



Full wwPDB EM Validation Report ⓘ

Mar 14, 2026 – 09:24 AM UTC

PDB ID : 8EYX / pdb_00008eyx
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 ⓘ 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:

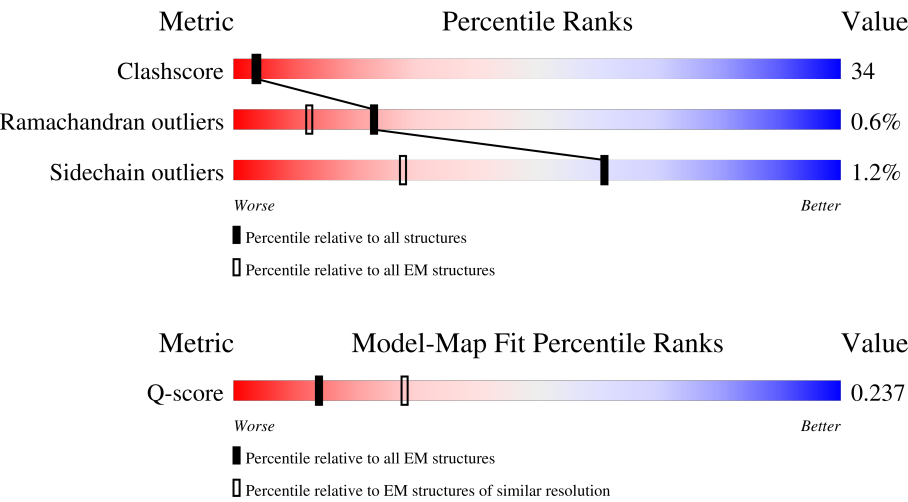
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2937 (4.00 - 5.00)

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

Mol	Chain	Length	Quality of chain
1	A	1345	29%31%39%
1	B	1345	26%31%43%
2	D	110	31%9%60%
2	E	110	28%15%56%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	110	14%25%57%
2	G	110	15%27%57%

2 Entry composition

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.

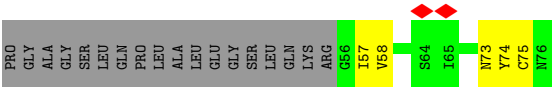
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	815	Total	C	N	O	S	0	0
			6572	4171	1135	1217	49		
1	B	772	Total	C	N	O	S	0	0
			6263	3983	1075	1165	40		

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.

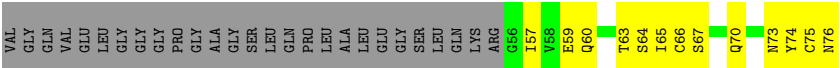
Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	44	Total	C	N	O	S	0	0
			347	220	56	65	6		
2	E	48	Total	C	N	O	S	0	0
			376	238	61	71	6		
2	F	47	Total	C	N	O	S	0	0
			370	235	60	69	6		
2	G	47	Total	C	N	O	S	0	0
			370	235	60	69	6		



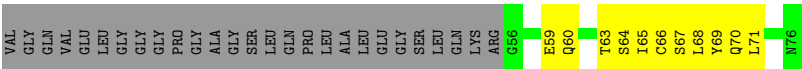
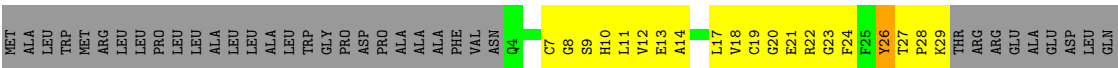
• Molecule 2: Insulin



• Molecule 2: Insulin



• Molecule 2: Insulin



4 Experimental information

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	0.31	1/6736 (0.0%)	0.45	1/9133 (0.0%)
1	B	0.24	0/6415	0.43	1/8693 (0.0%)
2	D	0.08	0/353	0.20	0/475
2	E	0.29	0/383	0.41	0/518
2	F	0.18	0/377	0.42	1/508 (0.2%)
2	G	0.24	0/377	0.49	0/508
All	All	0.28	1/14641 (0.0%)	0.43	3/19835 (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	8.60	1.76	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	548	PRO	CA-N-CD	-8.87	99.58	112.00
1	A	466	ALA	N-CA-C	6.57	119.30	108.99
2	F	25	PHE	N-CA-C	-5.13	106.28	112.54

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	441	0
1	B	6263	0	6099	453	0
2	D	347	0	317	10	0
2	E	376	0	346	13	0
2	F	370	0	344	37	0
2	G	370	0	344	27	0
All	All	14298	0	13837	953	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 34.

