



Full wwPDB EM Validation Report ⓘ

Mar 14, 2026 – 08:50 AM UTC

PDB ID : 7Q5S / pdb_00007q5s
EMDB ID : EMD-13846
Title : Protein community member fatty acid synthase complex from *C. thermophilum*
Authors : Chojnowski, G.; Skolidis, I.; Kyrilis, F.L.; Tueting, C.; Hamdi, F.; Kastritis, P.L.
Deposited on : 2021-11-04
Resolution : 4.47 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

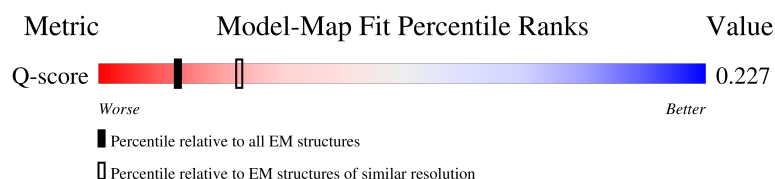
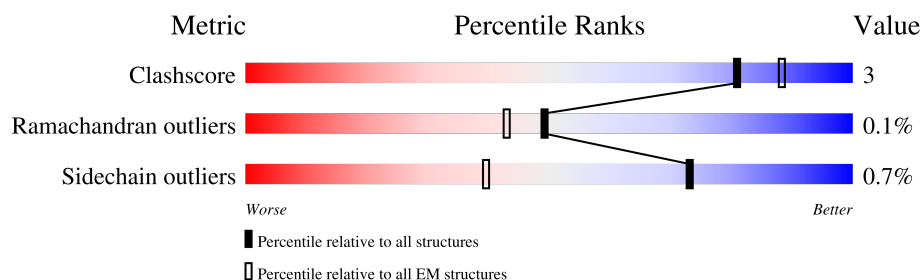
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 4.47 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.



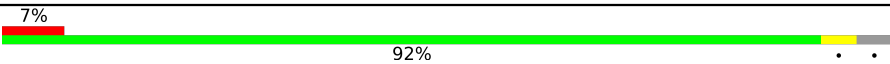
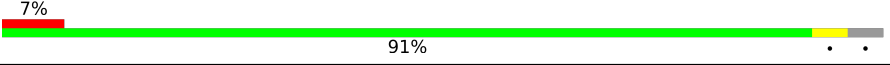
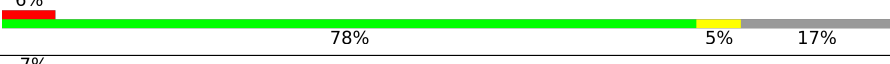
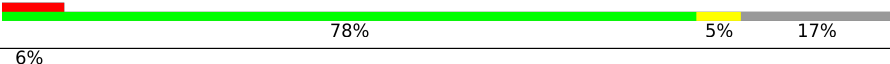
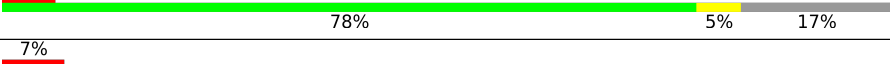
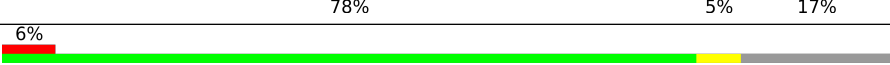
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2963 (3.97 - 4.97)

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	B	2122	7% 92% . .
1	C	2122	7% 91% . .
1	E	2122	7% 92% . .
1	G	2122	7% 91% . .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	I	2122	 92%
1	K	2122	 91%
2	A	1865	 78% 5% 17%
2	D	1865	 78% 5% 17%
2	F	1865	 78% 5% 17%
2	H	1865	 78% 5% 17%
2	J	1865	 78% 5% 17%
2	L	1865	 78% 5% 17%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 168624 atoms, of which 0 are hydrogens and 0 are deuteriums.

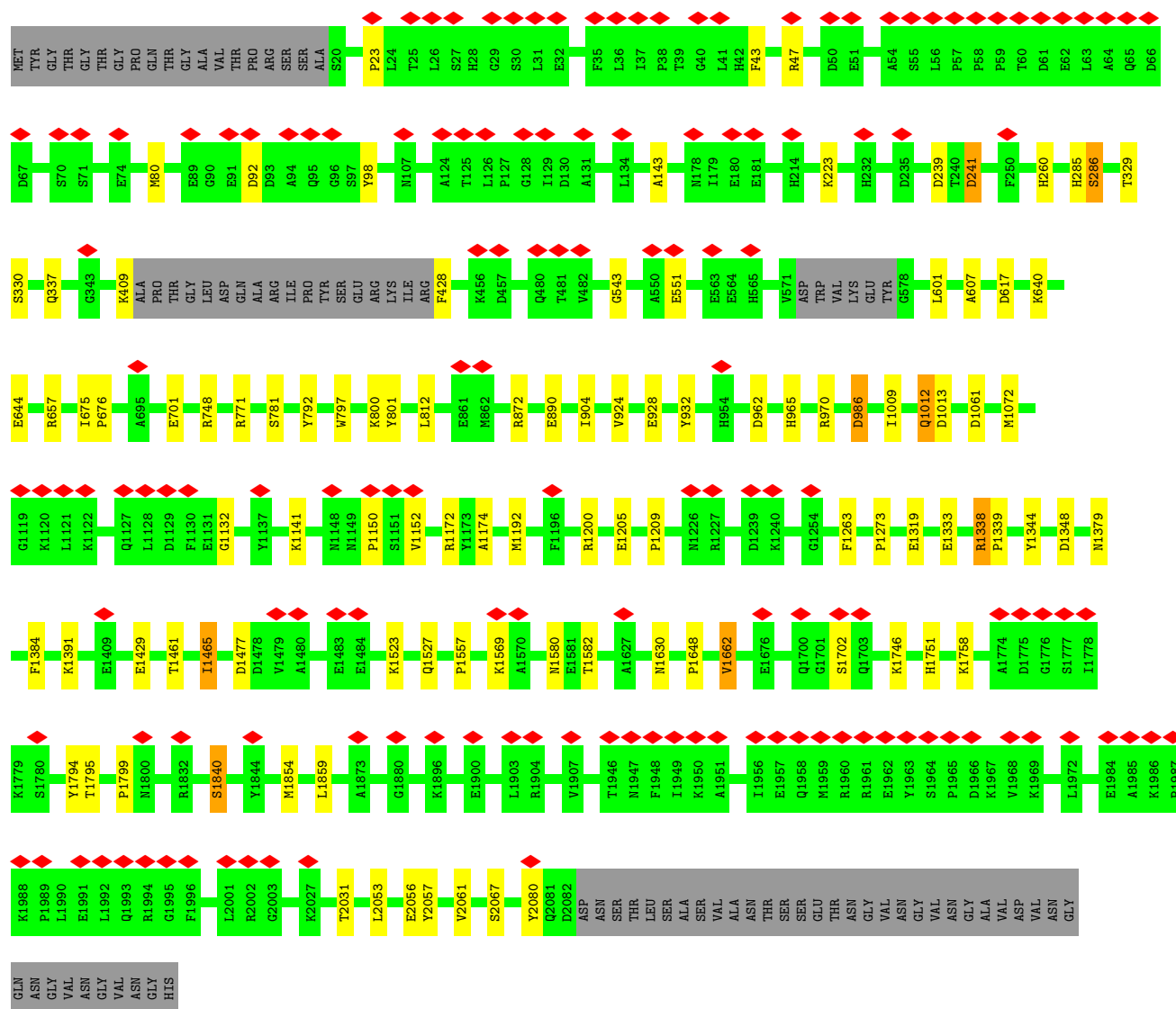
In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 3-hydroxyacyl-[acyl-carrier-protein] dehydratase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	2039	Total	C	N	O	S	0	0
			15987	10199	2739	2994	55		
1	C	2039	Total	C	N	O	S	0	0
			15987	10199	2739	2994	55		
1	E	2039	Total	C	N	O	S	0	0
			15987	10199	2739	2994	55		
1	G	2039	Total	C	N	O	S	0	0
			15987	10199	2739	2994	55		
1	I	2039	Total	C	N	O	S	0	0
			15987	10199	2739	2994	55		
1	K	2039	Total	C	N	O	S	0	0
			15987	10199	2739	2994	55		

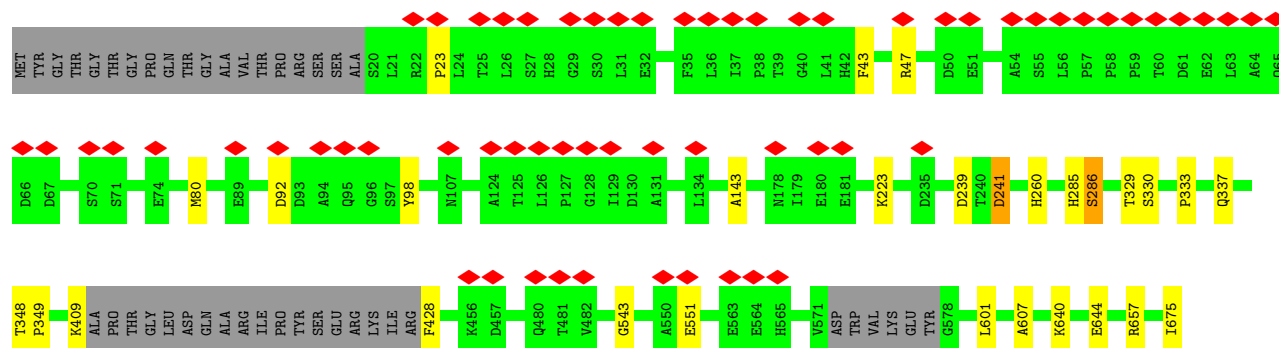
- Molecule 2 is a protein called 3-oxoacyl-[acyl-carrier-protein] reductase.

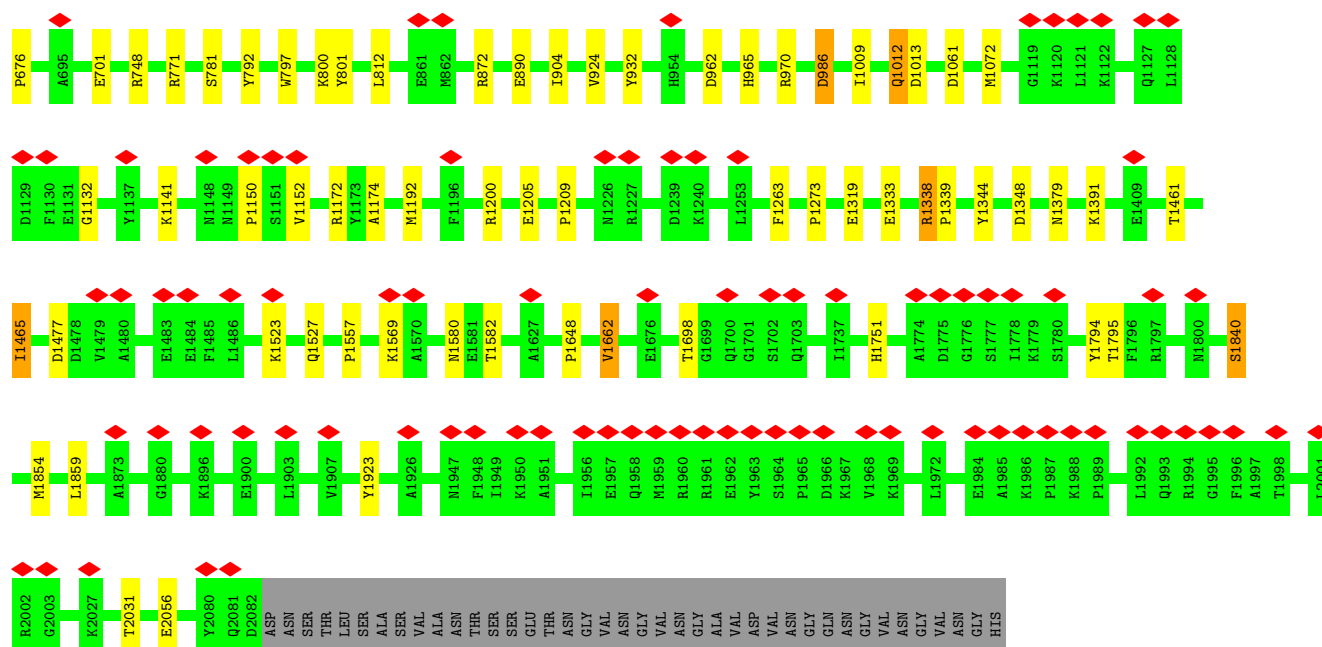
Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	1550	Total	C	N	O	S	0	0
			12117	7672	2079	2314	52		
2	D	1550	Total	C	N	O	S	0	0
			12117	7672	2079	2314	52		
2	F	1550	Total	C	N	O	S	0	0
			12117	7672	2079	2314	52		
2	H	1550	Total	C	N	O	S	0	0
			12117	7672	2079	2314	52		
2	J	1550	Total	C	N	O	S	0	0
			12117	7672	2079	2314	52		
2	L	1550	Total	C	N	O	S	0	0
			12117	7672	2079	2314	52		



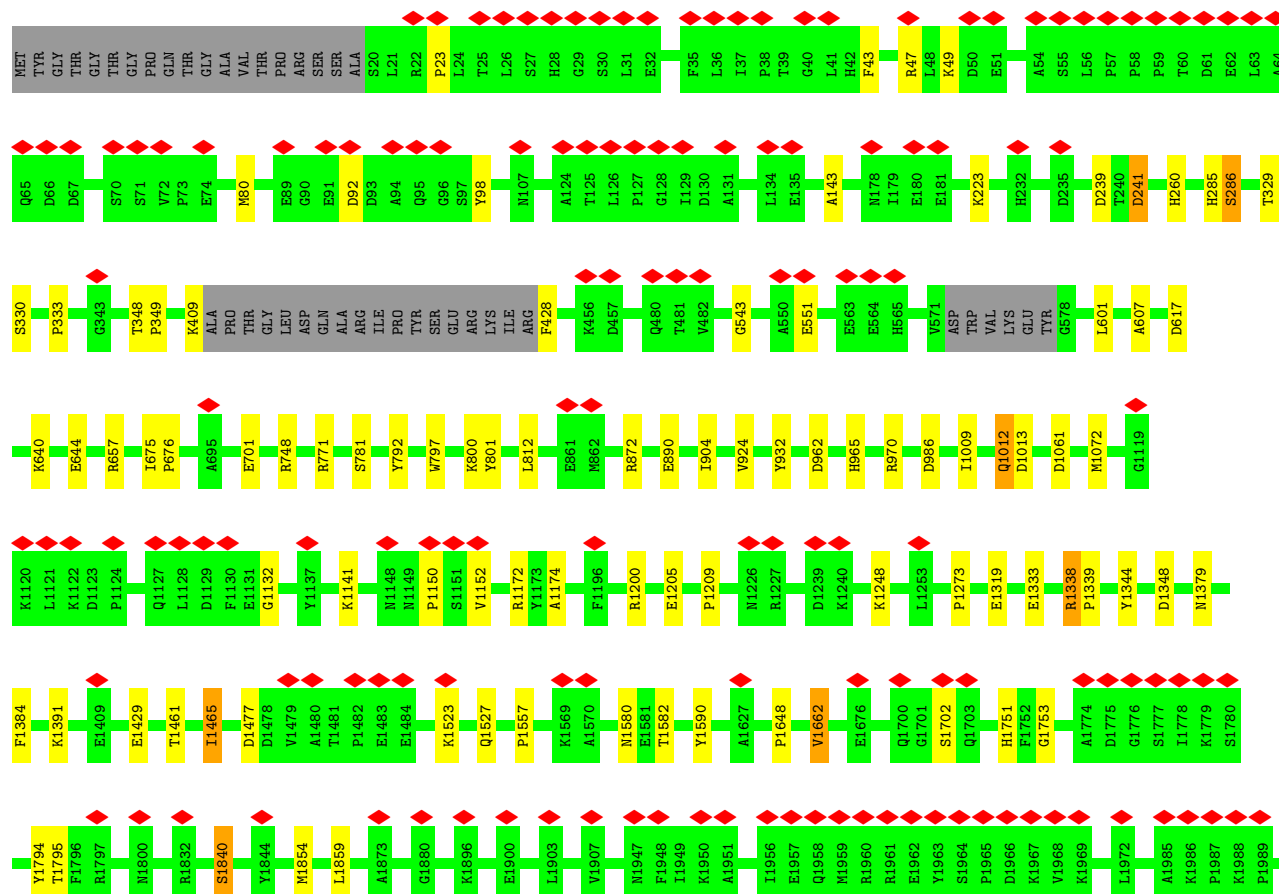
• Molecule 1: 3-hydroxyacyl-[acyl-carrier-protein] dehydratase

