	1.82	0.43
1:A:631:LEU:HD21	1:A:633:TYR:CZ	2.53	0.43
1:A:852:ARG:O	1:A:885:SER:N	2.50	0.43
1:A:475:PHE:CD1	1:A:487:LEU:HD11	2.54	0.43
1:A:869:ALA:HA	1:A:872:ARG:NH2	2.33	0.43
1:B:321:ILE:HD11	1:B:340:LEU:HD22	2.00	0.43
1:B:483:ASP:OD1	1:B:484:LYS:HG3	2.19	0.43
1:B:845:VAL:O	1:B:865:ARG:HG3	2.17	0.43
2:F:70:GLN:HA	2:F:73:ASN:OD1	2.18	0.43
1:A:508:LYS:HG2	1:A:529:TRP:CE2	2.54	0.43
1:A:632:VAL:O	1:A:761:PHE:HA	2.19	0.43
1:A:634:TRP:CE2	1:A:760:PRO:HB2	2.54	0.43
1:A:868:PHE:CD1	1:A:873:GLY:HA2	2.54	0.43
1:B:596:ASN:O	1:B:624:ASN:ND2	2.49	0.43
1:A:294:MET:HA	1:A:300:MET:O	2.18	0.43
1:B:479:ARG:HB3	1:B:486:LEU:HB3	2.00	0.43
1:B:838:LYS:HE2	1:B:838:LYS:HB2	1.86	0.43
1:B:277:TYR:HB3	1:B:284:CYS:SG	2.58	0.43
1:B:289:PRO:HG2	1:B:292:TYR:CD1	2.54	0.43
1:B:645:GLU:HA	1:B:866:LYS:HE3	2.01	0.43
1:B:778:PHE:N	1:B:807:THR:OG1	2.51	0.43
1:B:884:TYR:O	1:B:904:TYR:HA	2.19	0.43
2:E:60:GLN:OE1	2:E:60:GLN:N	2.45	0.43
1:A:394:GLU:OE2	1:A:395:ILE:HG22	2.19	0.43
1:A:476:SER:N	1:A:489:TRP:HA	2.33	0.43
1:A:508:LYS:CG	1:A:529:TRP:CG	3.01	0.43
1:A:518:PHE:CD1	1:A:521:GLN:CG	3.02	0.43
1:A:529:TRP:N	1:A:529:TRP:HE3	2.14	0.43
1:A:887:ARG:HH21	1:A:899:TRP:HB2	1.83	0.43
1:B:793:PRO:O	1:B:794:ASP:HB2	2.19	0.43
2:E:11:LEU:O	2:E:15:LEU:HD23	2.18	0.43
1:A:489:TRP:CE2	1:A:551:PRO:HB2	2.54	0.43
1:A:846:LEU:HD22	1:A:862:CYS:SG	2.59	0.43
1:B:371:ARG:NE	1:B:372:ARG:HH21	2.17	0.43
1:B:887:ARG:NH1	1:B:902:PRO:HD3	2.34	0.43
1:A:469:GLU:OE1	1:A:469:GLU:N	2.48	0.43
1:B:7:VAL:HG13	1:B:251:TRP:CZ2	2.53	0.43
1:B:458:ALA:HB3	1:B:461:THR:OG1	2.18	0.43
1:B:488:ARG:HH11	1:B:550:HIS:HB2	1.84	0.43
1:B:634:TRP:CE2	1:B:760:PRO:HB2	2.53	0.43
1:A:767:LYS:HG2	1:A:769:SER:H	1.82	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:ILE:O	1:B:385:LEU:N	2.52	0.42
2:F:15:LEU:CD2	2:F:26:TYR:HA	2.48	0.42
1:A:429:HIS:H	1:A:431:ASN:HD21	1.67	0.42
1:A:609:SER:HB3	1:A:612:GLN:HB2	2.01	0.42
1:A:853:ARG:HG3	1:A:883:ASN:O	2.19	0.42
1:A:195:ILE:HG23	1:A:207:CYS:SG	2.59	0.42
1:A:314:ILE:CG2	1:A:315:LEU:O	2.56	0.42
1:A:840:PRO:HG2	1:A:843:LEU:HA	2.00	0.42
1:B:222:PRO:HA	1:B:225:CYS:SG	2.59	0.42
1:B:280:HIS:HB2	1:B:301:CYS:SG	2.59	0.42
1:B:658:ARG:HH22	1:B:842:GLY:HA3	1.84	0.42
1:B:777:HIS:O	1:B:779:THR:HG23	2.20	0.42
1:B:816:ILE:HD12	1:B:900:THR:HG23	2.02	0.42
1:A:91:TYR:CE2	1:A:118:ARG:HB2	2.54	0.42
1:A:529:TRP:O	1:A:530:THR:OG1	2.34	0.42
1:B:474:LYS:HB2	1:B:490:GLU:CD	2.40	0.42
1:B:816:ILE:CD1	1:B:888:VAL:HG12	2.49	0.42
1:A:440:HIS:HA	1:A:443:GLU:OE1	2.20	0.42
1:A:454:ARG:NE	1:A:455:ASN:H	2.10	0.42
1:B:70:GLU:HB3	1:B:102:LYS:HE2	2.02	0.42
1:B:476:SER:N	1:B:488:ARG:O	2.52	0.42
1:B:492:TYR:CG	1:B:493:TRP:N	2.87	0.42
1:B:595:THR:OG1	1:B:596:ASN:N	2.52	0.42
1:B:789:ASN:ND2	1:B:796:ARG:HH12	2.17	0.42
1:B:823:GLU:HB2	1:B:831:HIS:HB3	2.02	0.42
2:E:57:ILE:HA	2:E:60:GLN:NE2	2.34	0.42
1:A:476:SER:H	1:A:489:TRP:HA	1.84	0.42
1:A:566:ILE:HD13	1:A:590:VAL:HG12	2.02	0.42
1:A:598:SER:HB3	1:A:622:ASP:H	1.85	0.42
1:B:120:GLU:HA	1:B:146:VAL:O	2.19	0.42
1:B:355:GLU:OE1	1:B:381:PHE:HA	2.20	0.42
1:B:558:LEU:HG	1:B:564:TYR:CZ	2.54	0.42
1:B:778:PHE:HA	1:B:807:THR:O	2.19	0.42
1:B:844:ILE:HG21	1:B:890:ALA:HB1	2.02	0.42
1:A:132:ASP:O	1:A:189:GLN:NE2	2.51	0.42
1:A:291:GLY:O	1:A:304:CYS:N	2.41	0.42
1:B:562:THR:HB	1:B:564:TYR:HE1	1.85	0.42
1:A:488:ARG:NH1	1:A:550:HIS:HB2	2.35	0.42
1:B:473:LEU:HB2	1:B:585:SER:HB3	2.02	0.42
1:A:63:LEU:HB2	1:A:95:ILE:HG12	2.02	0.42
1:B:399:SER:HB3	1:B:423:GLN:O	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:60:GLN:HA	2:G:64:SER:HB3	2.00	0.42
1:B:102:LYS:O	1:B:126:CYS:N	2.47	0.42
1:B:248:PHE:HB2	1:B:254:VAL:HG22	2.02	0.42
1:B:333:CYS:O	1:B:360:LEU:HB2	2.20	0.42
1:B:389:ARG:HA	1:B:422:THR:HB	2.01	0.42
1:B:398:TYR:CE2	1:B:427:PHE:HB2	2.55	0.42
1:B:70:GLU:HA	1:B:101:LEU:HA	2.01	0.41
1:B:271:LYS:N	1:B:274:CYS:SG	2.85	0.41
1:A:245:TYR:HB3	1:A:253:CYS:HB3	2.02	0.41
1:A:617:TRP:O	1:A:768:GLU:HB3	2.20	0.41
1:B:489:TRP:CZ3	1:B:552:GLY:HA2	2.55	0.41
1:A:193:PRO:HB2	1:A:195:ILE:HG22	2.01	0.41
1:A:202:THR:HG22	1:A:206:LEU:HB2	2.02	0.41
1:A:614:ILE:HG13	1:A:614:ILE:O	2.20	0.41
1:B:208:CYS:HB3	1:B:212:CYS:HB2	2.02	0.41
1:B:218:GLU:CD	1:B:224:LYS:NZ	2.74	0.41
1:A:91:TYR:CD2	1:A:118:ARG:HB2	2.55	0.41