All (953) 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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:314:ILE:HG21	1:B:318:GLU:C	1.94	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:294:MET:HE3	1:B:295:ASN:H	1.36	0.89
1:B:267:ARG:HG2	1:B:276:GLN:HE22	0.77	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:56:MET:HE1	1:B:83:ARG:H	1.50	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:517:GLU:CD	1:B:567:PHE:CZ	2.68	0.70
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:293:THR:OG1	1:A:304:CYS:SG	2.53	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:507:TYR:CD2	1:B:555:MET:HE1	2.30	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:PRO:HD3	1:A:185:HIS:HA	1.78	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:314:ILE:CG2	1:B:318:GLU:C	2.68	0.64
1:B:507:TYR:CG	1:B:555:MET:HE1	2.32	0.64
1:A:190:LYS:NZ	1:A:201:CYS:SG	2.70	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:260:GLN:C	1:A:264:PHE:CD2	2.75	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: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:260:GLN:C	1:A:264:PHE:HD2	2.06	0.62
1:A:471:GLU:HB2	1:A:583:ALA:HA	1.82	0.62
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:614:ILE:HB	1:B:616:LYS:HZ2	1.64	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
1:B:362:GLU:HG2	1:B:384:LYS:HB3	1.83	0.59
1:B:439:ILE:HA	1:B:442:MET:HE2	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:513:GLN:O	1:A:589:TYR:OH	2.19	0.58
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:161:GLY:O	1:A:162:THR:C	2.46	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:314:ILE:HG22	1:A:315:LEU:C	2.29	0.57
1:A:520:GLY:C	1:A:521:GLN:HG3	2.29	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:615:LEU:C	1:A:616:LYS:HD2	2.29	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:506:PHE:CB	1:B:529:TRP:CE2	2.77	0.57
1:A:483:ASP:C	1:A:484:LYS:HD3	2.30	0.56
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:B:218:GLU:OE1	1:B:224:LYS:NZ	2.33	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: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:314:ILE:HG22	1:A:315:LEU:N	2.21	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:A:270:ARG:O	1:A:271:LYS:C	2.48	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:160:PRO:O	1:A:161:GLY:C	2.49	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:159:CYS:O	1:A:160:PRO:C	2.49	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:A:504:MET:HE1	1:A:571:LEU:HB2	1.90	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:528:SER:C	1:A:529:TRP:HE3	2.16	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:587:ILE:HG22	1:B:589:TYR:HE1	1.75	0.52
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:B:765:VAL:H	1:B:767:LYS:HZ1	1.56	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:602:ASP:O	1:B:617:TRP:HA	2.11	0.51
2:G:27:THR:HG22	2:G:29:LYS:HZ1	1.75	0.51
1:A:164:LYS:O	1:A:165:GLY:C	2.52	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: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: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:F:24:PHE:HA	2:F:76:ASN:N	2.24	0.50
1:A:66:VAL:H	1:A:98:MET:HE1	1.75	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: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:E:64:SER:OG	2:E:65:ILE:N	2.43	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
1:B:831:HIS:CE1	1:B:833:MET:HE3	2.47	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:697:GLU:HA	1:B:700:GLU:CD	2.38	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:A:167:THR:O	1:A:168:ASN:C	2.55	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:791:ASP:N	1:A:791:ASP:OD1	2.44	0.49
1:A:102:LYS:C	1:A:125:LEU:HD12	2.37	0.49
1:A:629:HIS:CE1	1:A:791:ASP:HB3	2.48	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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:288:CYS:O	1:A:310:LYS:NZ	2.45	0.48
1:A:494:PRO:HG2	1:A:496:ASP:O	2.14	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:A:637:GLN:HB2	1:A:780:GLY:C	2.39	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:474:LYS:HB2	1:B:490:GLU:CD	2.40	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:262:LEU:HA	1:A:265:LYS:HZ2	1.80	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:B:765:VAL:O	1:B:767:LYS:NZ	2.42	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:218:GLU:CD	1:B:224:LYS:NZ	2.74	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: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: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:F:28:PRO:O	2:F:29:LYS:C	2.59	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:528:SER:C	1:A:529:TRP:CE3	2.93	0.45
1:A:642:GLU:HA	1:A:645:GLU:OE2	2.16	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:B:266:CYS:O	1:B:267:ARG:C	2.59	0.45
1:B:615:LEU:C	1:B:616:LYS:HD2	2.42	0.45
1:A:509:GLU:OE1	1:A:511:PRO:HD3	2.17	0.45
1:B:355:GLU:CD	1:B:383:ARG:HE	2.22	0.45
1:B:658:ARG:HH22	1:B:841:ASN:C	2.21	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:118:ARG:HH12	1:B:703:PHE:HZ	1.61	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
1:A:163:ALA:O	1:A:164:LYS:C	2.59	0.44
1:B:307:PRO:O	1:B:309:PRO:HD3	2.18	0.44
1:B:521:GLN:CD	1:B:527:ASN:N	2.75	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:267:ARG:O	1:B:268:ASN:C	2.60	0.44
1:B:312:CYS:HB3	1:B:330:LEU:HD12	2.00	0.44
1:B:832:LEU:O	1:B:833:MET:HE2	2.18	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:LEU:C	1:A:440:HIS:HD1	2.26	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:467:SER:C	1:B:469:GLU:H	2.24	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:793:PRO:O	1:A:794:ASP:HB2	2.19	0.43
1:B:120:GLU:CD	1:B:144:TYR:HE2	2.27	0.43
1:B:614:ILE:HB	1:B:616:LYS:NZ	2.33	0.43
1:B:617:TRP:C	1:B:618:LYS:HD2	2.43	0.43
1:B:844:ILE:HD13	1:B:890:ALA:HB1	2.00	0.43
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:509:GLU:CD	1:B:511:PRO:HD3	2.42	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:PHE:CD1	1:A:521:GLN:CG	3.02	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
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:298:ASN:CG	1:B:300:MET:HG2	2.43	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: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:619:PRO:HD3	1:B:768:GLU:CD	2.44	0.42
1:B:628:THR:HG1	1:B:629:HIS:CE1	2.37	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:G:9:SER:O	2:G:10:HIS:C	2.62	0.42
1:A:63:LEU:HB2	1:A:95:ILE:HG12	2.02	0.42
1:A:426:LEU:H	1:A:452:GLN:CD	2.27	0.42
1:B:399:SER:HB3	1:B:423:GLN:O	2.20	0.42
2:G:60:GLN:HA	2:G:64:SER:HB3	2.00	0.42
1:A:315:LEU:C	1:A:317:GLY:H	2.28	0.42
1:A:518:PHE:CD1	1:A:521:GLN:CD	2.94	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:B:553:TRP:CG	1:B:554:LEU:H	2.38	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:562:THR:C	1:A:591:GLN:HG2	2.46	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
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
1:B:713:ASN:O	1:B:714:VAL:C	2.61	0.41
2:D:6:LEU:C	2:D:11:LEU:HB2	2.46	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:469:GLU:HB3	1:B:583:ALA:C	2.45	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: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
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: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: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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	805/1345 (60%)	712 (88%)	87 (11%)	6 (1%)	18	55
1	B	760/1345 (56%)	691 (91%)	68 (9%)	1 (0%)	48	83
2	D	40/110 (36%)	37 (92%)	3 (8%)	0	100	100
2	E	44/110 (40%)	40 (91%)	4 (9%)	0	100	100
2	F	43/110 (39%)	38 (88%)	3 (7%)	2 (5%)	2	17
2	G	43/110 (39%)	38 (88%)	4 (9%)	1 (2%)	5	28
All	All	1735/3130 (55%)	1556 (90%)	169 (10%)	10 (1%)	23	58

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

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%)	731 (99%)	8 (1%)	65	74
1	B	704/1211 (58%)	696 (99%)	8 (1%)	65	74
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%)	13	35
2	G	42/88 (48%)	42 (100%)	0	100	100
All	All	1609/2774 (58%)	1590 (99%)	19 (1%)	61	73

All (19) 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	B	263	HIS
1	B	265	LYS
1	B	266	CYS
1	B	274	CYS
1	B	700	GLU
1	B	704	ARG
1	B	705	LYS
1	B	706	THR
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 (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	A	276	GLN
1	A	282	ASN
1	A	405	ASN
1	A	410	GLN
1	A	431	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	513	GLN
1	A	591	GLN
1	A	786	GLN
1	A	896	ASN
1	B	32	HIS
1	B	386	HIS
2	G	73	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

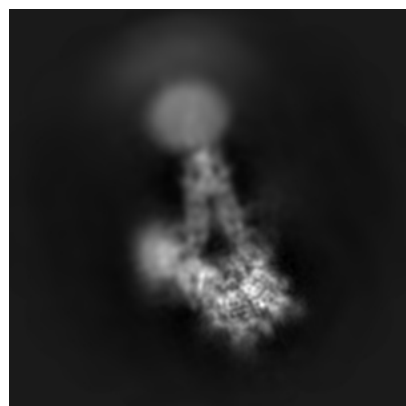
6 Map visualisation [i](#)

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.