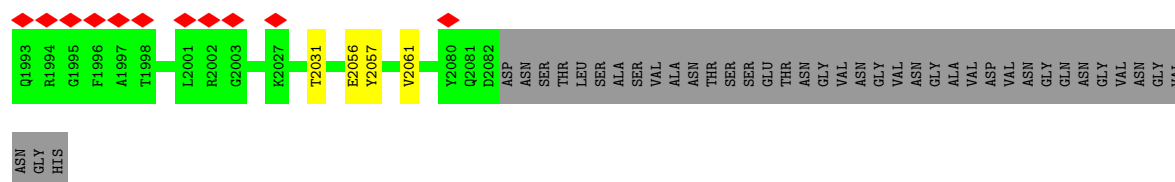
Chain E: 7% 92%



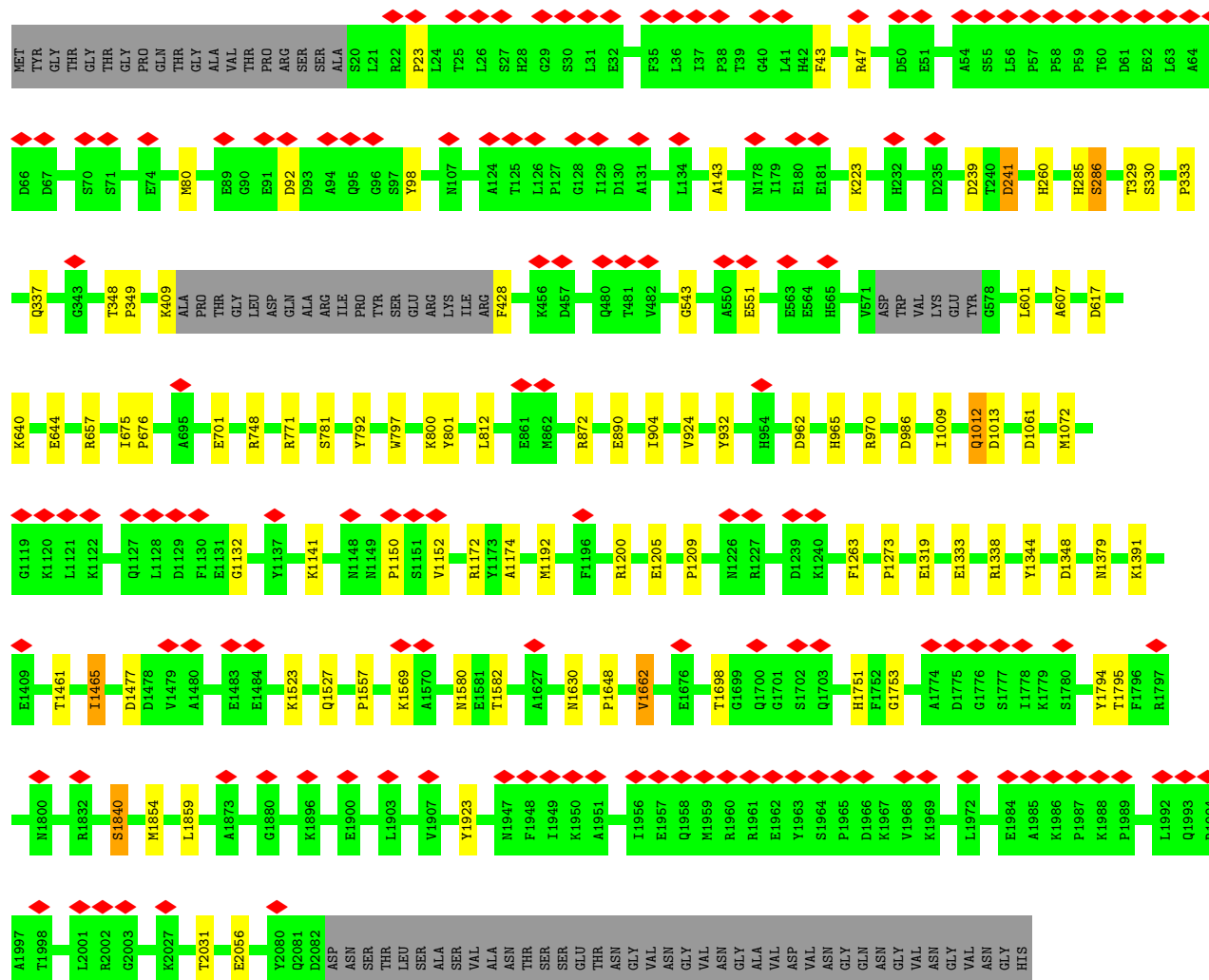


• Molecule 1: 3-hydroxyacyl-[acyl-carrier-protein] dehydratase

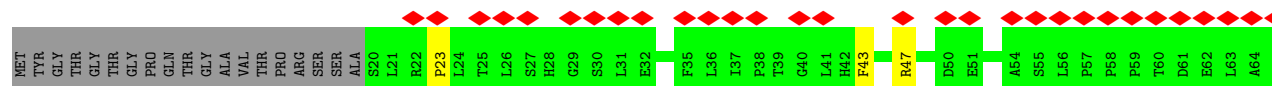


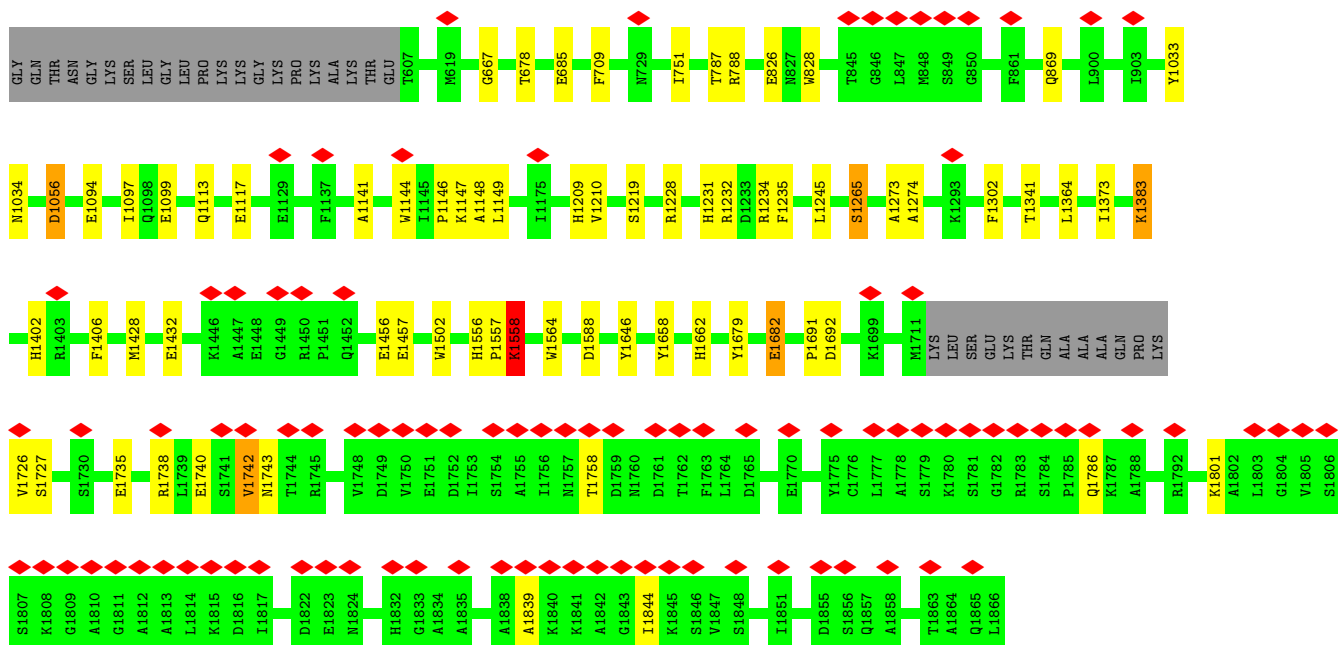


- Molecule 1: 3-hydroxyacyl-[acyl-carrier-protein] dehydratase

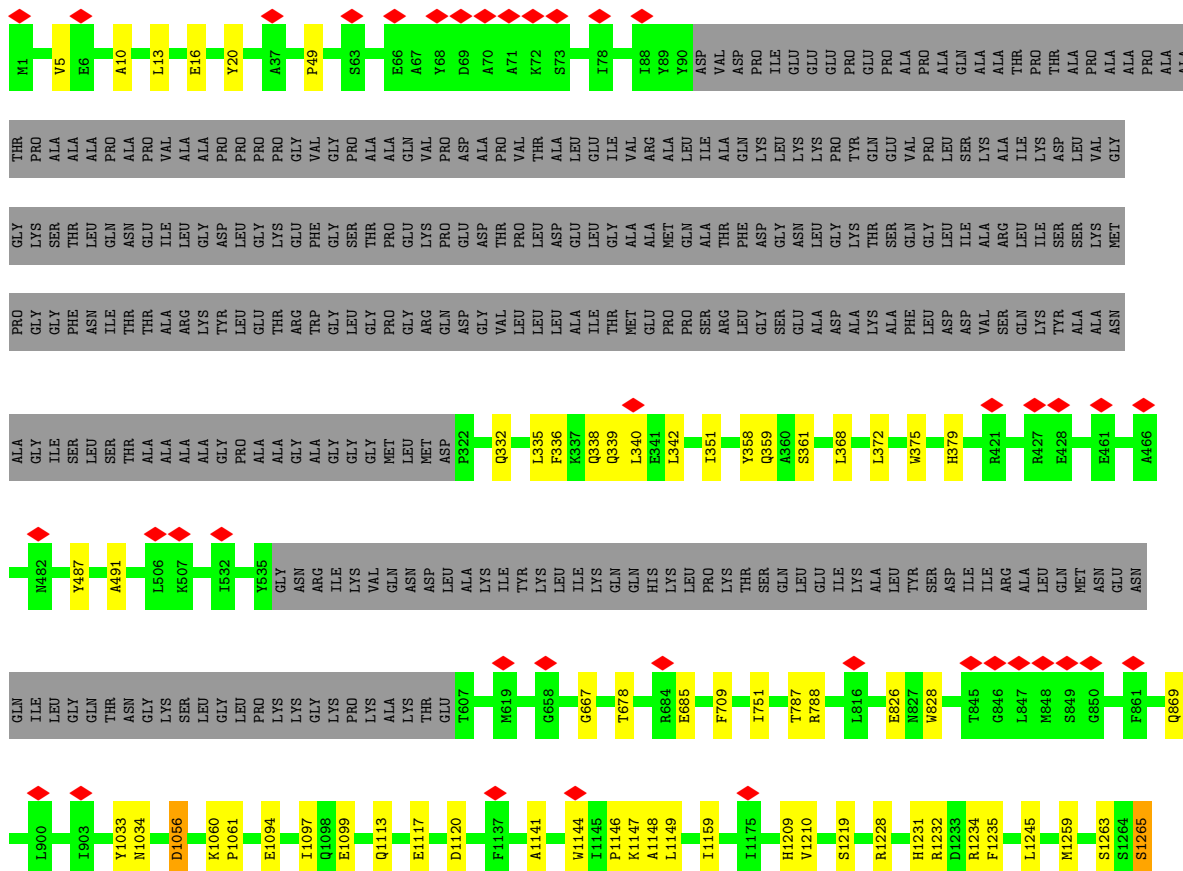
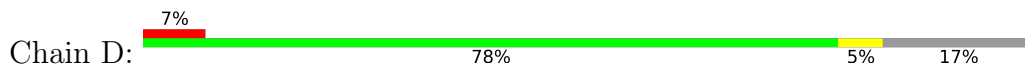


- Molecule 1: 3-hydroxyacyl-[acyl-carrier-protein] dehydratase





- Molecule 2: 3-oxoacyl-[acyl-carrier-protein] reductase



PHE	ASN	ILE	THR	ALA	ARG	LYS	TYR	LEU	GLU	THR	ARG	TRP	GLY	LEU	GLY	PRO	GLY	ASP	ARG	GLN	ASP	GLY	VAL	LEU	LEU	ALA	ILE	THR	THR	MET	GLU	PRO	PRO	SER	ARG	LEU	GLY	SER	GLU	ALA	ASP	LYS	ALA	ALA	PHE	LEU	ASP	ASP	VAL	SER	GLN	LYS	TYR	ALA	ASN	ALA	ASN	ALA	GLY	ILE
SER	LEU	SER	THR	ALA	ALA	ALA	GLY	ALA	PRO	ALA	ALA	GLY	ALA	GLY	GLY	GLY	MET	LEU	MET	ASP	P322	Q332	Q332	F336	K337	Q338	Q339	ILE	THR	THR	GLN	GLN	PRO	PRO	SER	ARG	LEU	GLY	SER	GLU	ALA	ASP	LYS	ALA	ALA	W375	H379	R421	R427	E428	E461	A466	N482	Y487						
A491	L506	K507	L532	Y535	ASN	ARG	ILE	LYS	VAL	GLN	ASN	ASP	LEU	ALA	LYS	ILE	TYR	LYS	LEU	ILE	LYS	LYS	ILE	LYS	GLN	GLN	HIS	LYS	LEU	PRO	LYS	THR	SER	GLN	LEU	ILE	LYS	ALA	LEU	TYR	SER	ASP	ILE	ARG	ALA	LEU	GLN	MET	ASN	GLU	ASN	GLN	ILE	GLY						
GLN	THR	ASN	GLY	LYS	SER	LEU	GLY	PRO	LYS	LYS	GLY	LYS	PRO	LYS	ALA	LYS	THR	GLU	T607	M619	G667	T678	R684	E685	F709	I751	R788	H799	F803	L816	R822	E826	R827	W828	T845	G846	L847	M848	S849	G850	F861	Q869																		
L900	I903	Y1033	N1034	D1056	L1092	H1093	E1094	I1097	Q1098	E1099	Q1113	R1116	E1117	H1118	G1119	D1120	F1137	A1141	W1144	I1145	K1147	A1148	L1149	I1159	H1209	V1210	S1219	R1228	H1231	R1232	F1235	M1259	S1265	A1273	A1274	K1293	F1302																							
Y1311	E1312	T1341	Q1350	L1364	I1373	K1383	I1384	R1400	E1401	H1402	R1403	F1406	M1428	K1446	A1447	E1448	G1449	R1450	P1451	Q1452	E1456	W1502	H1556	P1557	K1583	W1564	D1588	Y1646	Y1658	H1662	Y1679	E1682	P1691	D1692	K1699	G1702																								
M1711	LYS	SER	GLU	THR	GLN	ALA	ALA	ALA	GLN	PRO	LYS	V1726	S1727	S1730	E1735	R1738	L1739	E1740	S1741	V1742	N1743	T1744	R1745	V1748	D1749	V1750	E1751	D1752	A1755	I1756	N1757	T1758	D1759	N1760	T1762	F1763	L1764	D1765	R1766	E1770	Y1775	C1776	L1777	A1778	S1779	K1780	S1781	G1782												
R1783	S1784	P1785	K1787	A1788	R1792	L1803	G1804	V1805	S1806	S1807	K1808	G1809	A1810	G1811	A1812	A1813	L1814	K1815	D1816	I1817	V1821	D1822	E1823	N1824	H1832	A1835	A1838	A1839	K1840	K1841	A1842	G1843	I1844	K1845	S1846	V1847	S1848	I1851	D1855	S1856	Q1857	A1858	T1863	A1864	Q1865	L1866														

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	5231	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	95675	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	2.802	Depositor
Minimum map value	-1.002	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.243	Depositor
Recommended contour level	0.7	Depositor
Map size (Å)	401.3568, 401.3568, 401.3568	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.5678, 1.5678, 1.5678	Depositor