1:A:443:GLU:O	1:A:446:SER:OG	2.23	0.41
1:A:508:LYS:HB2	1:A:529:TRP:HB3	2.02	0.41
1:A:784:GLU:HG3	1:A:800:ALA:HB1	2.03	0.41
1:B:87:LEU:HD22	1:B:92:ALA:HB2	2.02	0.41
1:B:365:SER:HB2	1:B:391:GLU:OE1	2.20	0.41
1:B:376:LEU:HD11	1:B:381:PHE:HZ	1.84	0.41
1:B:633:TYR:CD1	1:B:761:PHE:HB3	2.55	0.41
1:B:852:ARG:NH2	1:B:858:GLU:HB2	2.35	0.41
2:G:27:THR:HG22	2:G:29:LYS:HZ1	1.85	0.41
1:B:314:ILE:HG21	1:B:318:GLU:CA	2.50	0.41
1:B:489:TRP:O	1:B:550:HIS:ND1	2.50	0.41
1:B:808:MET:SD	1:B:808:MET:N	2.85	0.41
1:B:831:HIS:CE1	1:B:833:MET:CE	3.03	0.41
1:A:231:PHE:HA	1:A:251:TRP:O	2.21	0.41
1:A:258:PHE:O	1:A:262:LEU:HG	2.21	0.41
1:A:648:TYR:HB3	1:A:653:LEU:HD13	2.03	0.41
1:A:709:ASP:HB3	2:D:58:VAL:HG21	2.03	0.41
1:A:825:PHE:HD1	1:A:829:VAL:O	2.04	0.41
1:A:831:HIS:HB2	1:A:875:ARG:CZ	2.51	0.41
1:B:354:LEU:O	1:B:358:LEU:HB2	2.14	0.41
1:B:469:GLU:HG3	1:B:584:LYS:HG3	2.03	0.41
1:B:884:TYR:HB2	1:B:905:PHE:CE1	2.55	0.41
2:E:56:GLY:O	2:E:74:TYR:OH	2.39	0.41
1:A:615:LEU:H	1:A:615:LEU:HD23	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:636:ARG:HH22	1:A:776:ARG:HB2	1.86	0.41
1:B:83:ARG:HA	1:B:113:THR:HB	2.02	0.41
2:F:28:PRO:O	2:F:29:LYS:C	2.59	0.41
1:A:379:LEU:HA	1:A:381:PHE:CE1	2.55	0.41
1:A:496:ASP:OD1	1:A:498:ARG:NH2	2.52	0.41
1:A:822:HIS:HB2	1:A:830:VAL:HG13	2.03	0.41
1:A:854:TYR:HE2	1:A:883:ASN:HB3	1.86	0.41
1:B:405:ASN:HB3	1:B:408:LEU:HD23	2.02	0.41
1:B:507:TYR:CD2	1:B:555:MET:HE1	2.56	0.41
1:B:765:VAL:H	1:B:767:LYS:HZ1	1.68	0.41
1:B:851:TYR:HB3	1:B:886:VAL:HG22	2.01	0.41
2:F:59:GLU:O	2:F:63:THR:HB	2.20	0.41
1:A:23:LEU:HD22	1:A:51:PHE:CD1	2.56	0.41
1:A:70:GLU:HG2	1:A:100:HIS:O	2.20	0.41
1:A:73:LYS:HG3	1:A:74:ASP:OD1	2.21	0.41
1:A:88:PHE:O	1:A:91:TYR:HB2	2.20	0.41
1:A:102:LYS:HA	1:A:124:GLU:O	2.21	0.41
1:A:197:LYS:HE2	1:A:197:LYS:HB2	1.90	0.41
1:A:365:SER:HA	1:A:389:ARG:HB2	2.03	0.41
1:A:561:TRP:N	1:A:592:THR:HG23	2.36	0.41
1:B:55:ILE:HG12	1:B:78:ASN:O	2.20	0.41
1:B:340:LEU:O	1:B:368:LEU:HD12	2.20	0.41
1:B:489:TRP:CE2	1:B:551:PRO:HG2	2.55	0.41
1:B:568:VAL:HG12	1:B:585:SER:HB3	2.02	0.41
1:A:260:GLN:HG3	1:A:264:PHE:CZ	2.53	0.41
1:A:314:ILE:HG21	1:A:318:GLU:N	2.36	0.41
1:A:345:ARG:NH1	1:B:699:GLU:OE1	2.54	0.41
1:B:342:ILE:O	1:B:373:SER:OG	2.39	0.41
1:B:692:SER:HA	1:B:695:LEU:HD12	2.03	0.41
2:F:18:VAL:HG12	2:F:19:CYS:SG	2.61	0.41
1:A:342:ILE:O	1:A:342:ILE:HG13	2.21	0.40
1:A:762:GLU:O	1:A:763:LYS:HD2	2.21	0.40
1:B:448:THR:HA	1:B:451:ARG:NE	2.36	0.40
1:B:513:GLN:HG2	1:B:589:TYR:CD2	2.55	0.40
1:B:704:ARG:HB2	1:B:704:ARG:CZ	2.51	0.40
1:A:135:ARG:HB2	1:A:136:ILE:HD12	2.02	0.40
1:B:65:ARG:HD2	2:D:12:VAL:HG11	2.03	0.40
1:B:266:CYS:O	1:B:267:ARG:C	2.59	0.40
1:B:342:ILE:HD13	1:B:370:ILE:CD1	2.51	0.40
1:B:362:GLU:O	1:B:385:LEU:HD12	2.20	0.40
1:B:410:GLN:OE1	1:B:413:ASP:N	2.54	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:615:LEU:C	1:B:616:LYS:HD2	2.42	0.40
1:A:88:PHE:CE1	1:B:710:TYR:CE2	3.08	0.40
1:A:314:ILE:CD1	1:A:336:ILE:HD11	2.51	0.40
1:A:528:SER:C	1:A:529:TRP:CE3	2.93	0.40
1:B:53:LYS:HA	1:B:226:VAL:HG13	2.02	0.40
1:B:321:ILE:HD11	1:B:340:LEU:HD13	2.02	0.40
1:B:355:GLU:CD	1:B:383:ARG:HE	2.22	0.40
1:B:658:ARG:HH22	1:B:841:ASN:C	2.21	0.40
1:A:12:ASP:OD1	1:A:34:GLN:HB2	2.22	0.40
1:A:90:ASN:O	1:A:91:TYR:HD1	2.04	0.40
1:A:362:GLU:HA	1:A:385:LEU:HA	2.03	0.40
1:A:496:ASP:OD1	1:A:498:ARG:NE	2.51	0.40
1:A:597:PRO:HB3	1:A:623:PRO:O	2.21	0.40
1:B:32:HIS:HD2	1:B:86:ARG:NH2	2.13	0.40
1:B:489:TRP:NE1	1:B:551:PRO:HG2	2.36	0.40
1:B:607:SER:HB3	1:B:613:ILE:HD12	2.03	0.40
1:B:790:GLN:HG2	1:B:793:PRO:HD2	2.03	0.40
1:B:848:GLU:O	1:B:888:VAL:HA	2.21	0.40
1:A:160:PRO:HD2	1:A:182:CYS:SG	2.61	0.40
1:A:269:SER:OG	1:A:271:LYS:HE2	2.21	0.40
1:B:469:GLU:CB	1:B:584:LYS:HG3	2.52	0.40
1:B:568:VAL:N	1:B:585:SER:OG	2.35	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	805/1345 (60%)	712 (88%)	87 (11%)	6 (1%)	22 62
1	B	760/1345 (56%)	691 (91%)	68 (9%)	1 (0%)	51 85
2	D	40/110 (36%)	37 (92%)	3 (8%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	E	44/110 (40%)	40 (91%)	4 (9%)	0	100 100
2	F	43/110 (39%)	38 (88%)	3 (7%)	2 (5%)	2 24
2	G	43/110 (39%)	38 (88%)	4 (9%)	1 (2%)	6 37
All	All	1735/3130 (55%)	1556 (90%)	169 (10%)	10 (1%)	29 65