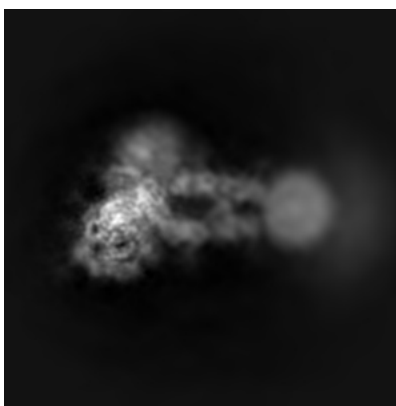
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

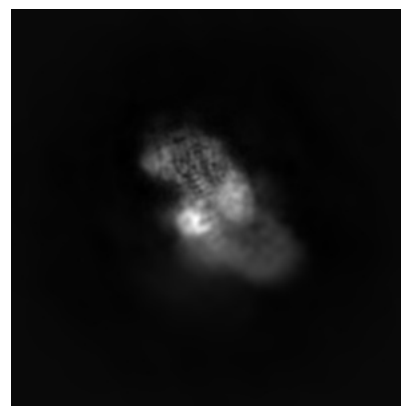
6.1.1 Primary map



X

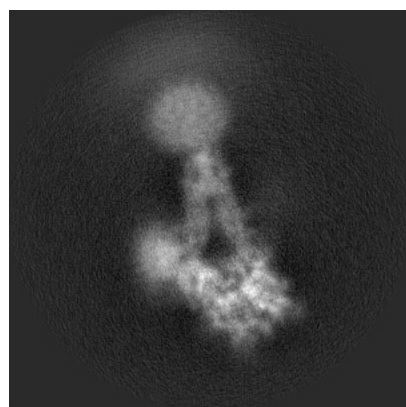


Y

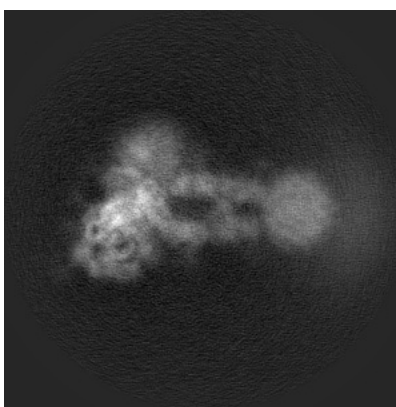


Z

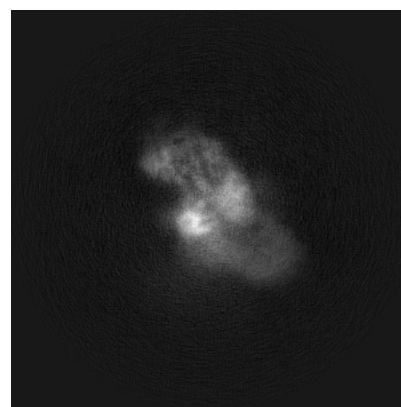
6.1.2 Raw map



X



Y

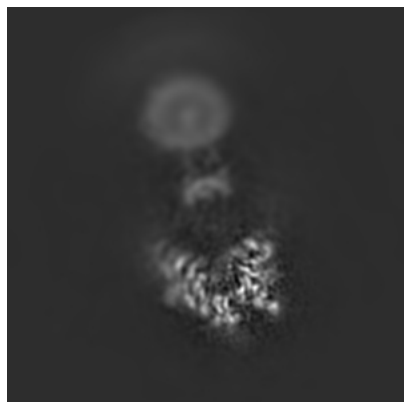


Z

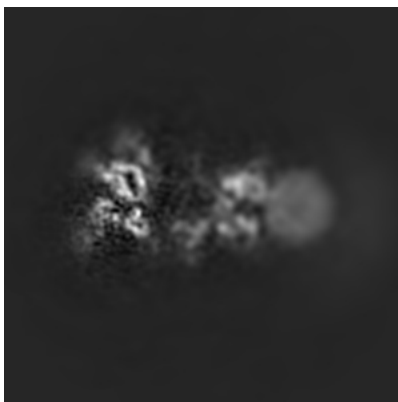
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

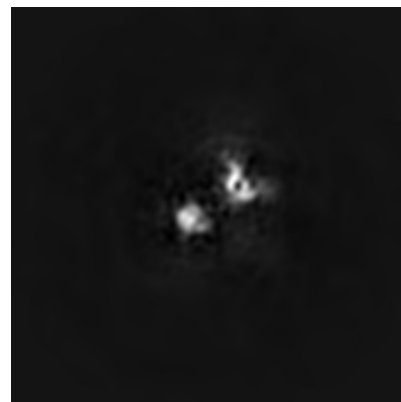
6.2.1 Primary map



X Index: 150

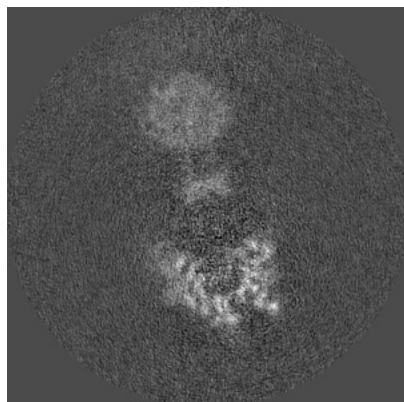


Y Index: 150

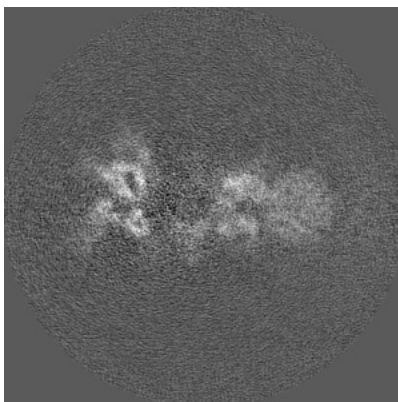


Z Index: 150

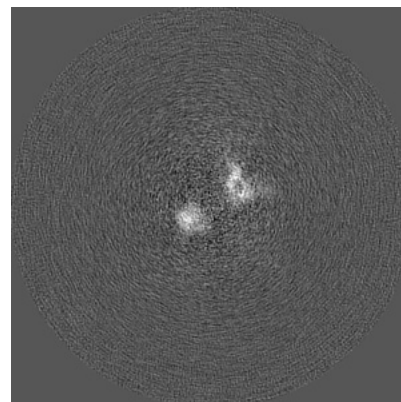
6.2.2 Raw map



X Index: 150



Y Index: 150

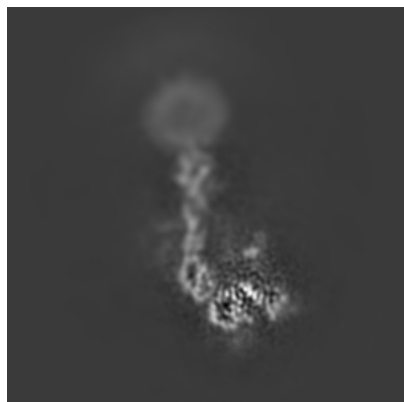


Z Index: 150

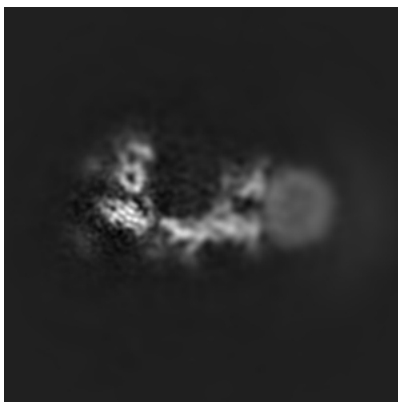
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