5 Model quality

5.1 Standard geometry

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	B	0.30	0/16355	0.54	2/22210 (0.0%)
1	C	0.30	0/16355	0.54	2/22210 (0.0%)
1	E	0.30	0/16355	0.54	2/22210 (0.0%)
1	G	0.30	0/16355	0.54	2/22210 (0.0%)
1	I	0.30	0/16355	0.54	2/22210 (0.0%)
1	K	0.30	0/16355	0.54	2/22210 (0.0%)
2	A	0.33	0/12356	0.60	2/16714 (0.0%)
2	D	0.33	0/12356	0.60	2/16714 (0.0%)
2	F	0.33	0/12356	0.60	2/16714 (0.0%)
2	H	0.33	0/12356	0.60	2/16714 (0.0%)
2	J	0.33	0/12356	0.60	2/16714 (0.0%)
2	L	0.33	0/12356	0.60	2/16714 (0.0%)
All	All	0.31	0/172266	0.57	24/233544 (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	B	0	1
1	C	0	1
1	E	0	1
1	G	0	1
1	I	0	1
1	K	0	1
2	A	0	1
2	D	0	1
2	F	0	1
2	H	0	1
2	J	0	1
2	L	0	1
All	All	0	12

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	286	SER	N-CA-CB	-9.09	95.13	110.49
1	G	286	SER	N-CA-CB	-9.09	95.13	110.49
1	B	286	SER	N-CA-CB	-9.09	95.14	110.49
1	K	286	SER	N-CA-CB	-9.08	95.14	110.49
1	E	286	SER	N-CA-CB	-9.06	95.17	110.49
1	C	286	SER	N-CA-CB	-9.06	95.18	110.49
1	G	1840	SER	N-CA-CB	-6.39	99.69	110.49
1	I	1840	SER	N-CA-CB	-6.39	99.69	110.49
1	K	1840	SER	N-CA-CB	-6.39	99.69	110.49
1	B	1840	SER	N-CA-CB	-6.38	99.71	110.49
1	E	1840	SER	N-CA-CB	-6.38	99.72	110.49
1	C	1840	SER	N-CA-CB	-6.37	99.72	110.49
2	J	1558	LYS	N-CA-CB	-5.36	101.42	110.49
2	F	1558	LYS	N-CA-CB	-5.36	101.43	110.49
2	L	1558	LYS	N-CA-CB	-5.36	101.43	110.49
2	H	1558	LYS	N-CA-CB	-5.35	101.44	110.49
2	D	1558	LYS	N-CA-CB	-5.33	101.47	110.49
2	A	1558	LYS	N-CA-CB	-5.32	101.50	110.49
2	F	1383	LYS	CG-CD-CE	5.07	122.97	111.30
2	D	1383	LYS	CG-CD-CE	5.07	122.95	111.30
2	H	1383	LYS	CG-CD-CE	5.07	122.95	111.30
2	L	1383	LYS	CG-CD-CE	5.07	122.95	111.30
2	A	1383	LYS	CG-CD-CE	5.06	122.95	111.30
2	J	1383	LYS	CG-CD-CE	5.06	122.93	111.30

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	1273	ALA	Peptide
1	B	285	HIS	Peptide
1	C	285	HIS	Peptide
2	D	1273	ALA	Peptide
1	E	285	HIS	Peptide
2	F	1273	ALA	Peptide
1	G	285	HIS	Peptide
2	H	1273	ALA	Peptide
1	I	285	HIS	Peptide
2	J	1273	ALA	Peptide
1	K	285	HIS	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	L	1273	ALA	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	15987	0	15963	78	0
1	C	15987	0	15963	89	0
1	E	15987	0	15963	70	0
1	G	15987	0	15963	86	0
1	I	15987	0	15963	77	0
1	K	15987	0	15963	74	0
2	A	12117	0	12052	126	0
2	D	12117	0	12052	143	0
2	F	12117	0	12052	144	0
2	H	12117	0	12052	141	0
2	J	12117	0	12052	122	0
2	L	12117	0	12052	142	0
All	All	168624	0	168090	883	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 3.

All (883) 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)
2:F:351:ILE:HG22	2:L:351:ILE:HG22	1.14	1.12
2:D:751:ILE:HB	2:H:826:GLU:OE2	1.53	1.06
2:A:351:ILE:HG22	2:J:351:ILE:HG22	1.31	1.05
2:D:351:ILE:HG22	2:H:351:ILE:HG22	1.34	1.04
2:A:751:ILE:HB	2:J:826:GLU:OE2	1.57	1.04
2:A:751:ILE:HG21	2:J:828:TRP:CD1	1.94	1.02
2:D:751:ILE:HG21	2:H:828:TRP:CD1	1.94	1.02
2:F:351:ILE:HG22	2:L:351:ILE:CG2	1.90	1.02
2:F:351:ILE:CG2	2:L:351:ILE:HG22	1.90	1.01
1:G:23:PRO:HG3	1:K:43:PHE:HE2	1.25	0.99