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	271	LYS
1	A	272	PRO
2	F	28	PRO
1	A	529	TRP
1	B	794	ASP
2	F	26	TYR
1	A	166	LYS
2	G	26	TYR
1	A	581	TYR
1	A	161	GLY

5.3.2 Protein sidechains [\(i\)](#)

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	739/1211 (61%)	729 (99%)	10 (1%)	67 81
1	B	704/1211 (58%)	697 (99%)	7 (1%)	76 86
2	D	39/88 (44%)	39 (100%)	0	100 100
2	E	43/88 (49%)	43 (100%)	0	100 100
2	F	42/88 (48%)	39 (93%)	3 (7%)	14 41
2	G	42/88 (48%)	42 (100%)	0	100 100
All	All	1609/2774 (58%)	1589 (99%)	20 (1%)	72 84

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	159	CYS
1	A	269	SER
1	A	270	ARG
1	A	282	ASN
1	A	467	SER
1	A	468	CYS
1	A	518	PHE
1	A	529	TRP
1	A	556	ARG
1	A	866	LYS
1	B	265	LYS
1	B	266	CYS
1	B	274	CYS
1	B	343	ASN
1	B	700	GLU
1	B	704	ARG
1	B	705	LYS
2	F	24	PHE
2	F	25	PHE
2	F	29	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	A	276	GLN
1	A	410	GLN
1	A	591	GLN
1	B	32	HIS
1	B	276	GLN

5.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [\(i\)](#)

There are no monosaccharides 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.

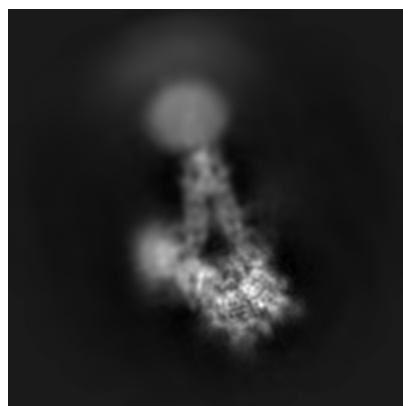
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-28723. These allow visual inspection of the internal detail of the map and identification of artifacts.

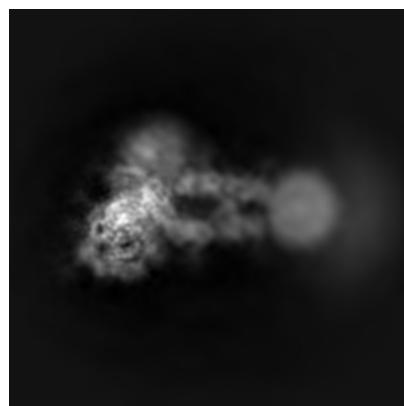
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