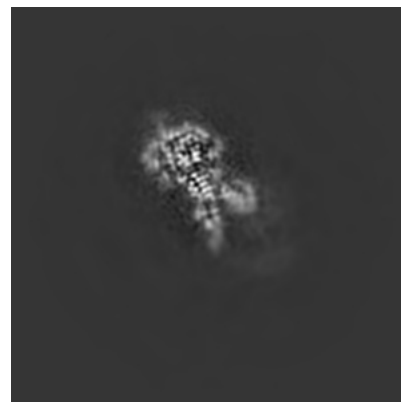
6.3.1 Primary map



X Index: 140

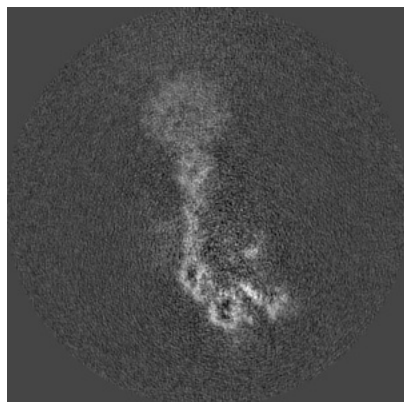


Y Index: 144

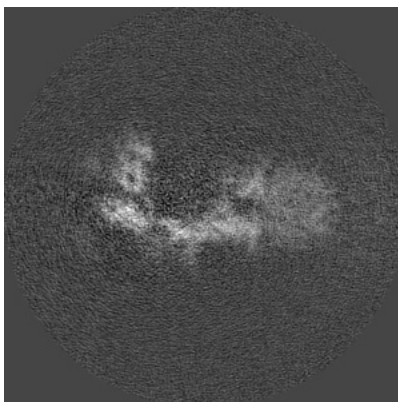


Z Index: 81

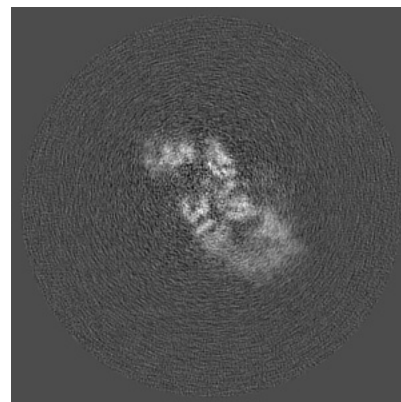
6.3.2 Raw map



X Index: 140



Y Index: 144

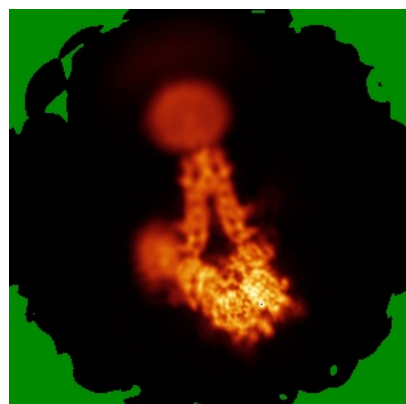


Z Index: 101

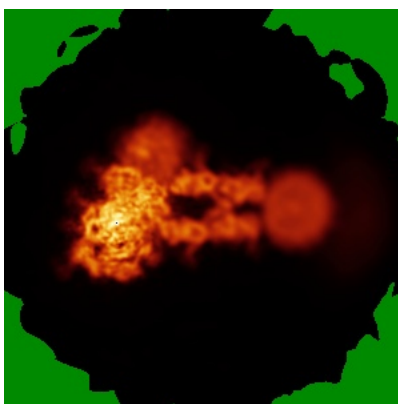
The images above show the largest variance slices of the map in three orthogonal directions.