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:43:PHE:HE2	1:I:23:PRO:HG3	1.31	0.95
2:D:368:LEU:HD22	2:H:372:LEU:HD11	1.51	0.93
1:C:43:PHE:HE2	1:E:23:PRO:HG3	1.33	0.91
2:F:826:GLU:OE2	2:L:751:ILE:HB	1.70	0.91
2:F:751:ILE:HB	2:L:826:GLU:OE2	1.71	0.89
1:G:43:PHE:CE2	1:I:23:PRO:HG3	2.09	0.88
1:G:23:PRO:HG3	1:K:43:PHE:CE2	2.07	0.88
2:A:368:LEU:HD22	2:J:372:LEU:HD11	1.56	0.87
2:A:1383:LYS:HD2	2:H:1679:TYR:OH	1.74	0.87
2:A:1679:TYR:OH	2:H:1383:LYS:HD2	1.74	0.87
1:C:43:PHE:CE2	1:E:23:PRO:HG3	2.10	0.86
1:B:330:SER:N	1:C:1333:GLU:OE1	2.10	0.85
2:D:351:ILE:CG2	2:H:351:ILE:HG22	2.07	0.84
2:F:828:TRP:CD1	2:L:751:ILE:HG21	2.12	0.84
1:B:23:PRO:HG3	1:E:43:PHE:HE2	1.43	0.83
2:F:751:ILE:HG21	2:L:828:TRP:CD1	2.13	0.83
2:F:1679:TYR:OH	2:J:1383:LYS:HD2	1.77	0.83
2:F:1383:LYS:HD2	2:J:1679:TYR:OH	1.79	0.83
2:A:351:ILE:CG2	2:J:351:ILE:HG22	2.08	0.83
1:I:43:PHE:HE2	1:K:23:PRO:HG3	1.43	0.82
2:A:1231:HIS:CE1	2:H:1228:ARG:HA	2.15	0.81
2:A:351:ILE:HG22	2:J:351:ILE:CG2	2.10	0.81
2:D:351:ILE:HG22	2:H:351:ILE:CG2	2.09	0.81
2:A:826:GLU:OE2	2:J:751:ILE:HB	1.82	0.80
1:B:43:PHE:HE2	1:C:23:PRO:HG3	1.45	0.80
2:A:828:TRP:CD1	2:J:751:ILE:HG21	2.17	0.80
2:A:1113:GLN:HB3	2:H:1147:LYS:HB2	1.66	0.78
2:A:1147:LYS:HB2	2:H:1113:GLN:HB3	1.66	0.78
2:D:1147:LYS:HB2	2:L:1113:GLN:HB3	1.66	0.77
1:C:1751:HIS:CG	2:H:788:ARG:HD2	2.20	0.77
2:D:1231:HIS:CE1	2:L:1228:ARG:HA	2.21	0.76
2:D:1113:GLN:HB3	2:L:1147:LYS:HB2	1.68	0.75
2:D:826:GLU:OE2	2:H:751:ILE:HB	1.85	0.75
2:A:1228:ARG:HA	2:H:1231:HIS:CE1	2.21	0.74
2:D:1383:LYS:HD2	2:L:1679:TYR:OH	1.87	0.74
2:F:1056:ASP:OD1	2:F:1056:ASP:N	2.16	0.74
1:B:23:PRO:HG3	1:E:43:PHE:CE2	2.23	0.74
2:H:1056:ASP:OD1	2:H:1056:ASP:N	2.16	0.74
2:D:1146:PRO:HB2	2:L:1117:GLU:HG2	1.70	0.73
2:F:372:LEU:HD11	2:L:368:LEU:HD22	1.71	0.73
2:F:379:HIS:HE1	2:L:379:HIS:HE1	1.37	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1056:ASP:OD1	2:D:1056:ASP:N	2.16	0.73
2:D:358:TYR:CE1	2:H:361:SER:OG	2.42	0.73
1:E:241:ASP:N	1:E:241:ASP:OD1	2.22	0.73
1:I:241:ASP:OD1	1:I:241:ASP:N	2.22	0.73
1:I:43:PHE:CE2	1:K:23:PRO:HG3	2.23	0.72
2:D:1146:PRO:C	2:L:1117:GLU:HG2	2.14	0.72
2:F:368:LEU:HD22	2:L:372:LEU:HD11	1.71	0.72
2:A:1146:PRO:HB2	2:H:1117:GLU:HG2	1.71	0.72
1:B:241:ASP:OD1	1:B:241:ASP:N	2.22	0.72
2:A:1383:LYS:CD	2:H:1679:TYR:OH	2.37	0.72
1:G:241:ASP:N	1:G:241:ASP:OD1	2.22	0.72
1:C:1702:SER:HB2	2:D:49:PRO:HG2	1.70	0.72
1:C:241:ASP:N	1:C:241:ASP:OD1	2.22	0.71
2:L:1056:ASP:OD1	2:L:1056:ASP:N	2.16	0.71
2:D:1679:TYR:OH	2:L:1383:LYS:HD2	1.90	0.71
1:K:241:ASP:OD1	1:K:241:ASP:N	2.22	0.71
2:A:1146:PRO:C	2:H:1117:GLU:HG2	2.14	0.71
1:B:329:THR:HB	1:C:1333:GLU:CD	2.16	0.70
2:D:828:TRP:CD1	2:H:751:ILE:HG21	2.26	0.70
2:F:1117:GLU:HG2	2:J:1146:PRO:C	2.17	0.70
1:G:329:THR:HB	1:I:1333:GLU:CD	2.16	0.69
2:A:1457:GLU:HG2	2:H:1406:PHE:CE2	2.27	0.69
2:F:1146:PRO:C	2:J:1117:GLU:HG2	2.17	0.69
2:D:1228:ARG:HA	2:L:1231:HIS:CE1	2.28	0.69
1:C:330:SER:N	1:E:1333:GLU:OE1	2.24	0.68
2:D:788:ARG:HD2	1:G:1751:HIS:CG	2.28	0.68
1:I:551:GLU:OE1	1:I:771:ARG:NH2	2.28	0.67
2:J:1682:GLU:CD	2:J:1682:GLU:H	2.03	0.67
1:G:551:GLU:OE1	1:G:771:ARG:NH2	2.28	0.67
2:A:1679:TYR:OH	2:H:1383:LYS:CD	2.43	0.67
2:A:1682:GLU:CD	2:A:1682:GLU:H	2.03	0.67
2:D:1117:GLU:HG2	2:L:1146:PRO:C	2.20	0.67
1:G:23:PRO:CG	1:K:43:PHE:CE2	2.78	0.67
1:B:43:PHE:CE2	1:C:23:PRO:HG3	2.29	0.67
2:A:1056:ASP:OD1	2:A:1056:ASP:N	2.16	0.67
1:C:551:GLU:OE1	1:C:771:ARG:NH2	2.28	0.67
1:E:551:GLU:OE1	1:E:771:ARG:NH2	2.28	0.67
1:G:330:SER:N	1:I:1333:GLU:OE1	2.23	0.67
2:D:368:LEU:HD22	2:H:372:LEU:CD1	2.23	0.66
1:I:330:SER:N	1:K:1333:GLU:OE1	2.27	0.66
1:B:551:GLU:OE1	1:B:771:ARG:NH2	2.28	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:551:GLU:OE1	1:K:771:ARG:NH2	2.28	0.66
2:F:1682:GLU:CD	2:F:1682:GLU:H	2.03	0.66
2:F:361:SER:OG	2:L:358:TYR:CE1	2.49	0.66
1:B:1333:GLU:OE1	1:E:330:SER:N	2.27	0.66
2:A:1117:GLU:HG2	2:H:1146:PRO:C	2.20	0.66
2:F:379:HIS:CE1	2:L:379:HIS:CE1	2.84	0.66
1:G:800:LYS:HE3	1:G:801:TYR:CE2	2.32	0.65
1:I:329:THR:HB	1:K:1333:GLU:CD	2.22	0.65
1:B:1333:GLU:CD	1:E:329:THR:HB	2.22	0.65
1:G:43:PHE:CE2	1:I:23:PRO:CG	2.78	0.65
1:C:800:LYS:HE3	1:C:801:TYR:CE2	2.32	0.65
1:E:800:LYS:HE3	1:E:801:TYR:CE2	2.32	0.65
2:F:358:TYR:CE1	2:L:361:SER:OG	2.49	0.65
1:C:1751:HIS:CD2	2:H:788:ARG:HD2	2.32	0.65
2:L:1682:GLU:CD	2:L:1682:GLU:H	2.03	0.65
2:F:1228:ARG:HA	2:J:1231:HIS:CE1	2.32	0.65
1:G:43:PHE:CE2	1:I:23:PRO:CD	2.80	0.64
1:B:800:LYS:HE3	1:B:801:TYR:CE2	2.31	0.64
2:A:1149:LEU:HD21	2:H:1113:GLN:NE2	2.13	0.64
2:H:1682:GLU:CD	2:H:1682:GLU:H	2.03	0.64
2:D:1682:GLU:H	2:D:1682:GLU:CD	2.03	0.64
1:I:800:LYS:HE3	1:I:801:TYR:CE2	2.32	0.64
1:K:800:LYS:HE3	1:K:801:TYR:CE2	2.32	0.64
2:F:1231:HIS:CE1	2:J:1228:ARG:HA	2.33	0.64
2:A:1117:GLU:HG2	2:H:1146:PRO:HB2	1.81	0.63
1:G:23:PRO:CD	1:K:43:PHE:CE2	2.81	0.63
2:F:375:TRP:CD1	2:L:375:TRP:CE2	2.87	0.63
2:J:1056:ASP:OD1	2:J:1056:ASP:N	2.16	0.63
2:A:358:TYR:CE1	2:J:361:SER:OG	2.52	0.62
2:D:1146:PRO:CB	2:L:1117:GLU:HG2	2.29	0.62
2:F:379:HIS:CE1	2:L:379:HIS:HE1	2.18	0.62
2:F:1679:TYR:OH	2:J:1383:LYS:CD	2.47	0.62
2:H:1094:GLU:HB2	2:H:1144:TRP:CZ2	2.35	0.62
2:L:1094:GLU:HB2	2:L:1144:TRP:CZ2	2.35	0.62
2:D:1149:LEU:HD21	2:L:1113:GLN:NE2	2.15	0.62
1:G:23:PRO:CG	1:K:43:PHE:HE2	2.05	0.62
2:A:1094:GLU:HB2	2:A:1144:TRP:CZ2	2.35	0.62
2:D:1094:GLU:HB2	2:D:1144:TRP:CZ2	2.35	0.62
2:F:1094:GLU:HB2	2:F:1144:TRP:CZ2	2.35	0.62
2:A:1146:PRO:CB	2:H:1117:GLU:HG2	2.30	0.61
2:F:375:TRP:CE2	2:L:375:TRP:CD1	2.87	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1147:LYS:HB2	2:J:1113:GLN:HB3	1.82	0.61
2:D:1117:GLU:HG2	2:L:1146:PRO:HB2	1.83	0.61
2:J:1097:ILE:HD12	2:J:1141:ALA:HB3	1.83	0.61
2:F:1113:GLN:HB3	2:J:1147:LYS:HB2	1.82	0.61
2:A:1097:ILE:HD12	2:A:1141:ALA:HB3	1.82	0.61
2:A:1146:PRO:HB2	2:H:1117:GLU:CG	2.31	0.61
2:D:358:TYR:HE1	2:H:361:SER:OG	1.83	0.61
2:H:1097:ILE:HD12	2:H:1141:ALA:HB3	1.82	0.61
2:D:1232:ARG:NH2	2:L:1235:PHE:CE2	2.68	0.61
2:J:1094:GLU:HB2	2:J:1144:TRP:CZ2	2.35	0.61
2:D:375:TRP:CE2	2:H:375:TRP:CD1	2.88	0.61
2:A:1457:GLU:HG2	2:H:1406:PHE:HE2	1.64	0.61
2:F:1402:HIS:CE1	2:J:1692:ASP:CG	2.79	0.60
2:A:1232:ARG:NH2	2:H:1235:PHE:CE2	2.68	0.60
1:G:23:PRO:HD3	1:K:43:PHE:CE2	2.35	0.60
2:D:1146:PRO:HB2	2:L:1117:GLU:CG	2.31	0.60
2:F:822:ARG:HH22	2:L:751:ILE:HA	1.67	0.60
2:D:1097:ILE:HD12	2:D:1141:ALA:HB3	1.83	0.60
2:D:368:LEU:CD2	2:H:372:LEU:HD11	2.30	0.60
2:F:1402:HIS:HE2	2:J:1692:ASP:H	1.49	0.60
2:F:1692:ASP:H	2:J:1402:HIS:HE2	1.48	0.60
2:A:1679:TYR:CZ	2:H:1383:LYS:HD2	2.37	0.60
2:D:379:HIS:HE1	2:H:379:HIS:HE1	1.48	0.60
2:F:751:ILE:HA	2:L:822:ARG:HH22	1.67	0.60
2:F:1097:ILE:HD12	2:F:1141:ALA:HB3	1.82	0.60
2:D:787:THR:CB	1:G:1751:HIS:O	2.50	0.60
2:D:751:ILE:HA	2:H:822:ARG:NH2	2.16	0.60
2:A:368:LEU:HD22	2:J:372:LEU:CD1	2.31	0.59
2:A:372:LEU:HD11	2:J:368:LEU:HD22	1.82	0.59
2:L:1097:ILE:HD12	2:L:1141:ALA:HB3	1.82	0.59
2:A:1692:ASP:CG	2:H:1402:HIS:CE1	2.80	0.59
2:A:787:THR:O	1:I:1753:GLY:HA3	2.03	0.59
2:F:1383:LYS:CD	2:J:1679:TYR:OH	2.49	0.59
2:A:1147:LYS:HD2	2:H:1113:GLN:OE1	2.02	0.59
1:C:43:PHE:CE2	1:E:23:PRO:CG	2.86	0.59
2:F:1235:PHE:CE2	2:J:1232:ARG:NH2	2.71	0.59
1:G:2061:VAL:HG21	2:H:13:LEU:HD11	1.83	0.59
2:D:1147:LYS:HD2	2:L:1113:GLN:OE1	2.03	0.59
2:A:1113:GLN:OE1	2:H:1147:LYS:HD2	2.04	0.58
1:G:1333:GLU:OE1	1:K:330:SER:N	2.32	0.58
1:K:601:LEU:HD11	1:K:657:ARG:NH2	2.18	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1691:PRO:HD3	2:H:1400:ARG:HB2	1.85	0.58
2:F:1692:ASP:CG	2:J:1402:HIS:CE1	2.82	0.58
1:G:601:LEU:HD11	1:G:657:ARG:NH2	2.18	0.58
2:D:1117:GLU:CD	2:L:1146:PRO:HB2	2.29	0.58
1:B:601:LEU:HD11	1:B:657:ARG:NH2	2.18	0.58
1:B:1333:GLU:OE2	1:E:329:THR:HG22	2.03	0.58
1:C:601:LEU:HD11	1:C:657:ARG:NH2	2.18	0.58
1:G:43:PHE:HE2	1:I:23:PRO:CG	2.07	0.58
1:I:601:LEU:HD11	1:I:657:ARG:NH2	2.18	0.58
1:E:601:LEU:HD11	1:E:657:ARG:NH2	2.18	0.57
1:G:1702:SER:HB2	2:H:49:PRO:HG2	1.85	0.57
2:H:338:GLN:O	2:H:342:LEU:HB2	2.04	0.57
1:B:1557:PRO:HA	1:B:1662:VAL:HG13	1.87	0.57
2:D:1692:ASP:CG	2:L:1402:HIS:CE1	2.82	0.57
1:E:1557:PRO:HA	1:E:1662:VAL:HG13	1.87	0.57
2:F:1406:PHE:CE2	2:J:1457:GLU:HG2	2.39	0.57
1:G:43:PHE:CE2	1:I:23:PRO:HD3	2.39	0.57
1:I:329:THR:HG22	1:K:1333:GLU:OE2	2.04	0.57
2:F:1556:HIS:CE1	2:F:1558:LYS:HA	2.39	0.57
2:H:1556:HIS:CE1	2:H:1558:LYS:HA	2.39	0.57
1:G:1557:PRO:HA	1:G:1662:VAL:HG13	1.86	0.57
2:A:338:GLN:O	2:A:342:LEU:HB2	2.04	0.57
2:F:338:GLN:O	2:F:342:LEU:HB2	2.04	0.57
2:F:822:ARG:NH2	2:L:751:ILE:HA	2.20	0.57
1:I:1557:PRO:HA	1:I:1662:VAL:HG13	1.86	0.57
2:J:1556:HIS:CE1	2:J:1558:LYS:HA	2.39	0.57
2:A:1117:GLU:CD	2:H:1146:PRO:HB2	2.28	0.57
2:L:338:GLN:O	2:L:342:LEU:HB2	2.04	0.57
2:D:787:THR:OG1	1:G:1751:HIS:O	2.18	0.57
2:A:1117:GLU:HG2	2:H:1146:PRO:CB	2.35	0.57
2:D:1556:HIS:CE1	2:D:1558:LYS:HA	2.39	0.57
2:J:338:GLN:O	2:J:342:LEU:HB2	2.04	0.57
1:K:1557:PRO:HA	1:K:1662:VAL:HG13	1.87	0.57
2:A:1146:PRO:HB2	2:H:1117:GLU:CD	2.30	0.57
1:C:1557:PRO:HA	1:C:1662:VAL:HG13	1.87	0.57
2:D:338:GLN:O	2:D:342:LEU:HB2	2.04	0.57
2:D:751:ILE:HA	2:H:822:ARG:HH22	1.69	0.57
2:D:1146:PRO:HB2	2:L:1117:GLU:CD	2.30	0.57
2:D:1383:LYS:CD	2:L:1679:TYR:OH	2.52	0.57
2:A:375:TRP:CE2	2:J:375:TRP:CD1	2.93	0.56
1:E:1012:GLN:OE1	1:E:1013:ASP:N	2.37	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:340:LEU:HD12	2:L:340:LEU:HD12	1.87	0.56
2:A:1556:HIS:CE1	2:A:1558:LYS:HA	2.39	0.56
2:L:1556:HIS:CE1	2:L:1558:LYS:HA	2.39	0.56
2:D:372:LEU:HD11	2:H:368:LEU:HD22	1.87	0.56
2:D:379:HIS:CE1	2:H:379:HIS:HE1	2.24	0.56
2:F:361:SER:HB3	2:L:361:SER:HB3	1.87	0.56
2:D:1113:GLN:OE1	2:L:1147:LYS:HD2	2.06	0.56
2:D:751:ILE:HD13	2:H:828:TRP:CE2	2.41	0.56
2:A:751:ILE:HD13	2:J:828:TRP:CE2	2.41	0.56
2:A:1406:PHE:CE2	2:H:1457:GLU:HG2	2.41	0.56
2:F:1117:GLU:HG2	2:J:1146:PRO:HB2	1.87	0.56
2:A:335:LEU:HD13	2:L:342:LEU:HD22	1.88	0.56
1:K:1012:GLN:OE1	1:K:1013:ASP:N	2.37	0.56
2:A:751:ILE:CG2	2:J:828:TRP:CD1	2.80	0.56
2:F:1113:GLN:NE2	2:J:1149:LEU:HD21	2.21	0.56
1:G:1012:GLN:OE1	1:G:1013:ASP:N	2.37	0.56
2:D:1691:PRO:HD3	2:L:1400:ARG:HB2	1.87	0.56
2:F:751:ILE:HA	2:L:822:ARG:NH2	2.20	0.56
2:F:1457:GLU:HG2	2:J:1406:PHE:CE2	2.40	0.56
2:D:751:ILE:CG2	2:H:828:TRP:CD1	2.80	0.55
2:F:358:TYR:HA	2:L:358:TYR:HD1	1.71	0.55
2:A:787:THR:O	1:I:1753:GLY:CA	2.54	0.55
1:G:1333:GLU:CD	1:K:329:THR:HB	2.32	0.55
2:D:358:TYR:CD1	2:H:361:SER:OG	2.58	0.55
2:A:361:SER:HB3	2:J:361:SER:HB3	1.88	0.55
1:C:1012:GLN:OE1	1:C:1013:ASP:N	2.37	0.55
2:D:787:THR:O	1:G:1753:GLY:HA3	2.07	0.55
1:G:890:GLU:CD	1:G:890:GLU:H	2.15	0.55
1:I:890:GLU:CD	1:I:890:GLU:H	2.15	0.55
2:A:1406:PHE:HE2	2:H:1457:GLU:HG2	1.72	0.55
1:C:890:GLU:H	1:C:890:GLU:CD	2.15	0.55
2:D:1117:GLU:HG2	2:L:1146:PRO:CB	2.37	0.55
1:E:890:GLU:CD	1:E:890:GLU:H	2.15	0.55
2:D:375:TRP:CD1	2:H:375:TRP:CE2	2.95	0.55
2:D:379:HIS:CE1	2:H:379:HIS:CE1	2.94	0.55
2:F:358:TYR:HD1	2:L:358:TYR:HA	1.71	0.55
1:B:329:THR:HB	1:C:1333:GLU:OE2	2.06	0.54
2:F:1146:PRO:HB2	2:J:1117:GLU:HG2	1.89	0.54
2:F:822:ARG:NH2	2:L:751:ILE:CB	2.71	0.54
1:G:1477:ASP:CG	1:G:1527:GLN:HE21	2.15	0.54
1:B:890:GLU:CD	1:B:890:GLU:H	2.15	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1751:HIS:O	2:H:787:THR:CB	2.55	0.54
1:K:890:GLU:H	1:K:890:GLU:CD	2.15	0.54
1:B:1477:ASP:CG	1:B:1527:GLN:HE21	2.15	0.54
1:K:1477:ASP:CG	1:K:1527:GLN:HE21	2.15	0.54
2:F:358:TYR:HE1	2:L:361:SER:OG	1.90	0.54
2:F:751:ILE:CB	2:L:822:ARG:NH2	2.71	0.53
1:E:1477:ASP:CG	1:E:1527:GLN:HE21	2.15	0.53
2:A:379:HIS:HE1	2:J:379:HIS:HE1	1.56	0.53
1:C:1477:ASP:CG	1:C:1527:GLN:HE21	2.15	0.53
2:A:751:ILE:HA	2:J:822:ARG:NH2	2.23	0.53
1:C:1172:ARG:HH12	1:C:1209:PRO:HA	1.74	0.53
2:D:751:ILE:CB	2:H:826:GLU:OE2	2.43	0.53
1:K:1172:ARG:HH12	1:K:1209:PRO:HA	1.74	0.53
2:A:1113:GLN:NE2	2:H:1149:LEU:HD21	2.24	0.53
1:C:92:ASP:CG	1:C:98:TYR:HB2	2.34	0.53
2:D:787:THR:O	1:G:1753:GLY:CA	2.56	0.53
2:F:379:HIS:HE1	2:L:379:HIS:CE1	2.18	0.53
1:B:1172:ARG:HH12	1:B:1209:PRO:HA	1.74	0.53
1:E:92:ASP:CG	1:E:98:TYR:HB2	2.33	0.53
1:G:1794:TYR:CG	1:G:1795:THR:N	2.77	0.53
1:B:1012:GLN:OE1	1:B:1013:ASP:N	2.37	0.53
2:F:361:SER:OG	2:L:358:TYR:HE1	1.90	0.53
1:K:92:ASP:CG	1:K:98:TYR:HB2	2.34	0.53
1:B:92:ASP:CG	1:B:98:TYR:HB2	2.34	0.53
1:C:1751:HIS:O	2:H:787:THR:HB	2.08	0.53
1:E:1794:TYR:CG	1:E:1795:THR:N	2.77	0.53
2:F:1259:MET:O	2:J:1384:ILE:HG12	2.08	0.53
1:I:1172:ARG:HH12	1:I:1209:PRO:HA	1.74	0.53
1:I:1477:ASP:CG	1:I:1527:GLN:HE21	2.15	0.52
1:I:92:ASP:CG	1:I:98:TYR:HB2	2.34	0.52
2:D:787:THR:HB	1:G:1751:HIS:O	2.10	0.52
2:F:1384:ILE:HG12	2:J:1259:MET:O	2.09	0.52
1:G:1172:ARG:HH12	1:G:1209:PRO:HA	1.74	0.52
1:I:1794:TYR:CG	1:I:1795:THR:N	2.77	0.52
2:A:1231:HIS:CE1	2:H:1228:ARG:CA	2.91	0.52
2:D:358:TYR:HA	2:H:358:TYR:HD1	1.75	0.52
2:D:1146:PRO:HG2	2:L:1118:HIS:CE1	2.44	0.52
1:B:1794:TYR:CG	1:B:1795:THR:N	2.77	0.52
2:F:1149:LEU:HD21	2:J:1113:GLN:NE2	2.24	0.52
2:A:1679:TYR:CZ	2:H:1383:LYS:CD	2.93	0.52
2:A:1117:GLU:CG	2:H:1146:PRO:HB2	2.38	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1172:ARG:HH12	1:E:1209:PRO:HA	1.74	0.52
2:F:1232:ARG:NH2	2:J:1235:PHE:CE2	2.73	0.52
1:G:92:ASP:CG	1:G:98:TYR:HB2	2.34	0.52
2:D:1458:TYR:HA	2:L:1406:PHE:CE2	2.45	0.52
1:K:1794:TYR:CG	1:K:1795:THR:N	2.77	0.52
2:A:358:TYR:HE1	2:J:361:SER:OG	1.93	0.51
2:D:335:LEU:HD13	2:J:342:LEU:HD22	1.92	0.51
2:H:332:GLN:HB3	2:H:336:PHE:CE2	2.46	0.51
1:C:329:THR:HB	1:E:1333:GLU:CD	2.35	0.51
2:D:332:GLN:HB3	2:D:336:PHE:CE2	2.46	0.51
2:F:332:GLN:HB3	2:F:336:PHE:CE2	2.46	0.51
2:F:361:SER:CB	2:L:361:SER:HB3	2.41	0.51
2:F:368:LEU:HD22	2:L:372:LEU:CD1	2.39	0.51
2:L:332:GLN:HB3	2:L:336:PHE:CE2	2.46	0.51
1:C:1794:TYR:CG	1:C:1795:THR:N	2.77	0.51
1:I:1012:GLN:OE1	1:I:1013:ASP:N	2.37	0.51
2:A:751:ILE:HD13	2:J:828:TRP:NE1	2.26	0.51
2:F:372:LEU:CD1	2:L:368:LEU:HD22	2.39	0.51
2:D:1117:GLU:CG	2:L:1146:PRO:HB2	2.40	0.51
1:G:601:LEU:HD11	1:G:657:ARG:HH22	1.76	0.51
2:D:751:ILE:HG13	2:H:822:ARG:NH2	2.26	0.51
2:J:332:GLN:HB3	2:J:336:PHE:CE2	2.46	0.51
2:A:1383:LYS:HD2	2:H:1679:TYR:CZ	2.46	0.50
2:D:1210:VAL:C	2:D:1265:SER:HG	2.18	0.50
2:H:1210:VAL:C	2:H:1265:SER:HG	2.17	0.50
1:B:1523:LYS:HE3	1:B:2031:THR:O	2.11	0.50
2:A:375:TRP:CD1	2:J:375:TRP:CE2	2.99	0.50
1:E:601:LEU:HD11	1:E:657:ARG:HH22	1.76	0.50
1:I:1523:LYS:HE3	1:I:2031:THR:O	2.11	0.50
2:A:1146:PRO:HG2	2:H:1118:HIS:CE1	2.46	0.50
2:A:1692:ASP:H	2:H:1402:HIS:HE2	1.60	0.50
2:H:491:ALA:HB3	2:H:869:GLN:NE2	2.27	0.50
2:A:332:GLN:HB3	2:A:336:PHE:CE2	2.46	0.50
1:C:601:LEU:HD11	1:C:657:ARG:HH22	1.76	0.50
2:D:751:ILE:HD13	2:H:828:TRP:NE1	2.26	0.50
2:F:1383:LYS:HD2	2:J:1679:TYR:CZ	2.47	0.50
2:L:1210:VAL:C	2:L:1265:SER:HG	2.18	0.50
2:D:491:ALA:HB3	2:D:869:GLN:NE2	2.27	0.50
1:B:329:THR:HG22	1:C:1333:GLU:OE2	2.11	0.50
2:A:491:ALA:HB3	2:A:869:GLN:NE2	2.27	0.50
1:C:1523:LYS:HE3	1:C:2031:THR:O	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:788:ARG:HD2	1:K:1751:HIS:CG	2.46	0.50
1:B:1702:SER:HB2	2:A:49:PRO:HG2	1.93	0.50
2:A:751:ILE:HA	2:J:822:ARG:HH22	1.76	0.50
2:F:1758:THR:HG21	2:F:1786:GLN:HA	1.94	0.50
2:J:1210:VAL:C	2:J:1265:SER:HG	2.18	0.50
1:K:1523:LYS:HE3	1:K:2031:THR:O	2.11	0.50
2:F:361:SER:HB3	2:L:361:SER:CB	2.41	0.49
2:F:1146:PRO:O	2:J:1117:GLU:HG2	2.12	0.49
2:F:1210:VAL:C	2:F:1265:SER:HG	2.18	0.49
1:G:329:THR:HG22	1:I:1333:GLU:OE2	2.12	0.49
1:G:1523:LYS:HE3	1:G:2031:THR:O	2.11	0.49
1:E:1523:LYS:HE3	1:E:2031:THR:O	2.11	0.49
2:A:1210:VAL:C	2:A:1265:SER:HG	2.18	0.49
2:H:1758:THR:HG21	2:H:1786:GLN:HA	1.94	0.49
2:L:491:ALA:HB3	2:L:869:GLN:NE2	2.27	0.49
1:E:1751:HIS:CG	2:L:788:ARG:HD2	2.47	0.49
1:I:337:GLN:HB2	1:K:1569:LYS:HE3	1.95	0.49
2:J:491:ALA:HB3	2:J:869:GLN:NE2	2.27	0.49
1:B:601:LEU:HD11	1:B:657:ARG:HH22	1.76	0.49
2:D:1235:PHE:CE1	2:L:1092:LEU:HG	2.47	0.49
2:F:1457:GLU:HG2	2:J:1406:PHE:HE2	1.77	0.49
2:J:1758:THR:HG21	2:J:1786:GLN:HA	1.94	0.49
2:F:375:TRP:CD1	2:L:375:TRP:NE1	2.81	0.49
2:F:491:ALA:HB3	2:F:869:GLN:NE2	2.27	0.49
2:A:1219:SER:HB2	2:A:1302:PHE:CZ	2.48	0.49
1:C:2067:SER:OG	2:D:16:GLU:OE2	2.28	0.49
2:D:1219:SER:HB2	2:D:1302:PHE:CZ	2.48	0.49
2:J:1219:SER:HB2	2:J:1302:PHE:CZ	2.48	0.49
1:B:1569:LYS:HE3	1:E:337:GLN:HB2	1.95	0.49
2:D:361:SER:OG	2:H:358:TYR:CE1	2.66	0.49
2:D:1758:THR:HG21	2:D:1786:GLN:HA	1.94	0.49
2:F:361:SER:CB	2:L:361:SER:CB	2.91	0.49
2:F:1092:LEU:HG	2:J:1235:PHE:CE1	2.47	0.49
1:I:601:LEU:HD11	1:I:657:ARG:HH22	1.76	0.49
2:L:1219:SER:HB2	2:L:1302:PHE:CZ	2.48	0.49
1:B:1150:PRO:HA	1:B:1200:ARG:CZ	2.43	0.49
2:A:1383:LYS:CD	2:H:1679:TYR:CZ	2.96	0.49
1:K:601:LEU:HD11	1:K:657:ARG:HH22	1.76	0.49
1:B:1751:HIS:CG	2:J:788:ARG:HD2	2.47	0.49
2:A:1679:TYR:CE1	2:H:1383:LYS:HD3	2.48	0.49
2:A:1758:THR:HG21	2:A:1786:GLN:HA	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1150:PRO:HA	1:C:1200:ARG:CZ	2.43	0.49
1:C:1751:HIS:CE1	2:H:788:ARG:HD2	2.48	0.49
2:D:788:ARG:HD2	1:G:1751:HIS:CE1	2.48	0.49
1:G:1150:PRO:HA	1:G:1200:ARG:CZ	2.43	0.49
1:I:1150:PRO:HA	1:I:1200:ARG:CZ	2.43	0.48
2:D:339:GLN:HA	2:D:342:LEU:HB3	1.95	0.48
2:D:1117:GLU:HG2	2:L:1146:PRO:O	2.12	0.48
2:D:1679:TYR:OH	2:L:1383:LYS:CD	2.60	0.48
2:F:1219:SER:HB2	2:F:1302:PHE:CZ	2.48	0.48
2:H:1219:SER:HB2	2:H:1302:PHE:CZ	2.48	0.48
2:J:339:GLN:HA	2:J:342:LEU:HB3	1.95	0.48
2:A:339:GLN:HA	2:A:342:LEU:HB3	1.95	0.48
2:D:788:ARG:HD2	1:G:1751:HIS:CD2	2.48	0.48
2:F:375:TRP:NE1	2:L:375:TRP:CD1	2.80	0.48
1:G:329:THR:HB	1:I:1333:GLU:OE2	2.13	0.48
1:G:2056:GLU:CD	1:G:2056:GLU:H	2.22	0.48
1:K:2056:GLU:CD	1:K:2056:GLU:H	2.22	0.48
2:L:1758:THR:HG21	2:L:1786:GLN:HA	1.94	0.48
2:A:361:SER:CB	2:J:361:SER:HB3	2.43	0.48
2:A:368:LEU:CD2	2:J:372:LEU:HD11	2.36	0.48
1:B:2056:GLU:CD	1:B:2056:GLU:H	2.22	0.48
2:D:787:THR:HA	1:G:1753:GLY:O	2.13	0.48
2:A:1692:ASP:CG	2:H:1402:HIS:HE1	2.22	0.48
2:A:1742:VAL:HG22	2:A:1743:ASN:H	1.78	0.48
2:H:339:GLN:HA	2:H:342:LEU:HB3	1.95	0.48
2:F:1679:TYR:CZ	2:J:1383:LYS:HD2	2.48	0.48
1:B:23:PRO:CG	1:E:43:PHE:CE2	2.95	0.48
2:A:1148:ALA:HB3	2:H:1116:ARG:HG2	1.96	0.48
1:C:1758:LYS:HE2	2:H:885:ASP:OD1	2.13	0.48
1:C:2056:GLU:H	1:C:2056:GLU:CD	2.22	0.48
2:F:1400:ARG:HB2	2:J:1691:PRO:HD3	1.96	0.48
2:A:787:THR:HB	1:I:1753:GLY:O	2.14	0.47
2:D:1113:GLN:NE2	2:L:1149:LEU:HD21	2.29	0.47
2:D:1117:GLU:OE1	2:L:1146:PRO:HB2	2.14	0.47
1:K:1150:PRO:HA	1:K:1200:ARG:CZ	2.43	0.47
1:K:1698:THR:HA	2:L:53:LEU:HD11	1.95	0.47
2:A:379:HIS:CE1	2:J:379:HIS:CE1	3.03	0.47
1:E:2056:GLU:H	1:E:2056:GLU:CD	2.22	0.47
2:F:751:ILE:HB	2:L:822:ARG:NH2	2.29	0.47
2:F:1117:GLU:HG2	2:J:1146:PRO:O	2.14	0.47
1:G:2057:TYR:CE1	2:H:13:LEU:HD21	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:1742:VAL:HG22	2:L:1743:ASN:H	1.79	0.47
1:C:1141:LYS:HE3	1:C:1205:GLU:HG3	1.96	0.47
1:E:1150:PRO:HA	1:E:1200:ARG:CZ	2.43	0.47
1:B:43:PHE:CE2	1:C:23:PRO:HD3	2.49	0.47
1:C:43:PHE:CE2	1:E:23:PRO:CD	2.98	0.47
1:C:2080:TYR:O	2:D:5:VAL:HG11	2.14	0.47
2:D:361:SER:HB3	2:H:361:SER:HB3	1.94	0.47
1:I:2056:GLU:CD	1:I:2056:GLU:H	2.22	0.47
2:L:339:GLN:HA	2:L:342:LEU:HB3	1.95	0.47
2:F:339:GLN:HA	2:F:342:LEU:HB3	1.95	0.47
2:F:1406:PHE:HE2	2:J:1457:GLU:HG2	1.77	0.47
2:F:1742:VAL:HG22	2:F:1743:ASN:H	1.79	0.47
1:G:1141:LYS:HE3	1:G:1205:GLU:HG3	1.97	0.47
2:H:1742:VAL:HG22	2:H:1743:ASN:H	1.78	0.47
1:K:607:ALA:HB2	1:K:812:LEU:HD13	1.97	0.47
1:B:1319:GLU:N	1:B:1319:GLU:CD	2.73	0.47
2:A:379:HIS:CE1	2:J:379:HIS:HE1	2.33	0.47
2:A:1117:GLU:HG2	2:H:1146:PRO:O	2.13	0.47
2:A:1228:ARG:CA	2:H:1231:HIS:CE1	2.95	0.47
2:D:1457:GLU:HG2	2:L:1406:PHE:CE2	2.50	0.47
1:E:1698:THR:HA	2:F:53:LEU:HD11	1.95	0.47
2:F:358:TYR:CD1	2:L:361:SER:OG	2.67	0.47
2:F:678:THR:HB	2:F:709:PHE:HB3	1.97	0.47
2:F:822:ARG:NH2	2:L:751:ILE:HB	2.29	0.47
1:K:1319:GLU:CD	1:K:1319:GLU:N	2.73	0.47
2:D:1679:TYR:CZ	2:L:1383:LYS:HD2	2.50	0.47
2:F:822:ARG:NH2	2:L:751:ILE:CA	2.78	0.47
1:I:1141:LYS:HE3	1:I:1205:GLU:CD	2.40	0.47
2:J:1742:VAL:HG22	2:J:1743:ASN:H	1.78	0.47
1:K:1141:LYS:HE3	1:K:1205:GLU:CD	2.40	0.47
1:C:1319:GLU:N	1:C:1319:GLU:CD	2.73	0.47
1:E:1141:LYS:HE3	1:E:1205:GLU:CD	2.40	0.47
2:H:678:THR:HB	2:H:709:PHE:HB3	1.97	0.47
1:B:970:ARG:HH21	1:B:1013:ASP:CG	2.23	0.47