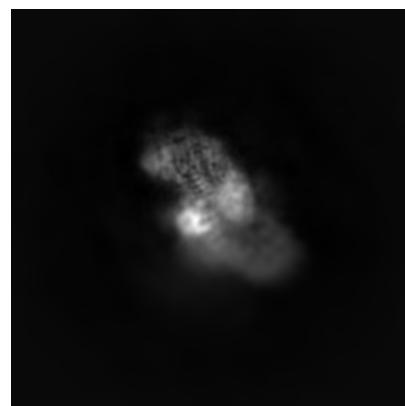
6.1.1 Primary map



X

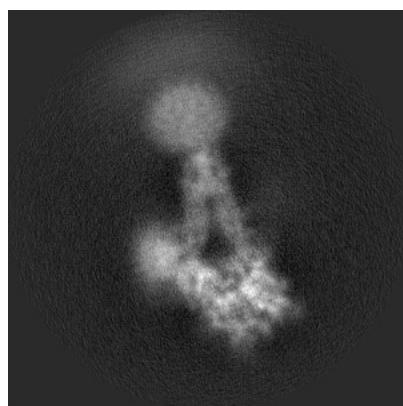


Y

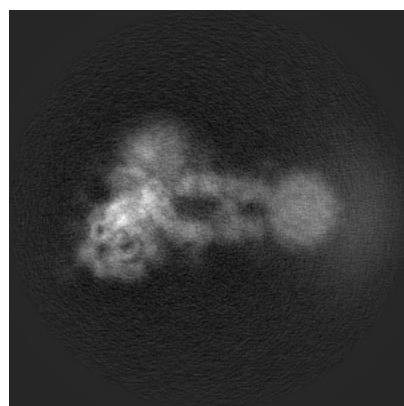


Z

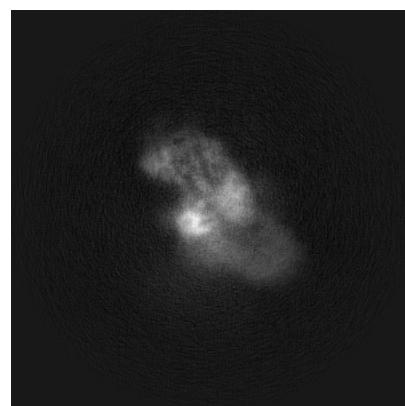
6.1.2 Raw map



X



Y

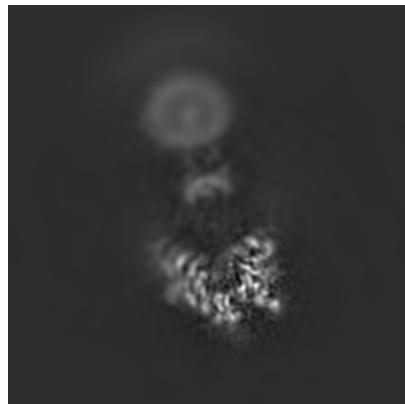


Z

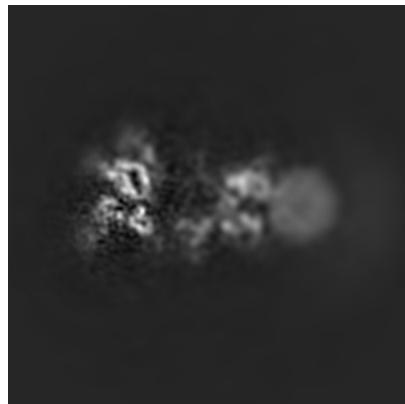
The images above show the map projected in three orthogonal directions.

6.2 Central slices [\(i\)](#)

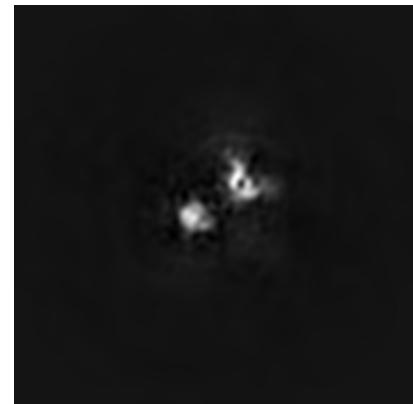
6.2.1 Primary map



X Index: 150

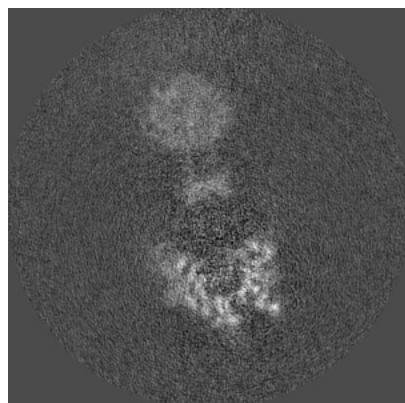


Y Index: 150

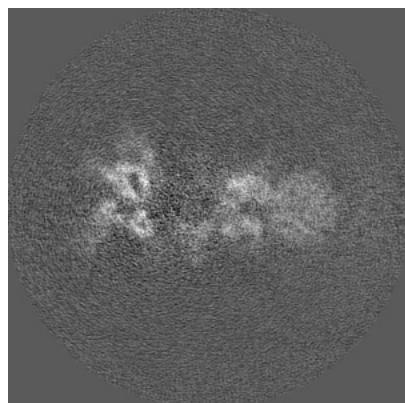


Z Index: 150

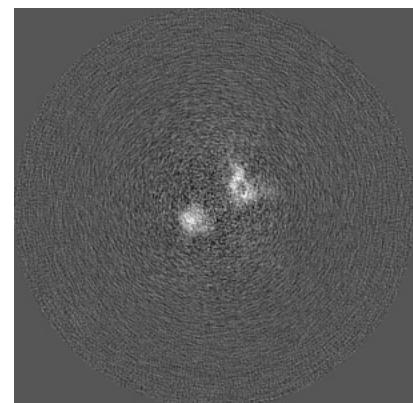
6.2.2 Raw map



X Index: 150



Y Index: 150

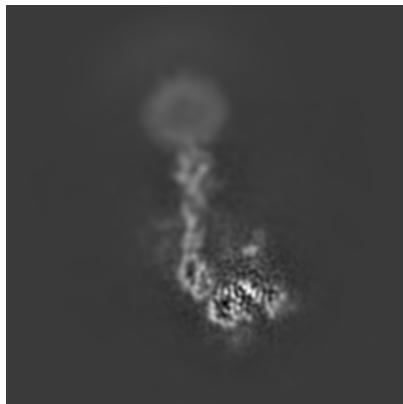


Z Index: 150

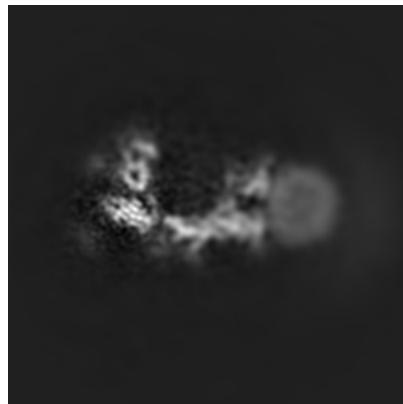
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [\(i\)](#)