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

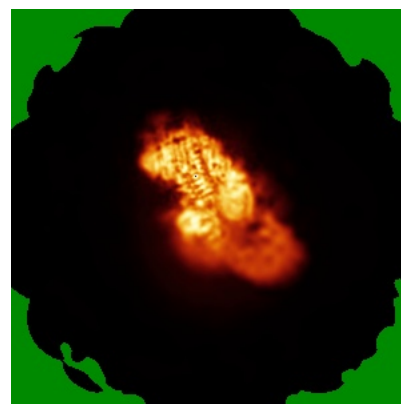
6.4.1 Primary map



X

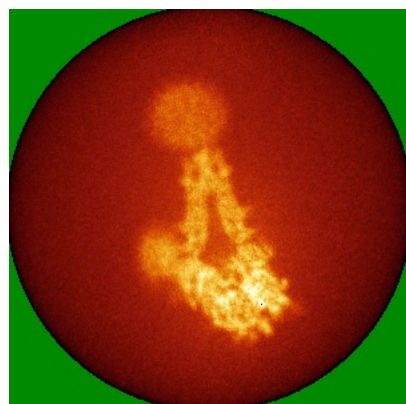


Y

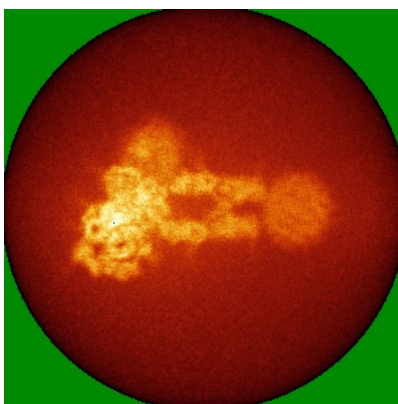


Z

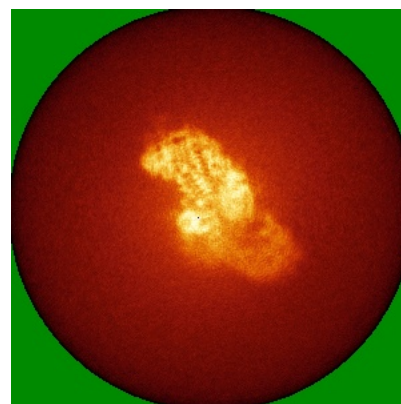
6.4.2 Raw map



X



Y

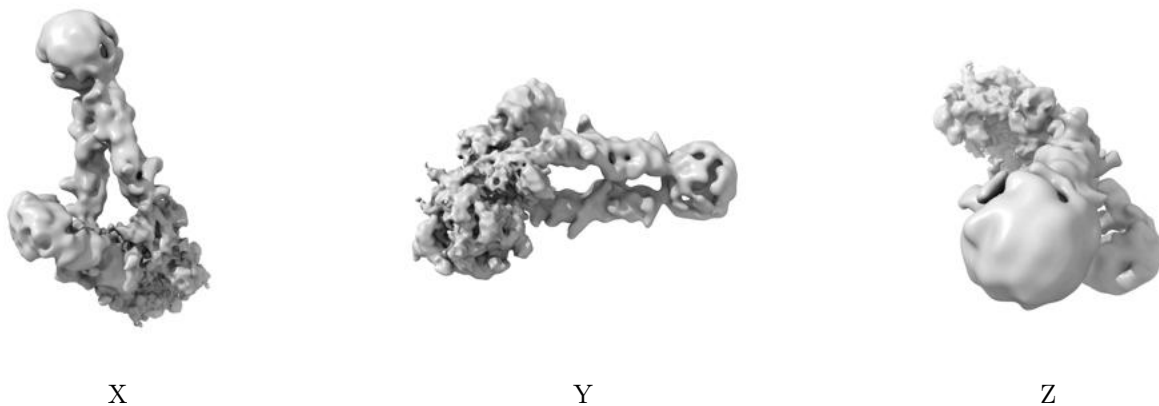


Z

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

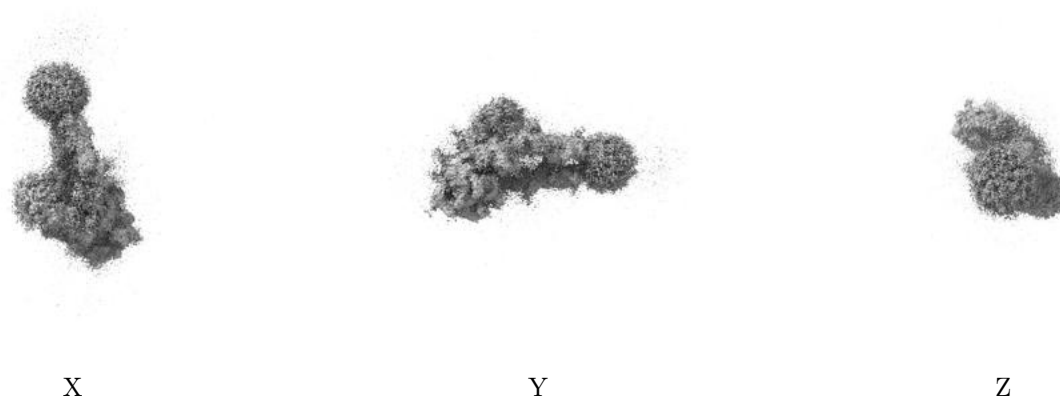
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

6.5.2 Raw map



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

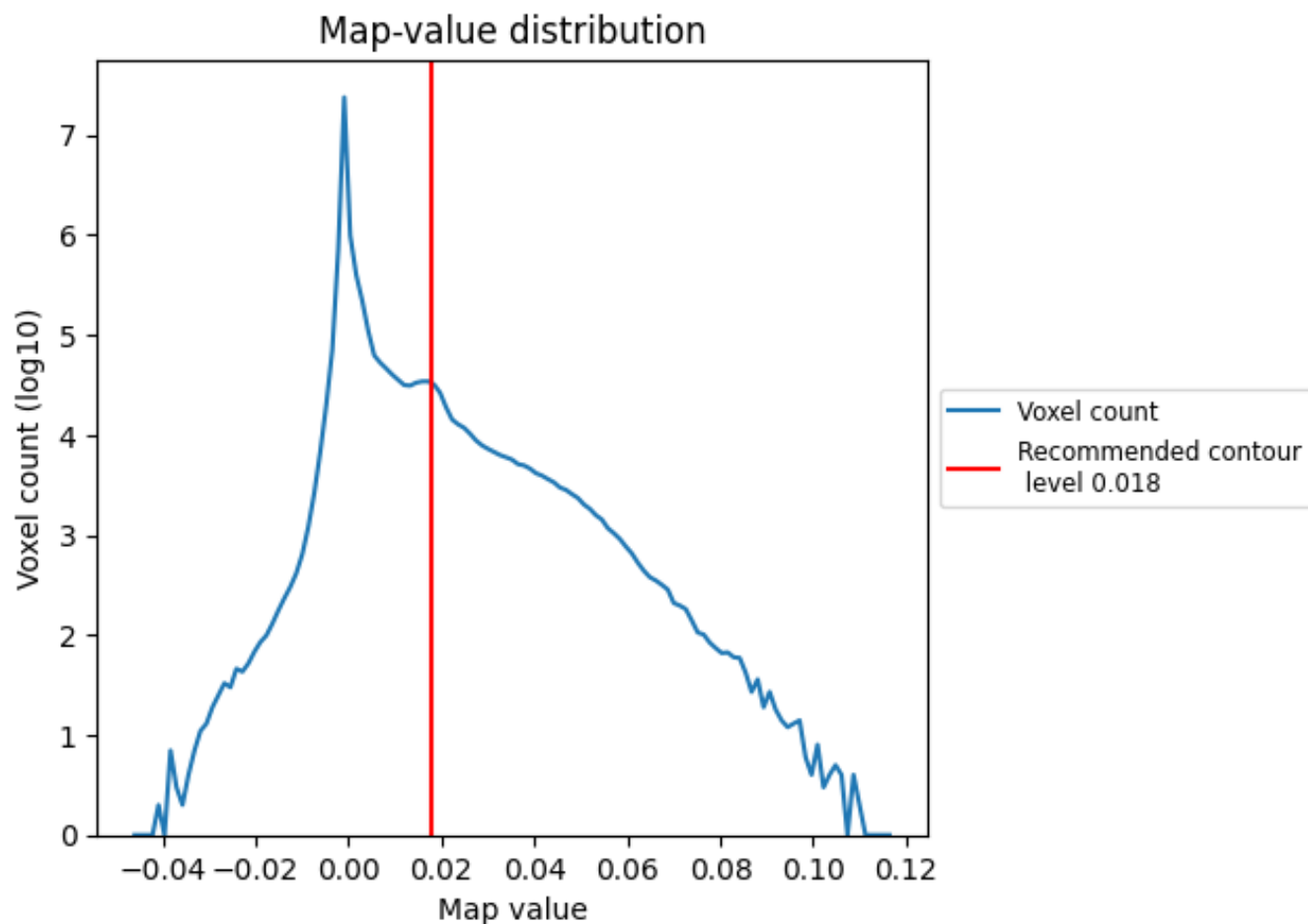
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