2:A:358:TYR:CD1	2:J:361:SER:OG	2.65	0.47
1:I:1319:GLU:CD	1:I:1319:GLU:N	2.73	0.47
1:K:1141:LYS:HE3	1:K:1205:GLU:HG3	1.97	0.47
2:D:1148:ALA:HB3	2:L:1116:ARG:HG2	1.97	0.46
1:E:1141:LYS:HE3	1:E:1205:GLU:HG3	1.96	0.46
2:F:751:ILE:HG13	2:L:822:ARG:NH2	2.30	0.46
2:F:751:ILE:CA	2:L:822:ARG:NH2	2.78	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1319:GLU:N	1:E:1319:GLU:CD	2.73	0.46
1:I:970:ARG:HH21	1:I:1013:ASP:CG	2.23	0.46
2:A:1117:GLU:OE1	2:H:1146:PRO:HB2	2.15	0.46
1:C:1141:LYS:HE3	1:C:1205:GLU:CD	2.40	0.46
2:D:1245:LEU:HD22	2:L:1312:GLU:HB2	1.98	0.46
2:D:1742:VAL:HG22	2:D:1743:ASN:H	1.79	0.46
2:F:375:TRP:HB2	2:L:375:TRP:CZ3	2.50	0.46
2:F:1235:PHE:CE1	2:J:1092:LEU:HG	2.51	0.46
1:G:1141:LYS:HE3	1:G:1205:GLU:CD	2.40	0.46
2:J:678:THR:HB	2:J:709:PHE:HB3	1.97	0.46
2:A:1235:PHE:CE2	2:H:1232:ARG:NH2	2.78	0.46
1:C:607:ALA:HB2	1:C:812:LEU:HD13	1.97	0.46
2:D:678:THR:HB	2:D:709:PHE:HB3	1.97	0.46
2:F:375:TRP:CZ3	2:L:375:TRP:HB2	2.50	0.46
1:G:1319:GLU:N	1:G:1319:GLU:CD	2.73	0.46
1:B:329:THR:CB	1:C:1333:GLU:OE2	2.63	0.46
1:B:1141:LYS:HE3	1:B:1205:GLU:CD	2.40	0.46
1:B:1141:LYS:HE3	1:B:1205:GLU:HG3	1.96	0.46
1:B:904:ILE:HG21	1:B:924:VAL:HG11	1.98	0.46
2:A:1235:PHE:CE1	2:H:1092:LEU:HG	2.50	0.46
2:D:340:LEU:HD12	2:H:340:LEU:HD12	1.97	0.46
1:E:607:ALA:HB2	1:E:812:LEU:HD13	1.97	0.46
1:G:970:ARG:HH21	1:G:1013:ASP:CG	2.23	0.46
1:C:970:ARG:HH21	1:C:1013:ASP:CG	2.23	0.46
2:F:1146:PRO:HB2	2:J:1117:GLU:CD	2.41	0.46
2:A:1402:HIS:HE2	2:H:1692:ASP:H	1.63	0.46
2:D:361:SER:CB	2:H:361:SER:HB3	2.46	0.46
2:D:751:ILE:CB	2:H:822:ARG:NH2	2.79	0.46
2:D:1147:LYS:HA	2:L:1117:GLU:HB2	1.97	0.46
1:E:640:LYS:HE2	1:E:644:GLU:OE1	2.16	0.46
1:I:1141:LYS:HE3	1:I:1205:GLU:HG3	1.97	0.46
1:B:1333:GLU:OE2	1:E:329:THR:CG2	2.64	0.46
2:A:788:ARG:HD2	1:I:1751:HIS:CG	2.51	0.46
2:A:1147:LYS:HA	2:H:1117:GLU:HB2	1.96	0.46
1:E:80:MET:HG2	1:E:143:ALA:HB2	1.98	0.46
1:I:607:ALA:HB2	1:I:812:LEU:HD13	1.97	0.46
1:K:80:MET:HG2	1:K:143:ALA:HB2	1.98	0.46
1:K:904:ILE:HG21	1:K:924:VAL:HG11	1.98	0.46
1:B:1569:LYS:HE3	1:E:333:PRO:O	2.16	0.45
1:C:1751:HIS:O	2:H:787:THR:OG1	2.28	0.45
2:F:822:ARG:NH2	2:L:751:ILE:CG1	2.79	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1341:THR:HG23	2:H:1588:ASP:HA	1.98	0.45
1:I:43:PHE:CE2	1:K:23:PRO:CG	2.96	0.45
1:K:601:LEU:HD11	1:K:657:ARG:CZ	2.46	0.45
1:C:80:MET:HG2	1:C:143:ALA:HB2	1.98	0.45
1:C:2061:VAL:HG21	2:D:13:LEU:HD11	1.98	0.45
2:D:788:ARG:HD2	1:G:1751:HIS:ND1	2.31	0.45
2:F:1117:GLU:HB2	2:J:1147:LYS:HA	1.97	0.45
2:F:1147:LYS:HA	2:J:1117:GLU:HB2	1.98	0.45
1:G:601:LEU:HD11	1:G:657:ARG:CZ	2.46	0.45
1:I:329:THR:CG2	1:K:1333:GLU:OE2	2.65	0.45
1:B:607:ALA:HB2	1:B:812:LEU:HD13	1.97	0.45
2:A:1146:PRO:HB2	2:H:1117:GLU:OE1	2.17	0.45
2:D:375:TRP:CD1	2:H:375:TRP:NE1	2.85	0.45
1:E:47:ARG:NH2	1:E:98:TYR:OH	2.50	0.45
2:F:375:TRP:CE2	2:L:375:TRP:CG	3.05	0.45
2:F:1402:HIS:HE1	2:J:1692:ASP:CG	2.25	0.45
1:G:640:LYS:HE2	1:G:644:GLU:OE1	2.16	0.45
1:K:970:ARG:HH21	1:K:1013:ASP:CG	2.23	0.45
1:B:601:LEU:HD11	1:B:657:ARG:CZ	2.47	0.45
1:C:792:TYR:HA	1:C:797:TRP:CD1	2.52	0.45
2:D:1231:HIS:CE1	2:L:1228:ARG:CA	2.97	0.45
1:E:601:LEU:HD11	1:E:657:ARG:CZ	2.46	0.45
2:F:1117:GLU:CD	2:J:1146:PRO:HB2	2.42	0.45
1:I:640:LYS:HE2	1:I:644:GLU:OE1	2.16	0.45
2:L:678:THR:HB	2:L:709:PHE:HB3	1.97	0.45
2:A:678:THR:HB	2:A:709:PHE:HB3	1.97	0.45
1:E:970:ARG:HH21	1:E:1013:ASP:CG	2.23	0.45
1:G:607:ALA:HB2	1:G:812:LEU:HD13	1.97	0.45
1:I:333:PRO:O	1:K:1569:LYS:HE3	2.17	0.45
1:I:904:ILE:HG21	1:I:924:VAL:HG11	1.98	0.45
1:C:47:ARG:NH2	1:C:98:TYR:OH	2.50	0.45
1:C:932:TYR:CZ	1:C:1009:ILE:HA	2.52	0.45
2:D:1341:THR:HG23	2:D:1588:ASP:HA	1.98	0.45
2:F:1117:GLU:HG2	2:J:1146:PRO:CB	2.46	0.45
1:I:80:MET:HG2	1:I:143:ALA:HB2	1.98	0.45
1:K:792:TYR:HA	1:K:797:TRP:CD1	2.52	0.45
1:B:43:PHE:CE2	1:C:23:PRO:CG	3.00	0.45
1:B:47:ARG:NH2	1:B:98:TYR:OH	2.50	0.45
1:B:329:THR:CG2	1:C:1333:GLU:OE2	2.65	0.45
1:B:1319:GLU:CD	1:B:1319:GLU:H	2.25	0.45
2:A:361:SER:OG	2:J:358:TYR:CE1	2.70	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:487:TYR:CD2	2:A:667:GLY:HA2	2.52	0.45
1:C:904:ILE:HG21	1:C:924:VAL:HG11	1.98	0.45
2:F:822:ARG:NH2	2:L:751:ILE:HG13	2.30	0.45
1:G:80:MET:HG2	1:G:143:ALA:HB2	1.98	0.45
2:J:1341:THR:HG23	2:J:1588:ASP:HA	1.98	0.45
2:L:487:TYR:CD2	2:L:667:GLY:HA2	2.52	0.45
2:D:375:TRP:CG	2:H:375:TRP:CE2	3.04	0.45
2:D:1456:GLU:HG2	2:D:1738:ARG:HH12	1.82	0.45
2:F:361:SER:OG	2:L:358:TYR:CD1	2.66	0.45
2:F:751:ILE:CG1	2:L:822:ARG:NH2	2.80	0.45
1:K:932:TYR:CZ	1:K:1009:ILE:HA	2.52	0.45
1:C:601:LEU:HD11	1:C:657:ARG:CZ	2.46	0.45
2:D:487:TYR:CD2	2:D:667:GLY:HA2	2.52	0.45
2:F:1456:GLU:HG2	2:F:1738:ARG:HH12	1.82	0.45
1:G:904:ILE:HG21	1:G:924:VAL:HG11	1.98	0.45
2:H:1432:GLU:CD	2:H:1801:LYS:HZ3	2.25	0.45
2:H:1456:GLU:HG2	2:H:1738:ARG:HH12	1.82	0.45
1:B:43:PHE:CE2	1:C:23:PRO:CD	3.00	0.45
2:A:1456:GLU:HG2	2:A:1738:ARG:HH12	1.82	0.45
1:C:1751:HIS:ND1	2:H:788:ARG:HD2	2.32	0.45
2:F:1432:GLU:CD	2:F:1801:LYS:HZ3	2.25	0.45
1:G:330:SER:OG	1:I:1630:ASN:ND2	2.49	0.45
1:G:792:TYR:HA	1:G:797:TRP:CD1	2.52	0.45
2:H:487:TYR:CD2	2:H:667:GLY:HA2	2.52	0.45
1:K:47:ARG:NH2	1:K:98:TYR:OH	2.50	0.45
1:K:1319:GLU:CD	1:K:1319:GLU:H	2.25	0.45
2:L:1341:THR:HG23	2:L:1588:ASP:HA	1.98	0.45
1:B:792:TYR:HA	1:B:797:TRP:CD1	2.51	0.44
1:C:640:LYS:HE2	1:C:644:GLU:OE1	2.16	0.44
2:F:487:TYR:CD2	2:F:667:GLY:HA2	2.52	0.44
1:G:47:ARG:NH2	1:G:98:TYR:OH	2.50	0.44
2:J:487:TYR:CD2	2:J:667:GLY:HA2	2.52	0.44
2:L:1456:GLU:HG2	2:L:1738:ARG:HH12	1.82	0.44
1:B:80:MET:HG2	1:B:143:ALA:HB2	1.98	0.44
1:C:701:GLU:CD	1:C:701:GLU:H	2.26	0.44
1:C:2053:LEU:HD21	2:D:10:ALA:HA	1.98	0.44
2:D:1146:PRO:HB2	2:L:1117:GLU:OE1	2.17	0.44
2:D:1726:VAL:HG22	2:D:1727:SER:H	1.82	0.44
1:E:904:ILE:HG21	1:E:924:VAL:HG11	1.98	0.44
2:F:1117:GLU:CG	2:J:1146:PRO:HB2	2.46	0.44
2:F:1691:PRO:HD3	2:J:1400:ARG:HB2	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:601:LEU:HD11	1:I:657:ARG:CZ	2.47	0.44
1:I:701:GLU:H	1:I:701:GLU:CD	2.26	0.44
1:I:1319:GLU:CD	1:I:1319:GLU:H	2.25	0.44
1:B:23:PRO:CD	1:E:43:PHE:CE2	3.00	0.44
1:B:640:LYS:HE2	1:B:644:GLU:OE1	2.16	0.44
2:D:375:TRP:CZ3	2:H:375:TRP:HB2	2.52	0.44
1:G:329:THR:CG2	1:I:1333:GLU:OE2	2.66	0.44
1:G:932:TYR:CZ	1:G:1009:ILE:HA	2.52	0.44
2:J:1456:GLU:HG2	2:J:1738:ARG:HH12	1.82	0.44
1:C:1319:GLU:CD	1:C:1319:GLU:H	2.25	0.44
2:D:751:ILE:HG21	2:H:828:TRP:NE1	2.30	0.44
2:D:1263:SER:OG	2:L:1384:ILE:HG13	2.17	0.44
2:F:375:TRP:CG	2:L:375:TRP:CE2	3.05	0.44
1:B:260:HIS:CE1	1:B:543:GLY:HA2	2.53	0.44
1:C:1702:SER:CB	2:D:49:PRO:HG2	2.44	0.44
2:D:751:ILE:CA	2:H:822:ARG:NH2	2.80	0.44
1:E:792:TYR:HA	1:E:797:TRP:CD1	2.52	0.44
1:E:800:LYS:HE3	1:E:801:TYR:CZ	2.52	0.44
1:E:1319:GLU:CD	1:E:1319:GLU:H	2.25	0.44
2:H:1726:VAL:HG22	2:H:1727:SER:H	1.82	0.44
1:I:47:ARG:NH2	1:I:98:TYR:OH	2.50	0.44
1:I:1698:THR:HA	2:J:53:LEU:HD11	1.98	0.44
1:K:640:LYS:HE2	1:K:644:GLU:OE1	2.16	0.44
2:L:1726:VAL:HG22	2:L:1727:SER:H	1.82	0.44
1:E:932:TYR:CZ	1:E:1009:ILE:HA	2.52	0.44
2:F:1118:HIS:CE1	2:J:1146:PRO:HG2	2.52	0.44
2:F:1341:THR:HG23	2:F:1588:ASP:HA	1.98	0.44
1:G:800:LYS:HE3	1:G:801:TYR:CZ	2.52	0.44
1:K:260:HIS:CE1	1:K:543:GLY:HA2	2.53	0.44
1:C:1461:THR:O	1:C:1465:ILE:HG13	2.18	0.44
1:G:1319:GLU:CD	1:G:1319:GLU:H	2.25	0.44
1:I:260:HIS:CE1	1:I:543:GLY:HA2	2.53	0.44
2:J:1432:GLU:CD	2:J:1801:LYS:HZ1	2.25	0.44
2:J:1557:PRO:HG3	2:J:1564:TRP:CZ3	2.53	0.44
1:B:701:GLU:H	1:B:701:GLU:CD	2.26	0.44
1:B:932:TYR:CZ	1:B:1009:ILE:HA	2.52	0.44
2:A:1234:ARG:CZ	2:H:1311:TYR:HE1	2.31	0.44
2:D:1146:PRO:HD2	2:L:1118:HIS:CE1	2.53	0.44
2:D:1557:PRO:HG3	2:D:1564:TRP:CZ3	2.53	0.44
2:F:1726:VAL:HG22	2:F:1727:SER:H	1.82	0.44
1:I:792:TYR:HA	1:I:797:TRP:CD1	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:800:LYS:HE3	1:I:801:TYR:CZ	2.52	0.44
2:L:1557:PRO:HG3	2:L:1564:TRP:CZ3	2.53	0.44
2:A:1341:THR:HG23	2:A:1588:ASP:HA	1.98	0.44
2:A:1557:PRO:HG3	2:A:1564:TRP:CZ3	2.53	0.44
2:D:1384:ILE:HG12	2:L:1259:MET:O	2.17	0.44
2:F:358:TYR:CD1	2:L:358:TYR:HA	2.51	0.44
1:I:932:TYR:CZ	1:I:1009:ILE:HA	2.52	0.44
2:A:1432:GLU:CD	2:A:1801:LYS:HZ3	2.25	0.43
1:C:1580:ASN:HD21	1:C:1648:PRO:HD3	1.83	0.43
1:E:260:HIS:CE1	1:E:543:GLY:HA2	2.53	0.43
1:G:260:HIS:CE1	1:G:543:GLY:HA2	2.53	0.43
2:H:1557:PRO:HG3	2:H:1564:TRP:CZ3	2.53	0.43
1:K:701:GLU:CD	1:K:701:GLU:H	2.26	0.43
1:B:337:GLN:HB2	1:C:1569:LYS:HE3	2.00	0.43
1:B:1580:ASN:HD21	1:B:1648:PRO:HD3	1.83	0.43
1:C:2057:TYR:CD1	2:D:13:LEU:HD21	2.53	0.43
2:F:1146:PRO:HB2	2:J:1117:GLU:CG	2.48	0.43
1:G:1461:THR:O	1:G:1465:ILE:HG13	2.18	0.43
1:K:1461:THR:O	1:K:1465:ILE:HG13	2.18	0.43
1:K:1580:ASN:HD21	1:K:1648:PRO:HD3	1.84	0.43
1:C:260:HIS:CE1	1:C:543:GLY:HA2	2.53	0.43
2:D:1117:GLU:HB2	2:L:1147:LYS:HA	2.00	0.43
2:D:1146:PRO:O	2:L:1117:GLU:HG2	2.18	0.43
1:E:1461:THR:O	1:E:1465:ILE:HG13	2.18	0.43
2:F:1557:PRO:HG3	2:F:1564:TRP:CZ3	2.53	0.43
1:I:43:PHE:CE2	1:K:23:PRO:CD	3.01	0.43
2:A:378:GLU:CD	2:J:714:VAL:HG12	2.43	0.43
2:F:372:LEU:HD11	2:L:368:LEU:CD2	2.46	0.43
1:K:800:LYS:HE3	1:K:801:TYR:CZ	2.52	0.43
1:C:800:LYS:HE3	1:C:801:TYR:CZ	2.52	0.43
2:D:1232:ARG:HH21	2:L:1235:PHE:HE2	1.59	0.43
1:E:1580:ASN:HD21	1:E:1648:PRO:HD3	1.83	0.43
1:B:800:LYS:HE3	1:B:801:TYR:CZ	2.52	0.43
2:A:751:ILE:HG13	2:J:822:ARG:NH2	2.34	0.43
2:A:1726:VAL:HG22	2:A:1727:SER:H	1.82	0.43
2:F:1373:ILE:HG21	2:F:1502:TRP:CZ2	2.54	0.43
1:G:1580:ASN:HD21	1:G:1648:PRO:HD3	1.83	0.43
1:I:962:ASP:HA	1:I:965:HIS:CD2	2.54	0.43
1:I:1580:ASN:HD21	1:I:1648:PRO:HD3	1.83	0.43
2:D:1402:HIS:CE1	2:L:1692:ASP:CG	2.96	0.43
1:E:748:ARG:NE	1:E:1072:MET:SD	2.92	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1461:THR:O	1:I:1465:ILE:HG13	2.18	0.43
2:J:1364:LEU:HD23	2:J:1646:TYR:CD2	2.54	0.43
2:J:1726:VAL:HG22	2:J:1727:SER:H	1.82	0.43
2:A:1402:HIS:CE1	2:H:1692:ASP:CG	2.97	0.43
1:C:748:ARG:NE	1:C:1072:MET:SD	2.92	0.43
2:D:1033:TYR:CG	2:D:1034:ASN:N	2.87	0.43
1:E:962:ASP:HA	1:E:965:HIS:CD2	2.54	0.43
2:F:1364:LEU:HD23	2:F:1646:TYR:CD2	2.54	0.43
1:K:748:ARG:NE	1:K:1072:MET:SD	2.92	0.43
2:D:751:ILE:CG1	2:H:822:ARG:NH2	2.82	0.43
2:F:1146:PRO:CB	2:J:1117:GLU:HG2	2.47	0.43
1:G:701:GLU:H	1:G:701:GLU:CD	2.26	0.43
2:H:1033:TYR:CG	2:H:1034:ASN:N	2.87	0.43
1:I:748:ARG:NE	1:I:1072:MET:SD	2.92	0.43
2:L:1373:ILE:HG21	2:L:1502:TRP:CZ2	2.54	0.43
2:A:751:ILE:CB	2:J:826:GLU:OE2	2.47	0.43
1:C:601:LEU:HD11	1:C:657:ARG:NH1	2.34	0.43
1:G:748:ARG:NE	1:G:1072:MET:SD	2.92	0.43
2:H:1373:ILE:HG21	2:H:1502:TRP:CZ2	2.54	0.43
2:J:1658:TYR:CE2	2:J:1662:HIS:CE1	3.07	0.43
2:A:361:SER:HB3	2:J:361:SER:CB	2.49	0.42
2:A:1658:TYR:CE2	2:A:1662:HIS:CE1	3.07	0.42
2:D:1235:PHE:CE2	2:L:1232:ARG:NH2	2.81	0.42
2:D:1658:TYR:CE2	2:D:1662:HIS:CE1	3.07	0.42
2:F:1113:GLN:OE1	2:J:1147:LYS:HD2	2.18	0.42
1:B:748:ARG:NE	1:B:1072:MET:SD	2.92	0.42
1:B:962:ASP:HA	1:B:965:HIS:CD2	2.54	0.42
2:A:1146:PRO:O	2:H:1117:GLU:HG2	2.17	0.42
2:A:1364:LEU:HD23	2:A:1646:TYR:CD2	2.54	0.42
2:D:361:SER:OG	2:H:358:TYR:HE1	2.02	0.42
1:E:1923:TYR:HB3	2:F:29:ILE:HD12	2.01	0.42
2:F:1147:LYS:HD2	2:J:1113:GLN:OE1	2.19	0.42
2:F:1272:VAL:HG21	2:J:1272:VAL:HG21	2.01	0.42
1:G:962:ASP:HA	1:G:965:HIS:CD2	2.54	0.42
1:B:1461:THR:O	1:B:1465:ILE:HG13	2.18	0.42
2:A:1373:ILE:HG21	2:A:1502:TRP:CZ2	2.54	0.42
1:C:43:PHE:CE2	1:E:23:PRO:HD3	2.55	0.42
2:D:358:TYR:HD1	2:H:358:TYR:HA	1.84	0.42
1:E:701:GLU:CD	1:E:701:GLU:H	2.26	0.42
1:G:601:LEU:HD11	1:G:657:ARG:NH1	2.34	0.42
1:G:1333:GLU:OE2	1:K:329:THR:HG22	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1364:LEU:HD23	2:H:1646:TYR:CD2	2.54	0.42
2:L:1658:TYR:CE2	2:L:1662:HIS:CE1	3.07	0.42
1:B:330:SER:H	1:C:1333:GLU:CD	2.18	0.42
2:F:358:TYR:HA	2:L:358:TYR:CD1	2.51	0.42
1:G:872:ARG:NH2	1:G:1061:ASP:OD2	2.53	0.42
2:J:1373:ILE:HG21	2:J:1502:TRP:CZ2	2.54	0.42
1:C:675:ILE:HB	1:C:676:PRO:HD3	2.02	0.42
1:C:872:ARG:NH2	1:C:1061:ASP:OD2	2.53	0.42
2:F:1146:PRO:HB2	2:J:1117:GLU:OE1	2.20	0.42
1:K:601:LEU:HD11	1:K:657:ARG:NH1	2.34	0.42
1:K:872:ARG:NH2	1:K:1061:ASP:OD2	2.53	0.42
1:C:337:GLN:HB2	1:E:1569:LYS:HE3	2.00	0.42
2:F:685:GLU:H	2:F:685:GLU:CD	2.28	0.42
1:G:409:LYS:HE3	1:G:428:PHE:O	2.20	0.42
2:H:1658:TYR:CE2	2:H:1662:HIS:CE1	3.07	0.42
1:I:409:LYS:HE3	1:I:428:PHE:O	2.20	0.42
2:L:1364:LEU:HD23	2:L:1646:TYR:CD2	2.54	0.42
1:K:675:ILE:HB	1:K:676:PRO:HD3	2.02	0.42
2:A:1033:TYR:CG	2:A:1034:ASN:N	2.87	0.42
2:F:1033:TYR:CG	2:F:1034:ASN:N	2.87	0.42
2:H:685:GLU:CD	2:H:685:GLU:H	2.28	0.42
1:I:43:PHE:CE2	1:K:23:PRO:HD3	2.55	0.42
2:L:1033:TYR:CG	2:L:1034:ASN:N	2.87	0.42
1:C:928:GLU:CD	2:D:1659:ARG:HE	2.27	0.42
1:I:1923:TYR:HB3	2:J:29:ILE:HD12	2.02	0.42
2:J:1033:TYR:CG	2:J:1034:ASN:N	2.87	0.42
1:K:409:LYS:HE3	1:K:428:PHE:O	2.20	0.42
1:B:409:LYS:HE3	1:B:428:PHE:O	2.20	0.42
1:B:872:ARG:NH2	1:B:1061:ASP:OD2	2.53	0.42
1:B:1132:GLY:HA3	1:B:1152:VAL:HG11	2.02	0.42
1:B:1344:TYR:HA	1:B:1391:LYS:HA	2.02	0.42
1:C:2053:LEU:HD11	2:D:10:ALA:HB2	2.01	0.42
2:D:1364:LEU:HD23	2:D:1646:TYR:CD2	2.54	0.42
2:D:1373:ILE:HG21	2:D:1502:TRP:CZ2	2.54	0.42
2:F:1383:LYS:NZ	2:J:1679:TYR:CE1	2.67	0.42
1:K:1338:ARG:HD3	1:K:1339:PRO:HD2	2.02	0.42
1:B:23:PRO:HD3	1:E:43:PHE:CE2	2.55	0.41
2:A:1245:LEU:HD22	2:H:1312:GLU:HB2	2.02	0.41
1:E:1854:MET:SD	1:E:1859:LEU:HA	2.60	0.41
2:F:335:LEU:HD13	2:H:342:LEU:HD22	2.02	0.41
1:G:675:ILE:HB	1:G:676:PRO:HD3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:348:THR:HB	1:I:349:PRO:HD2	2.02	0.41
1:I:601:LEU:HD11	1:I:657:ARG:NH1	2.34	0.41
2:J:685:GLU:H	2:J:685:GLU:CD	2.28	0.41
1:K:223:LYS:NZ	1:K:239:ASP:OD2	2.53	0.41
1:K:1344:TYR:HA	1:K:1391:LYS:HA	2.02	0.41
1:C:409:LYS:HE3	1:C:428:PHE:O	2.20	0.41
1:C:962:ASP:HA	1:C:965:HIS:CD2	2.54	0.41
1:C:1338:ARG:HD3	1:C:1339:PRO:HD2	2.02	0.41
1:E:348:THR:HB	1:E:349:PRO:HD2	2.02	0.41
1:E:409:LYS:HE3	1:E:428:PHE:O	2.20	0.41
1:E:872:ARG:NH2	1:E:1061:ASP:OD2	2.53	0.41
2:F:751:ILE:HB	2:L:822:ARG:HH21	1.85	0.41
1:G:1344:TYR:HA	1:G:1391:LYS:HA	2.02	0.41
1:B:675:ILE:HB	1:B:676:PRO:HD3	2.02	0.41
2:A:1146:PRO:HD2	2:H:1118:HIS:CE1	2.54	0.41
2:D:375:TRP:HB2	2:H:375:TRP:CZ3	2.55	0.41
1:E:601:LEU:HD11	1:E:657:ARG:NH1	2.34	0.41
1:G:49:LYS:HE2	1:G:49:LYS:HB3	1.99	0.41
1:B:348:THR:HB	1:B:349:PRO:HD2	2.02	0.41
1:B:601:LEU:HD11	1:B:657:ARG:NH1	2.34	0.41
1:B:1854:MET:SD	1:B:1859:LEU:HA	2.60	0.41
2:A:358:TYR:HA	2:J:358:TYR:HD1	1.85	0.41
1:E:986:ASP:OD1	1:E:986:ASP:N	2.54	0.41
2:F:36:LEU:HD22	2:F:61:LEU:HD21	2.03	0.41
1:I:1854:MET:SD	1:I:1859:LEU:HA	2.60	0.41
1:K:1854:MET:SD	1:K:1859:LEU:HA	2.60	0.41
1:C:986:ASP:OD1	1:C:986:ASP:N	2.53	0.41
2:D:685:GLU:CD	2:D:685:GLU:H	2.28	0.41
1:E:1174:ALA:HB1	1:E:1273:PRO:HG2	2.03	0.41
1:E:1344:TYR:HA	1:E:1391:LYS:HA	2.02	0.41
1:K:962:ASP:HA	1:K:965:HIS:CD2	2.54	0.41
1:K:1132:GLY:HA3	1:K:1152:VAL:HG11	2.02	0.41
1:K:1923:TYR:HB3	2:L:29:ILE:HD12	2.01	0.41
2:L:685:GLU:CD	2:L:685:GLU:H	2.28	0.41
2:A:1117:GLU:HB2	2:H:1147:LYS:HA	2.01	0.41
2:A:1148:ALA:HB3	2:H:1116:ARG:CG	2.50	0.41
2:F:1311:TYR:HE1	2:J:1234:ARG:CZ	2.33	0.41
1:I:223:LYS:NZ	1:I:239:ASP:OD2	2.53	0.41
1:I:1132:GLY:HA3	1:I:1152:VAL:HG11	2.02	0.41
1:K:1384:PHE:CE2	1:K:1429:GLU:HG3	2.56	0.41
1:B:1174:ALA:HB1	1:B:1273:PRO:HG2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1753:GLY:HA3	2:J:787:THR:O	2.21	0.41
2:A:685:GLU:H	2:A:685:GLU:CD	2.28	0.41
2:A:1147:LYS:CA	2:H:1117:GLU:HB2	2.51	0.41
1:C:223:LYS:NZ	1:C:239:ASP:OD2	2.53	0.41
1:E:675:ILE:HB	1:E:676:PRO:HD3	2.02	0.41
1:G:1854:MET:SD	1:G:1859:LEU:HA	2.60	0.41
2:A:361:SER:CB	2:J:361:SER:CB	2.99	0.41
2:D:1259:MET:O	2:L:1384:ILE:HG12	2.21	0.41
1:I:1174:ALA:HB1	1:I:1273:PRO:HG2	2.03	0.41
1:K:1174:ALA:HB1	1:K:1273:PRO:HG2	2.03	0.41
1:B:223:LYS:NZ	1:B:239:ASP:OD2	2.54	0.41
1:B:1384:PHE:CE2	1:B:1429:GLU:HG3	2.56	0.41
2:A:1383:LYS:HD3	2:H:1679:TYR:OH	2.20	0.41
1:C:1132:GLY:HA3	1:C:1152:VAL:HG11	2.02	0.41
1:C:1384:PHE:CE2	1:C:1429:GLU:HG3	2.56	0.41
1:C:1854:MET:SD	1:C:1859:LEU:HA	2.60	0.41
2:D:1159:ILE:HG12	2:D:1350:GLN:HE21	1.86	0.41
2:D:1692:ASP:CG	2:L:1402:HIS:HE1	2.28	0.41
2:F:1117:GLU:OE1	2:J:1146:PRO:HB2	2.21	0.41
2:F:1209:HIS:CD2	2:F:1691:PRO:HA	2.56	0.41
2:F:1383:LYS:CD	2:J:1679:TYR:CZ	3.03	0.41
1:G:348:THR:HB	1:G:349:PRO:HD2	2.02	0.41
1:G:617:ASP:OD1	1:G:617:ASP:N	2.54	0.41
1:I:617:ASP:OD1	1:I:617:ASP:N	2.54	0.41
1:B:986:ASP:OD1	1:B:986:ASP:N	2.53	0.41
1:C:617:ASP:OD1	1:C:617:ASP:N	2.54	0.41
2:D:1234:ARG:CZ	2:L:1311:TYR:HE1	2.34	0.41
1:E:1132:GLY:HA3	1:E:1152:VAL:HG11	2.02	0.41
1:E:1192:MET:HE3	1:E:1263:PHE:CZ	2.56	0.41
1:G:223:LYS:NZ	1:G:239:ASP:OD2	2.53	0.41
2:H:36:LEU:HD22	2:H:61:LEU:HD21	2.02	0.41
2:J:1839:ALA:HA	2:J:1844:ILE:HD12	2.03	0.41
2:L:1341:THR:CG2	2:L:1588:ASP:HA	2.51	0.41
1:B:1338:ARG:HD3	1:B:1339:PRO:HD2	2.02	0.40
1:C:1192:MET:HE3	1:C:1263:PHE:CZ	2.56	0.40
2:D:1147:LYS:CA	2:L:1117:GLU:HB2	2.51	0.40
2:D:1209:HIS:CD2	2:D:1691:PRO:HA	2.56	0.40
2:D:1341:THR:CG2	2:D:1588:ASP:HA	2.51	0.40
2:F:358:TYR:HB2	2:L:358:TYR:HB2	2.03	0.40
1:G:1338:ARG:HD3	1:G:1339:PRO:HD2	2.02	0.40
2:H:1159:ILE:HG12	2:H:1350:GLN:HE21	1.86	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:675:ILE:HB	1:I:676:PRO:HD3	2.02	0.40
1:I:872:ARG:NH2	1:I:1061:ASP:OD2	2.53	0.40
1:K:617:ASP:OD1	1:K:617:ASP:N	2.54	0.40
1:B:1248:LYS:HE3	1:B:1590:TYR:O	2.22	0.40
1:C:2067:SER:HB2	2:D:20:TYR:CE2	2.57	0.40
2:D:1148:ALA:HB3	2:L:1116:ARG:CG	2.51	0.40
2:D:1228:ARG:CA	2:L:1231:HIS:CE1	3.02	0.40
2:F:822:ARG:HH22	2:L:751:ILE:HG13	1.86	0.40
2:H:1839:ALA:HA	2:H:1844:ILE:HD12	2.03	0.40
2:J:36:LEU:HD22	2:J:61:LEU:HD21	2.03	0.40
1:B:617:ASP:OD1	1:B:617:ASP:N	2.54	0.40
2:A:1209:HIS:CD2	2:A:1691:PRO:HA	2.56	0.40
1:C:1174:ALA:HB1	1:C:1273:PRO:HG2	2.03	0.40
1:C:1344:TYR:HA	1:C:1391:LYS:HA	2.02	0.40
1:C:1746:LYS:HE2	1:C:1799:PRO:O	2.22	0.40
1:E:223:LYS:NZ	1:E:239:ASP:OD2	2.54	0.40
2:F:1159:ILE:HG12	2:F:1350:GLN:HE21	1.86	0.40
2:F:1341:THR:CG2	2:F:1588:ASP:HA	2.52	0.40
2:F:1839:ALA:HA	2:F:1844:ILE:HD12	2.03	0.40
1:G:1132:GLY:HA3	1:G:1152:VAL:HG11	2.02	0.40
1:G:1174:ALA:HB1	1:G:1273:PRO:HG2	2.03	0.40
1:I:1192:MET:HE3	1:I:1263:PHE:CZ	2.56	0.40
1:K:1702:SER:HB2	2:L:49:PRO:HG2	2.04	0.40
2:L:1792:ARG:HH22	2:L:1821:VAL:HG13	1.86	0.40
1:B:1693:THR:HA	2:A:43:ARG:O	2.20	0.40
2:A:1232:ARG:HH21	2:H:1235:PHE:HE2	1.59	0.40
2:A:1341:THR:CG2	2:A:1588:ASP:HA	2.51	0.40
2:A:1839:ALA:HA	2:A:1844:ILE:HD12	2.03	0.40
2:D:1060:LYS:HB3	2:D:1061:PRO:HD3	2.03	0.40
2:D:1792:ARG:HH22	2:D:1821:VAL:HG13	1.86	0.40
1:E:1338:ARG:HD3	1:E:1339:PRO:HD2	2.02	0.40
2:F:1679:TYR:CZ	2:J:1383:LYS:CD	3.04	0.40
2:F:1697:GLU:HA	2:F:1704:LEU:HD23	2.04	0.40
1:G:1248:LYS:HE3	1:G:1590:TYR:O	2.22	0.40
1:G:1384:PHE:CE2	1:G:1429:GLU:HG3	2.56	0.40
2:H:1209:HIS:CD2	2:H:1691:PRO:HA	2.57	0.40
2:H:1341:THR:CG2	2:H:1588:ASP:HA	2.51	0.40
1:I:1344:TYR:HA	1:I:1391:LYS:HA	2.02	0.40
1:K:348:THR:HB	1:K:349:PRO:HD2	2.02	0.40
1:K:1192:MET:HE3	1:K:1263:PHE:CZ	2.56	0.40
2:L:1159:ILE:HG12	2:L:1350:GLN:HE21	1.86	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:1209:HIS:CD2	2:L:1691:PRO:HA	2.56	0.40
2:L:1839:ALA:HA	2:L:1844:ILE:HD12	2.03	0.40
2:A:36:LEU:HD22	2:A:61:LEU:HD21	2.02	0.40
2:D:1839:ALA:HA	2:D:1844:ILE:HD12	2.03	0.40
2:F:1692:ASP:CG	2:J:1402:HIS:HE1	2.27	0.40
1:G:333:PRO:O	1:I:1569:LYS:HE3	2.21	0.40
1:G:2057:TYR:CD1	2:H:13:LEU:HD21	2.56	0.40
2:J:1209:HIS:CD2	2:J:1691:PRO:HA	2.56	0.40
2:J:1341:THR:CG2	2:J:1588:ASP:HA	2.51	0.40
2:J:1697:GLU:HA	2:J:1704:LEU:HD23	2.04	0.40
1:K:1746:LYS:HE2	1:K:1799:PRO:O	2.22	0.40
2:L:36:LEU:HD22	2:L:61:LEU:HD21	2.02	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	B	2033/2122 (96%)	1987 (98%)	44 (2%)	2 (0%)	48	83
1	C	2033/2122 (96%)	1987 (98%)	44 (2%)	2 (0%)	48	83
1	E	2033/2122 (96%)	1987 (98%)	44 (2%)	2 (0%)	48	83
1	G	2033/2122 (96%)	1987 (98%)	44 (2%)	2 (0%)	48	83
1	I	2033/2122 (96%)	1987 (98%)	44 (2%)	2 (0%)	48	83
1	K	2033/2122 (96%)	1987 (98%)	44 (2%)	2 (0%)	48	83
2	A	1542/1865 (83%)	1491 (97%)	49 (3%)	2 (0%)	48	83
2	D	1542/1865 (83%)	1490 (97%)	50 (3%)	2 (0%)	48	83
2	F	1542/1865 (83%)	1489 (97%)	51 (3%)	2 (0%)	48	83
2	H	1542/1865 (83%)	1490 (97%)	50 (3%)	2 (0%)	48	83