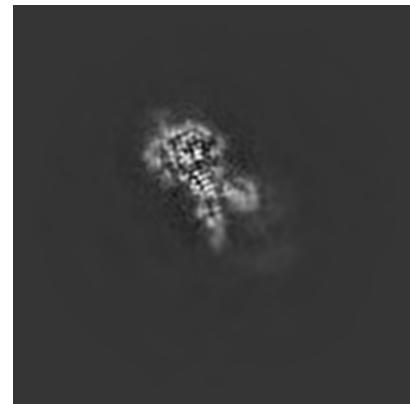
6.3.1 Primary map



X Index: 140

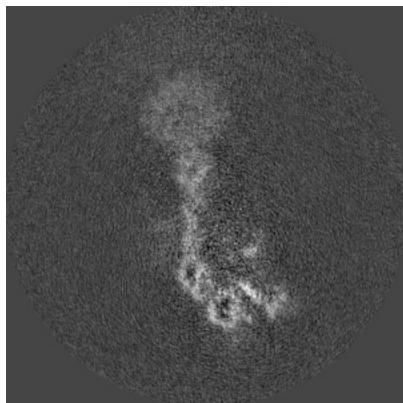


Y Index: 144

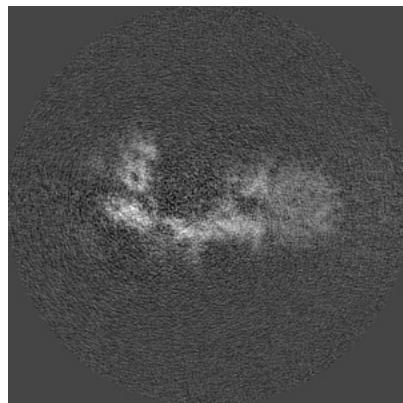


Z Index: 81

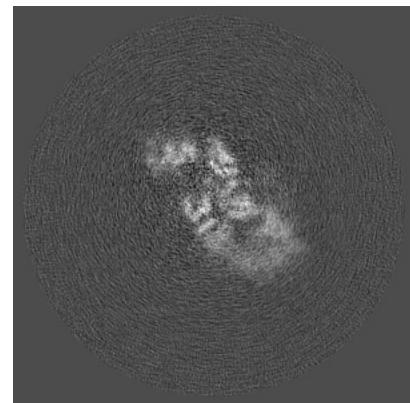
6.3.2 Raw map



X Index: 140



Y Index: 144

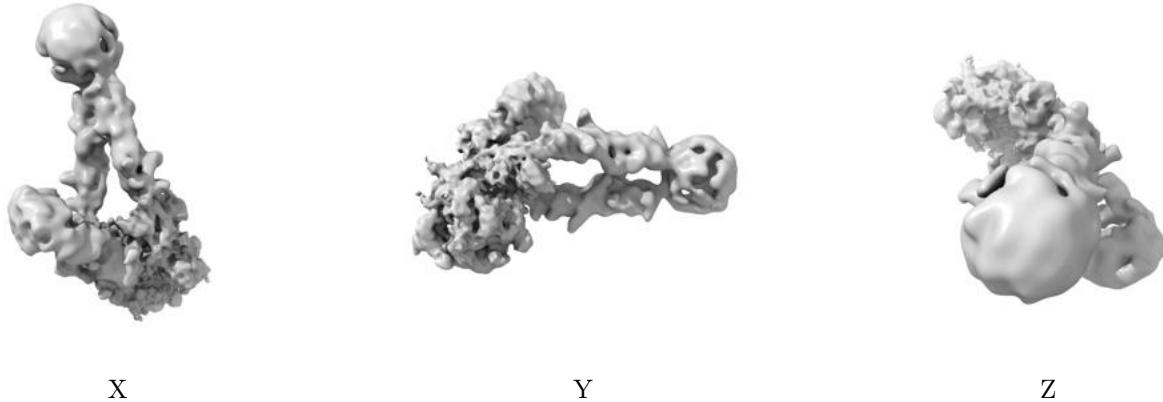


Z Index: 101

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

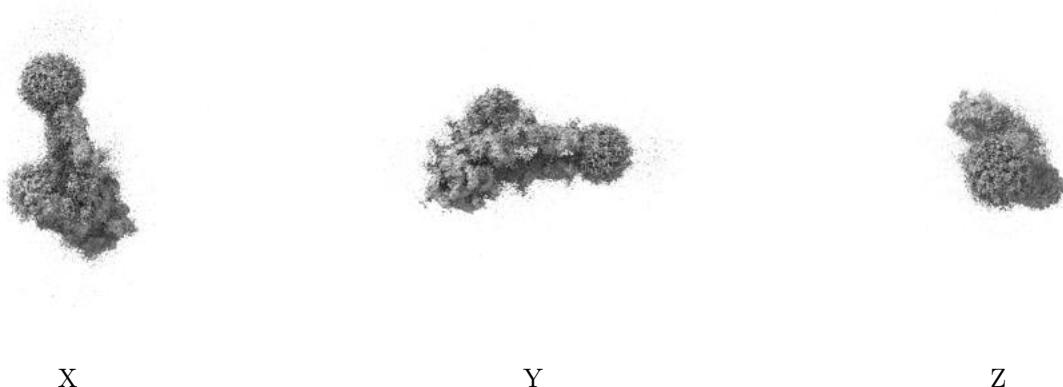
6.4 Orthogonal surface views [\(i\)](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.018. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

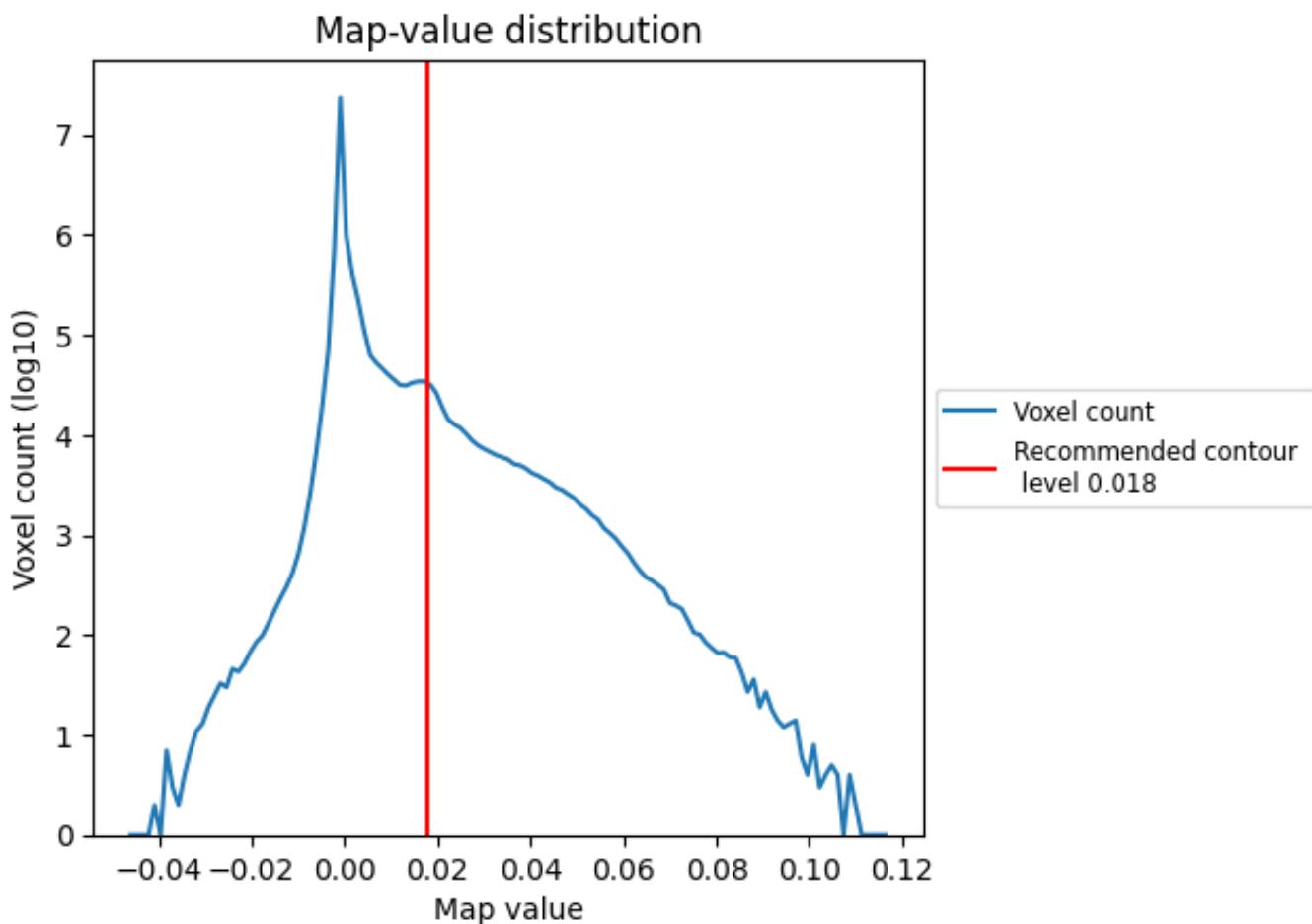
6.5 Mask visualisation [\(i\)](#)