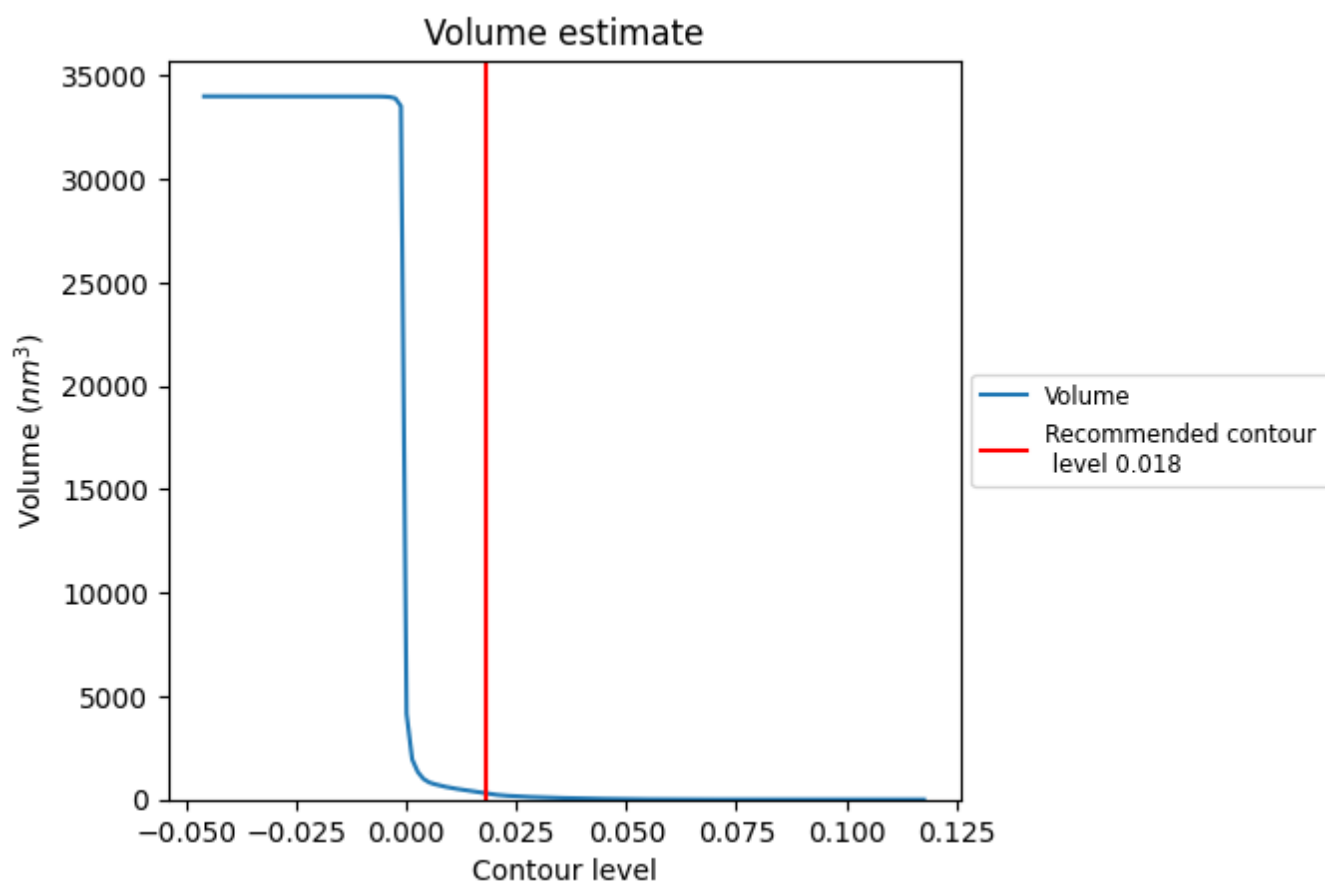
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

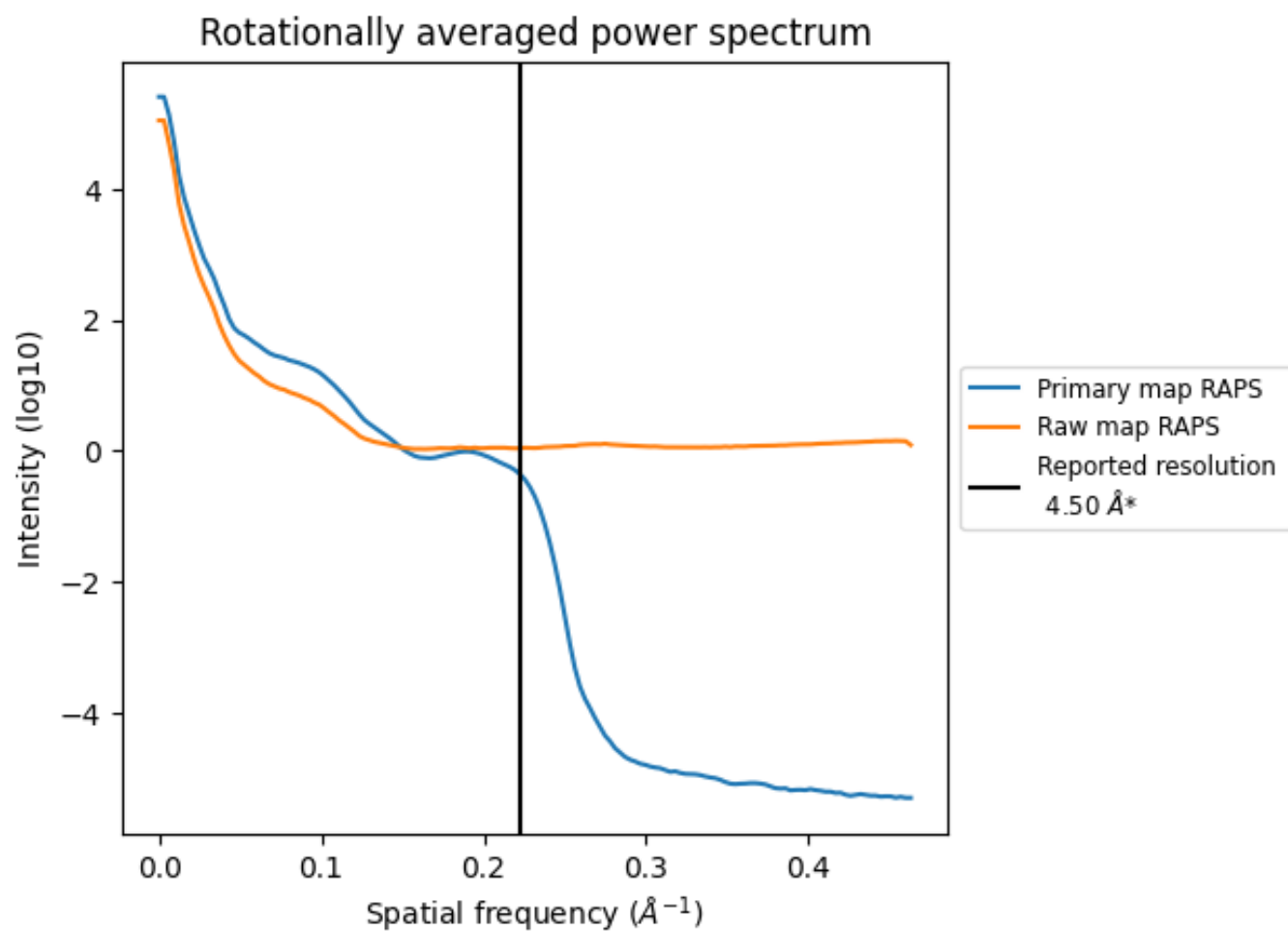
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 306 nm³; 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 ⓘ