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	1542/1865 (83%)	1490 (97%)	50 (3%)	2 (0%)	48	83
2	L	1542/1865 (83%)	1490 (97%)	50 (3%)	2 (0%)	48	83
All	All	21450/23922 (90%)	20862 (97%)	564 (3%)	24 (0%)	49	83

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	286	SER
1	B	1840	SER
2	A	1274	ALA
2	A	1558	LYS
1	C	286	SER
1	C	1840	SER
2	D	1274	ALA
2	D	1558	LYS
1	E	286	SER
1	E	1840	SER
2	F	1274	ALA
2	F	1558	LYS
1	G	286	SER
1	G	1840	SER
2	H	1274	ALA
2	H	1558	LYS
1	I	286	SER
1	I	1840	SER
2	J	1274	ALA
2	J	1558	LYS
1	K	286	SER
1	K	1840	SER
2	L	1274	ALA
2	L	1558	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	1718/1782 (96%)	1708 (99%)	10 (1%)	78	80
1	C	1718/1782 (96%)	1707 (99%)	11 (1%)	78	80
1	E	1718/1782 (96%)	1708 (99%)	10 (1%)	78	80
1	G	1718/1782 (96%)	1708 (99%)	10 (1%)	78	80
1	I	1718/1782 (96%)	1708 (99%)	10 (1%)	78	80
1	K	1718/1782 (96%)	1708 (99%)	10 (1%)	78	80
2	A	1285/1523 (84%)	1276 (99%)	9 (1%)	76	79
2	D	1285/1523 (84%)	1275 (99%)	10 (1%)	73	77
2	F	1285/1523 (84%)	1275 (99%)	10 (1%)	73	77
2	H	1285/1523 (84%)	1276 (99%)	9 (1%)	76	79
2	J	1285/1523 (84%)	1275 (99%)	10 (1%)	73	77
2	L	1285/1523 (84%)	1275 (99%)	10 (1%)	73	77
All	All	18018/19830 (91%)	17899 (99%)	119 (1%)	73	79