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

7 Map analysis (i)

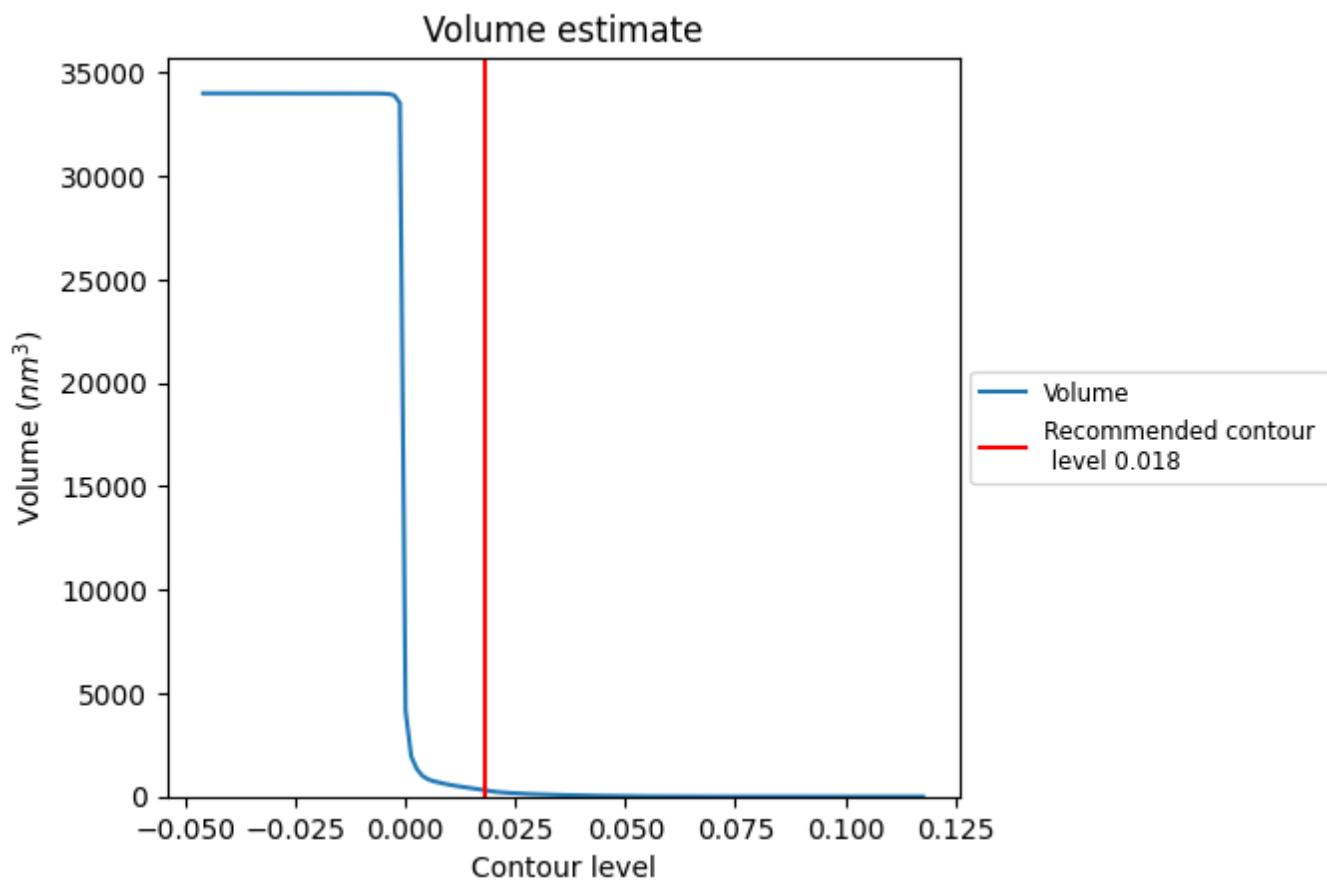
This section contains the results of statistical analysis of the map.

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.

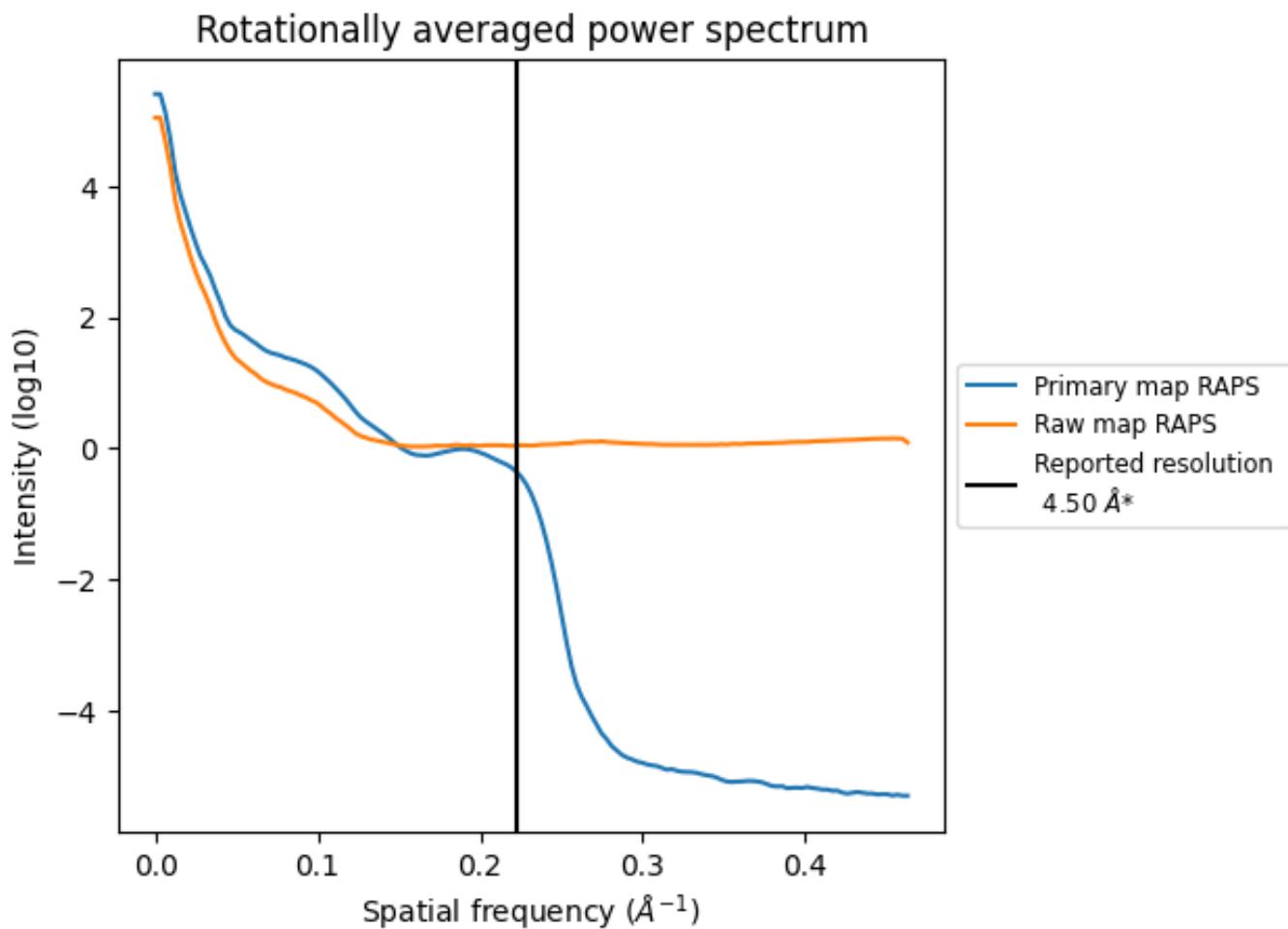
7.2 Volume estimate (i)



The volume at the recommended contour level is 306 nm^3 ; this corresponds to an approximate mass of 276 kDa.