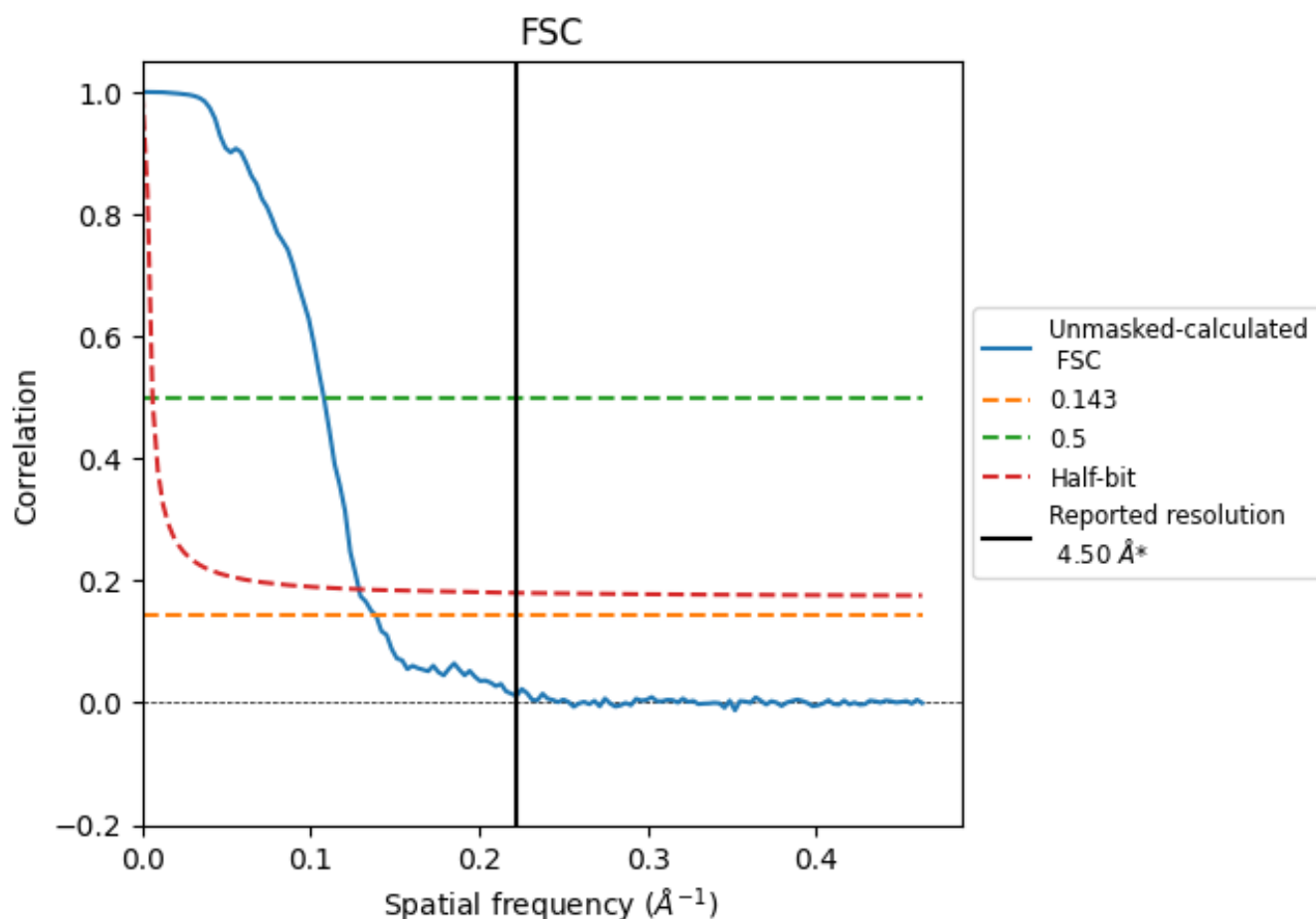


*Reported resolution corresponds to spatial frequency of 0.222 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.222 Å⁻¹

8.2 Resolution estimates [i](#)

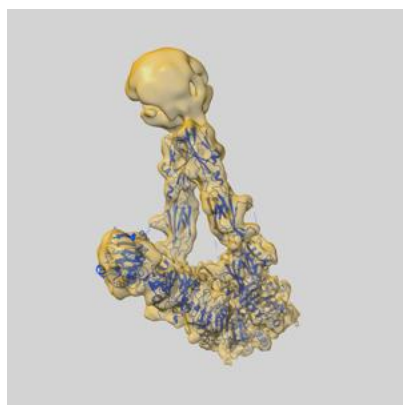
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.22	9.28	7.77

*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 %

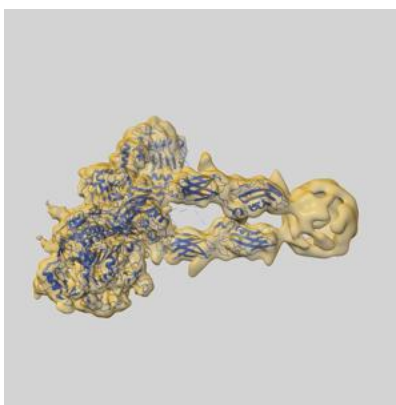
9 Map-model fit [i](#)

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 5.

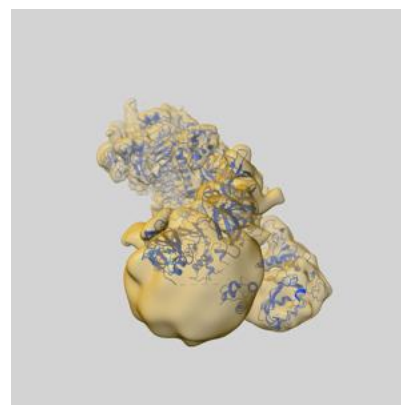
9.1 Map-model overlay [i](#)