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	241	ASP
1	B	781	SER
1	B	986	ASP
1	B	1012	GLN
1	B	1338	ARG
1	B	1348	ASP
1	B	1379	ASN
1	B	1465	ILE
1	B	1582	THR
1	B	1662	VAL
2	A	359	GLN
2	A	1056	ASP
2	A	1099	GLU
2	A	1265	SER
2	A	1428	MET
2	A	1682	GLU
2	A	1735	GLU
2	A	1740	GLU
2	A	1742	VAL
1	C	241	ASP
1	C	781	SER
1	C	986	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	1012	GLN
1	C	1338	ARG
1	C	1348	ASP
1	C	1379	ASN
1	C	1465	ILE
1	C	1582	THR
1	C	1630	ASN
1	C	1662	VAL
2	D	359	GLN
2	D	1056	ASP
2	D	1099	GLU
2	D	1120	ASP
2	D	1265	SER
2	D	1428	MET
2	D	1682	GLU
2	D	1735	GLU
2	D	1740	GLU
2	D	1742	VAL
1	E	241	ASP
1	E	781	SER
1	E	986	ASP
1	E	1012	GLN
1	E	1338	ARG
1	E	1348	ASP
1	E	1379	ASN
1	E	1465	ILE
1	E	1582	THR
1	E	1662	VAL
2	F	359	GLN
2	F	1056	ASP
2	F	1099	GLU
2	F	1120	ASP
2	F	1265	SER
2	F	1428	MET
2	F	1682	GLU
2	F	1735	GLU
2	F	1740	GLU
2	F	1742	VAL
1	G	241	ASP
1	G	781	SER
1	G	986	ASP
1	G	1012	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	1338	ARG
1	G	1348	ASP
1	G	1379	ASN
1	G	1465	ILE
1	G	1582	THR
1	G	1662	VAL
2	H	359	GLN
2	H	1056	ASP
2	H	1099	GLU
2	H	1265	SER
2	H	1428	MET
2	H	1682	GLU
2	H	1735	GLU
2	H	1740	GLU
2	H	1742	VAL
1	I	241	ASP
1	I	781	SER
1	I	986	ASP
1	I	1012	GLN
1	I	1338	ARG
1	I	1348	ASP
1	I	1379	ASN
1	I	1465	ILE
1	I	1582	THR
1	I	1662	VAL
2	J	359	GLN
2	J	1056	ASP
2	J	1099	GLU
2	J	1120	ASP
2	J	1265	SER
2	J	1428	MET
2	J	1682	GLU
2	J	1735	GLU
2	J	1740	GLU
2	J	1742	VAL
1	K	241	ASP
1	K	781	SER
1	K	986	ASP
1	K	1012	GLN
1	K	1338	ARG
1	K	1348	ASP
1	K	1379	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	1465	ILE
1	K	1582	THR
1	K	1662	VAL
2	L	359	GLN
2	L	1056	ASP
2	L	1099	GLU
2	L	1120	ASP
2	L	1265	SER
2	L	1428	MET
2	L	1682	GLU
2	L	1735	GLU
2	L	1740	GLU
2	L	1742	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (146) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	44	HIS
1	B	262	GLN
1	B	362	GLN
1	B	662	ASN
1	B	714	HIS
1	B	1106	ASN
1	B	1140	HIS
1	B	1456	GLN
1	B	1580	ASN
1	B	2081	GLN
2	A	451	HIS
2	A	691	GLN
2	A	874	ASN
2	A	888	GLN
2	A	976	ASN
2	A	1032	ASN
2	A	1105	GLN
2	A	1231	HIS
2	A	1241	GLN
2	A	1393	GLN
2	A	1465	HIS
2	A	1473	GLN
2	A	1532	GLN
2	A	1662	HIS
1	C	44	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	262	GLN
1	C	362	GLN
1	C	662	ASN
1	C	714	HIS
1	C	912	GLN
1	C	1007	GLN
1	C	1106	ASN
1	C	1140	HIS
1	C	1456	GLN
1	C	1630	ASN
1	C	1751	HIS
1	C	1810	GLN
1	C	2081	GLN
2	D	451	HIS
2	D	691	GLN
2	D	874	ASN
2	D	935	ASN
2	D	957	ASN
2	D	976	ASN
2	D	1032	ASN
2	D	1105	GLN
2	D	1231	HIS
2	D	1241	GLN
2	D	1393	GLN
2	D	1473	GLN
2	D	1532	GLN
2	D	1662	HIS
1	E	262	GLN
1	E	362	GLN
1	E	662	ASN
1	E	714	HIS
1	E	1106	ASN
1	E	1140	HIS
1	E	1456	GLN
1	E	1580	ASN
1	E	1958	GLN
1	E	2081	GLN
2	F	379	HIS
2	F	451	HIS
2	F	691	GLN
2	F	874	ASN
2	F	976	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	1105	GLN
2	F	1231	HIS
2	F	1241	GLN
2	F	1393	GLN
2	F	1473	GLN
2	F	1532	GLN
1	G	44	HIS
1	G	262	GLN
1	G	337	GLN
1	G	362	GLN
1	G	662	ASN
1	G	714	HIS
1	G	912	GLN
1	G	1007	GLN
1	G	1106	ASN
1	G	1140	HIS
1	G	1456	GLN
1	G	1539	HIS
1	G	1751	HIS
1	G	2081	GLN
2	H	379	HIS
2	H	451	HIS
2	H	691	GLN
2	H	874	ASN
2	H	957	ASN
2	H	976	ASN
2	H	1032	ASN
2	H	1105	GLN
2	H	1231	HIS
2	H	1241	GLN
2	H	1393	GLN
2	H	1473	GLN
2	H	1532	GLN
2	H	1662	HIS
1	I	262	GLN
1	I	362	GLN
1	I	662	ASN
1	I	714	HIS
1	I	912	GLN
1	I	1106	ASN
1	I	1140	HIS
1	I	1456	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	1580	ASN
1	I	2081	GLN
2	J	379	HIS
2	J	451	HIS
2	J	691	GLN
2	J	874	ASN
2	J	976	ASN
2	J	1105	GLN
2	J	1231	HIS
2	J	1241	GLN
2	J	1393	GLN
2	J	1473	GLN
2	J	1532	GLN
2	J	1662	HIS
1	K	362	GLN
1	K	628	GLN
1	K	662	ASN
1	K	714	HIS
1	K	1106	ASN
1	K	1140	HIS
1	K	1580	ASN
1	K	1810	GLN
1	K	2081	GLN
2	L	379	HIS
2	L	451	HIS
2	L	691	GLN
2	L	874	ASN
2	L	976	ASN
2	L	1032	ASN
2	L	1093	HIS
2	L	1105	GLN
2	L	1231	HIS
2	L	1241	GLN
2	L	1393	GLN
2	L	1473	GLN
2	L	1532	GLN
2	L	1662	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