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

7.3 Rotationally averaged power spectrum [\(i\)](#)

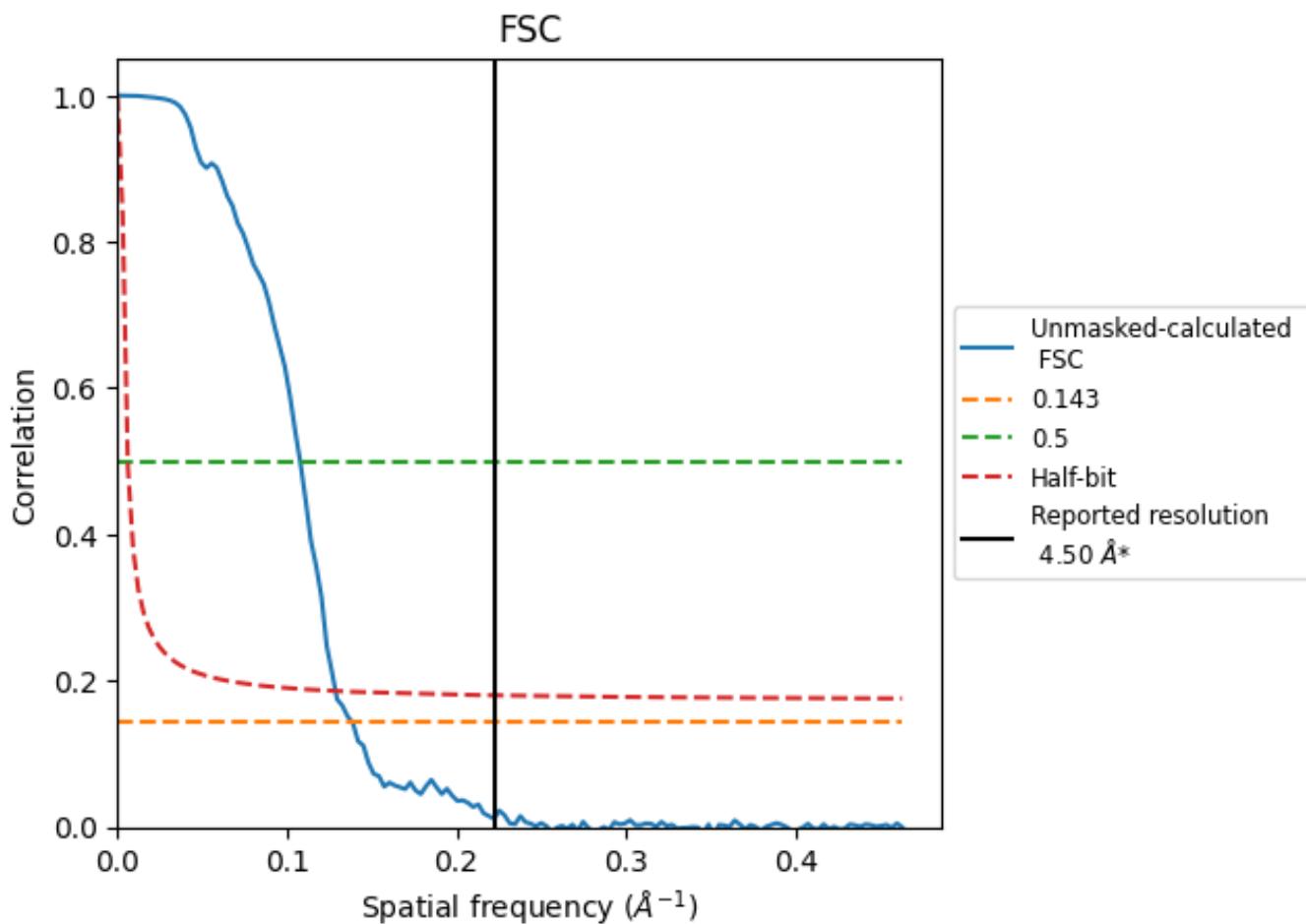


*Reported resolution corresponds to spatial frequency of 0.222 \AA^{-1}

8 Fourier-Shell correlation [\(i\)](#)

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

8.1 FSC [\(i\)](#)



*Reported resolution corresponds to spatial frequency of 0.222 \AA^{-1}

8.2 Resolution estimates [\(i\)](#)

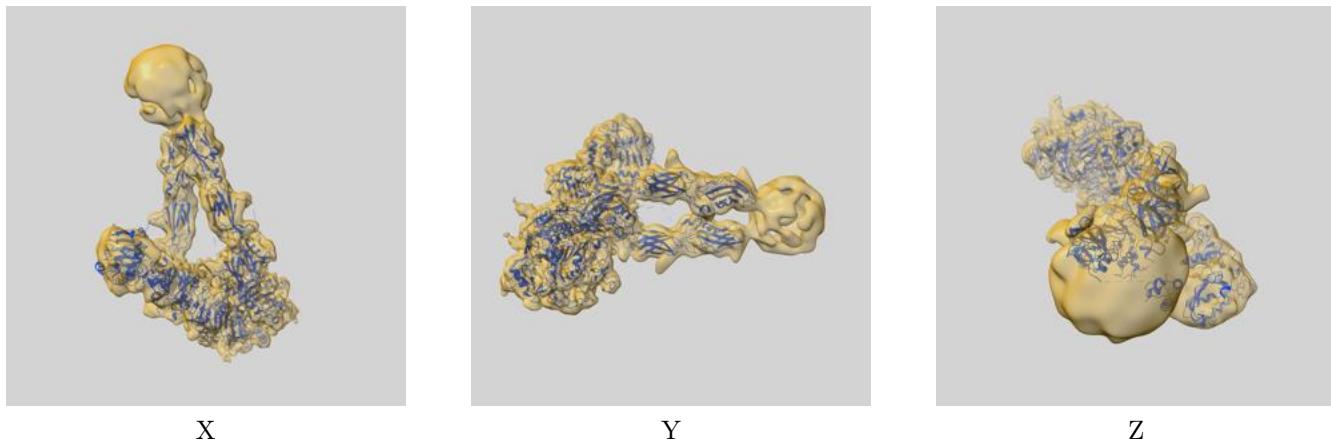
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.22	9.28	7.77

*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 7.22 differs from the reported value 4.5 by more than 10 %