X



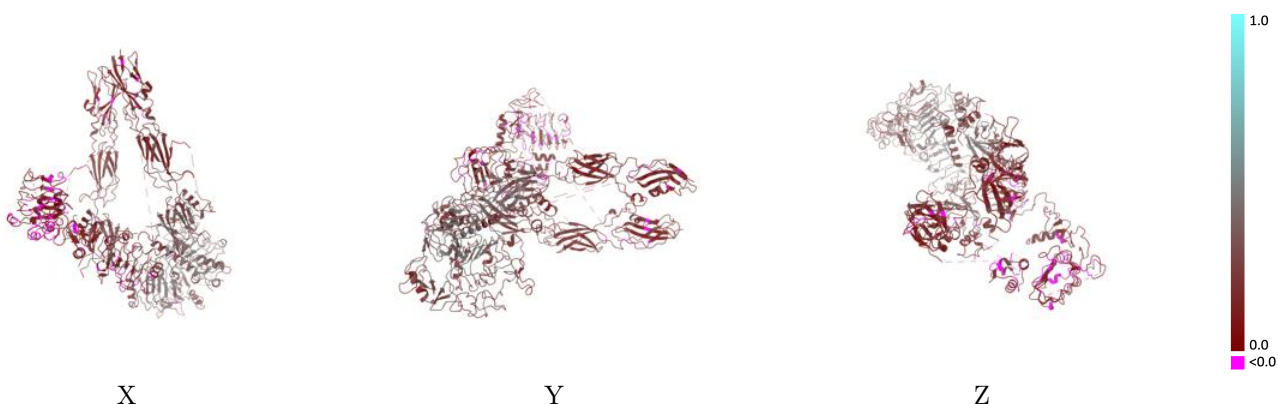
Y



Z

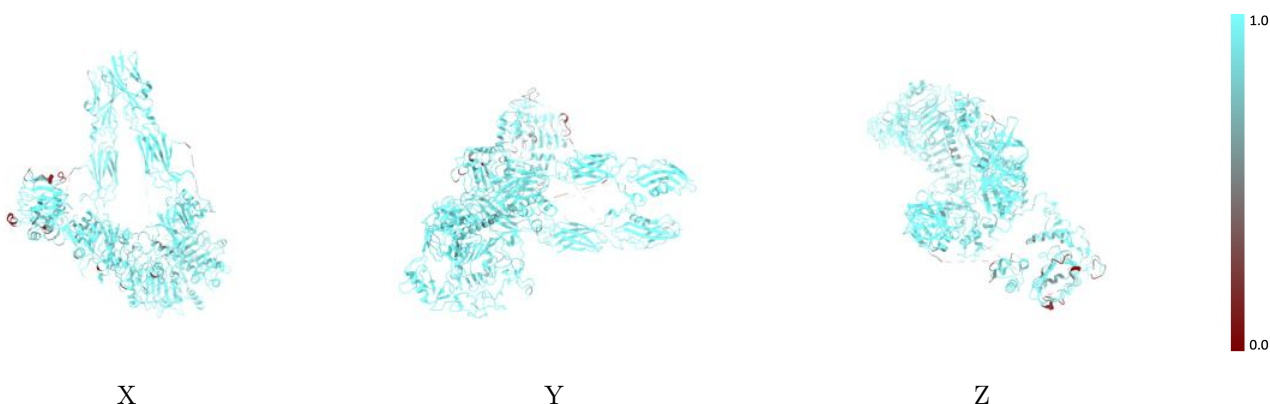
The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



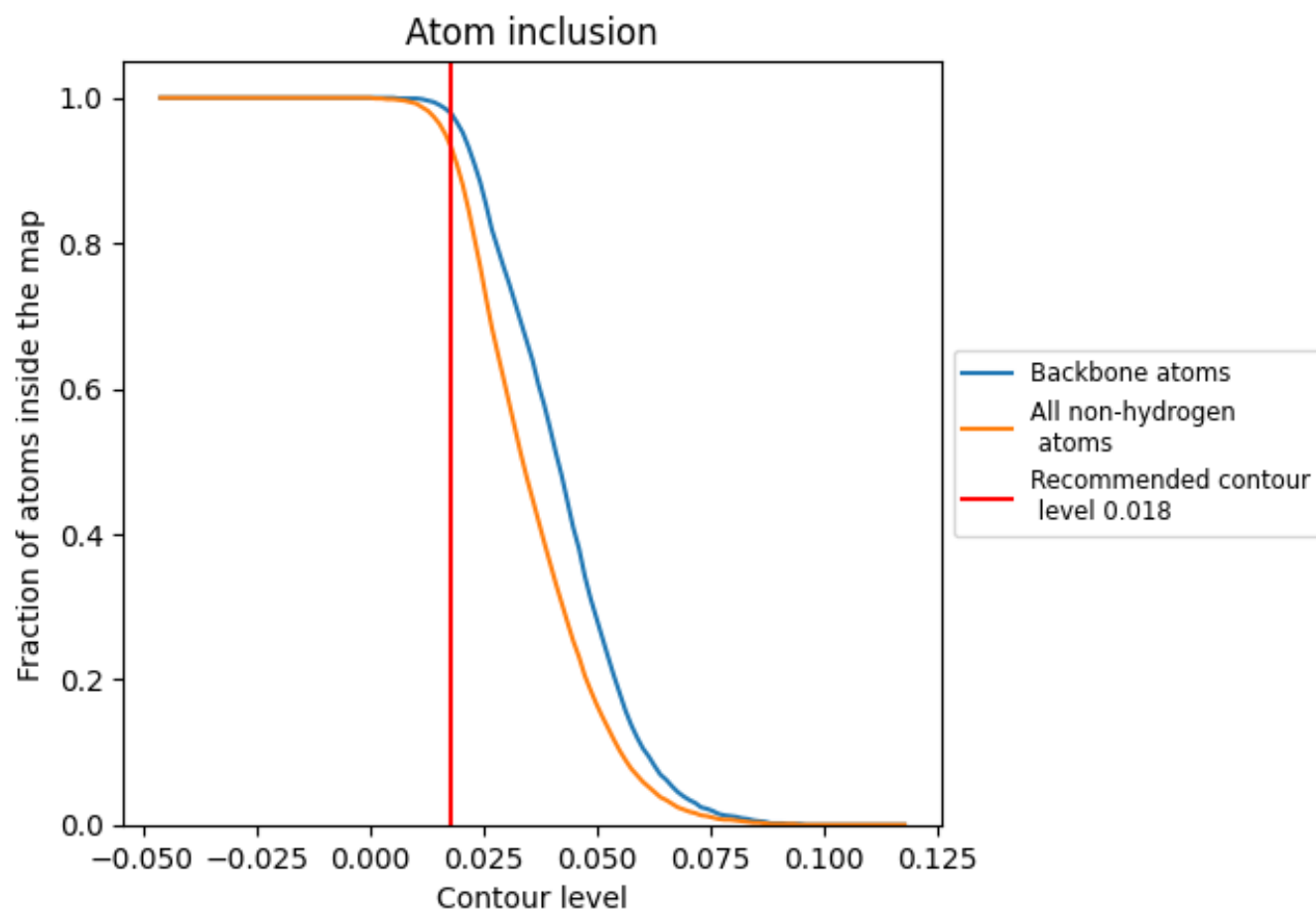
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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	0.9310	0.2370
A	0.9550	0.2840
B	0.9030	0.1910
D	0.8890	0.0890
E	0.9780	0.3360
F	0.9510	0.1920
G	0.9480	0.2620

1.0

0.0

<0.0