9 Map-model fit i

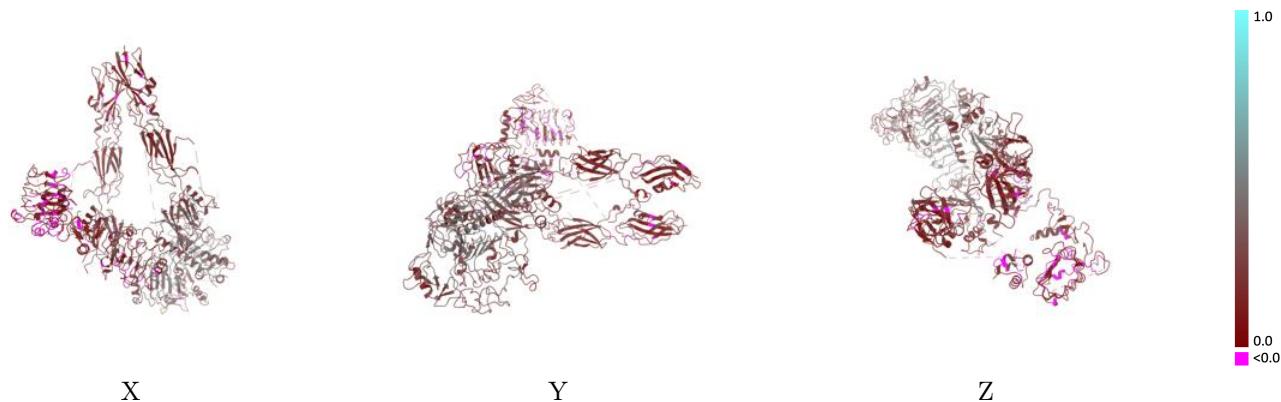
This section contains information regarding the fit between EMDB map EMD-28723 and PDB model 8EYX. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay i



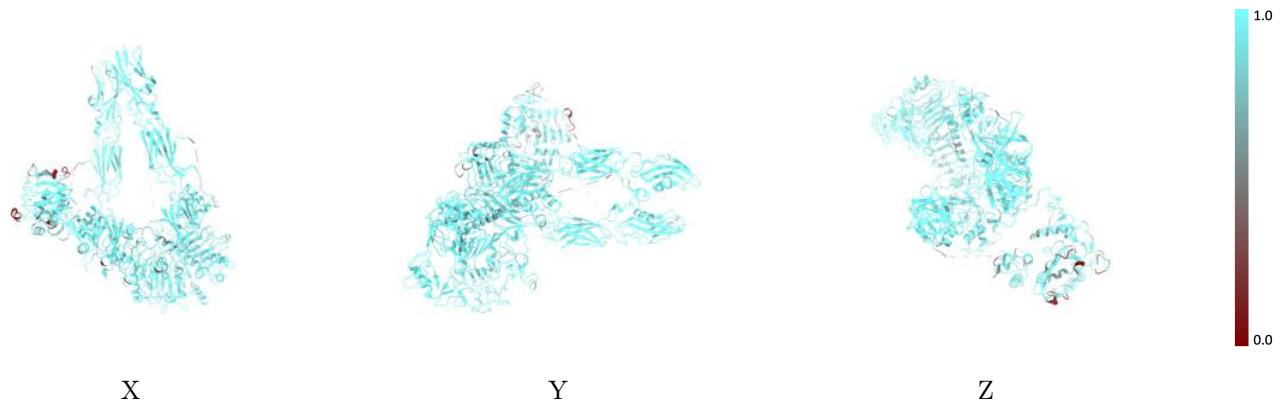
The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



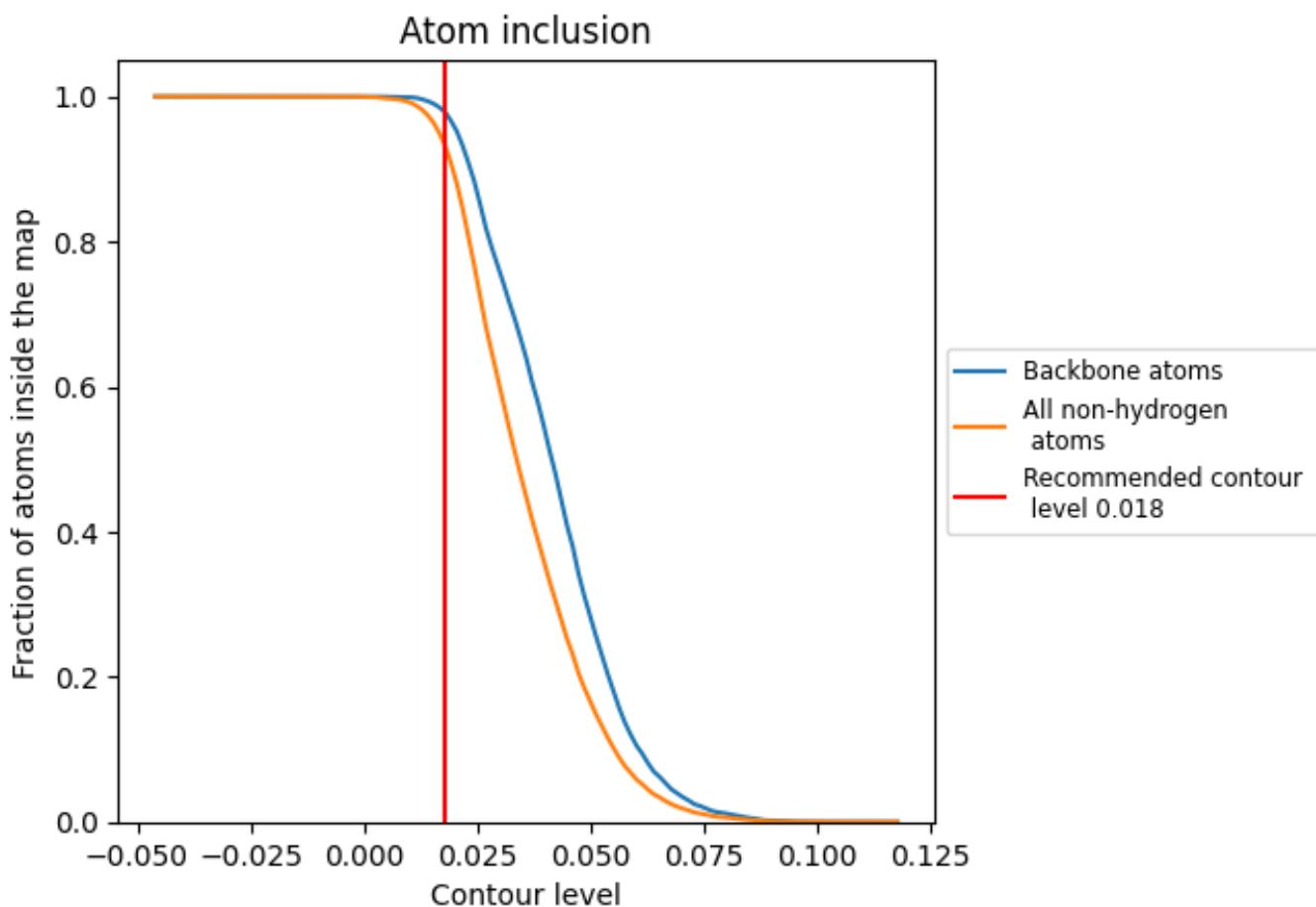
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.018).

9.4 Atom inclusion [\(i\)](#)



At the recommended contour level, 98% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9309	0.2370
A	0.9547	0.2840
B	0.9032	0.1910
D	0.8886	0.0890
E	0.9784	0.3360
F	0.9505	0.1920
G	0.9478	0.2620