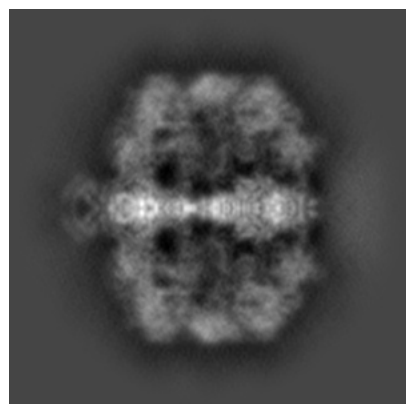
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13846. These allow visual inspection of the internal detail of the map and identification of artifacts.

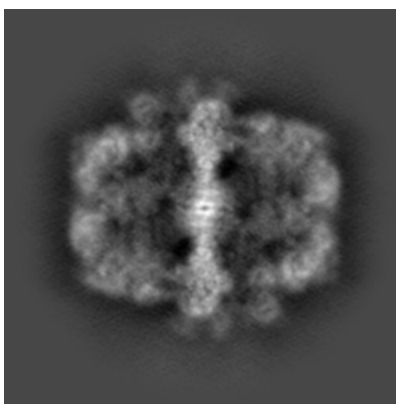
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

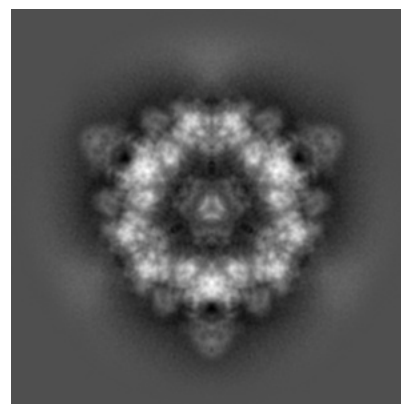
6.1.1 Primary map



X

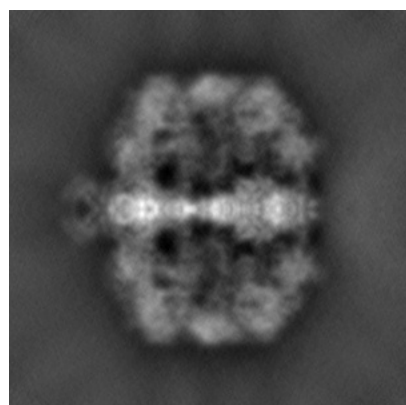


Y

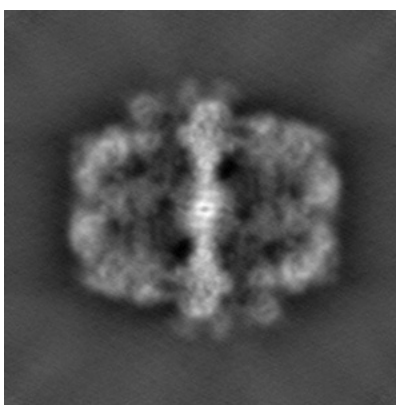


Z

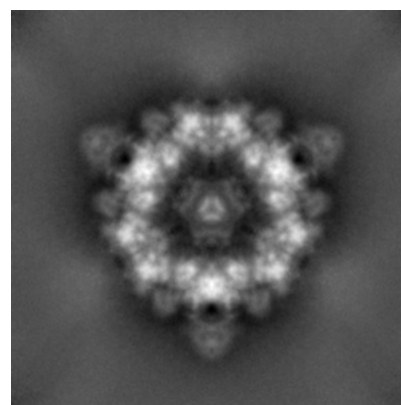
6.1.2 Raw map



X



Y

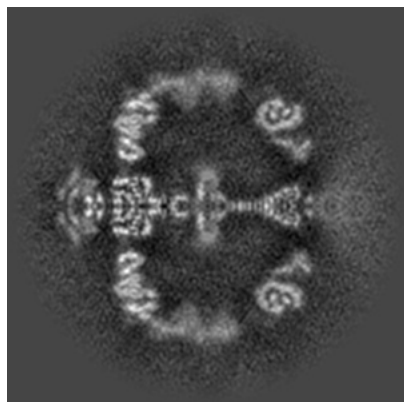


Z

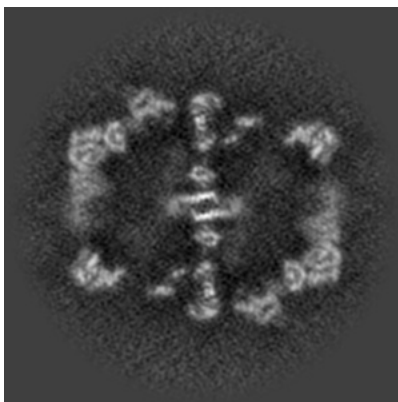
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

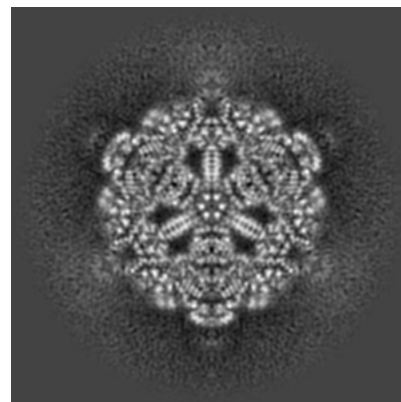
6.2.1 Primary map



X Index: 128

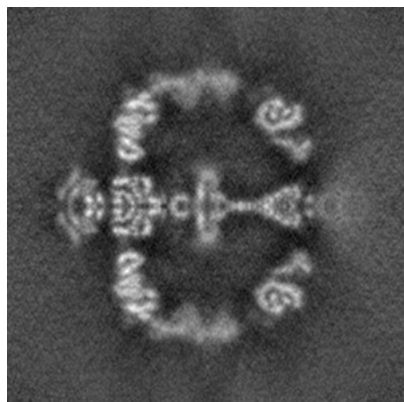


Y Index: 128

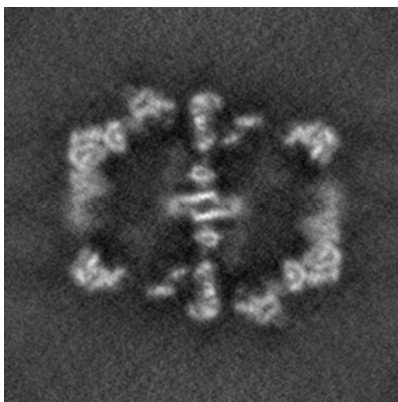


Z Index: 128

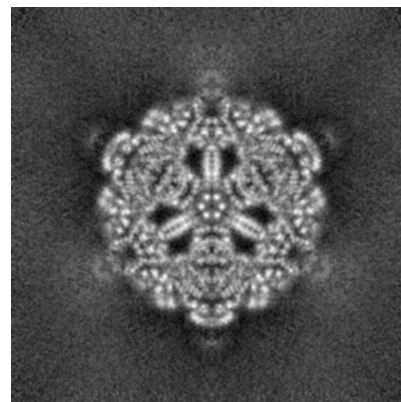
6.2.2 Raw map



X Index: 128



Y Index: 128

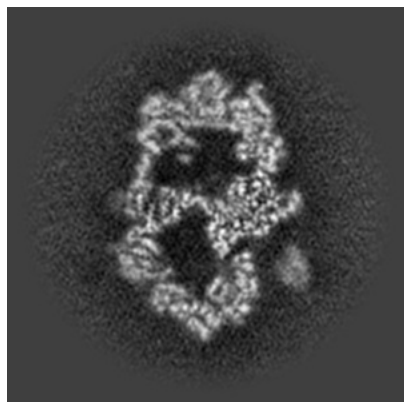


Z Index: 128

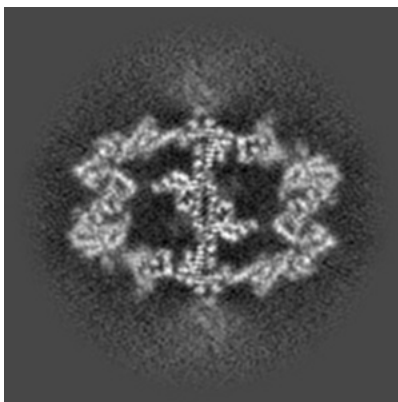
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

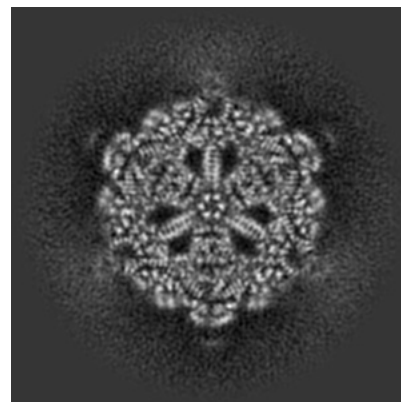
6.3.1 Primary map



X Index: 87

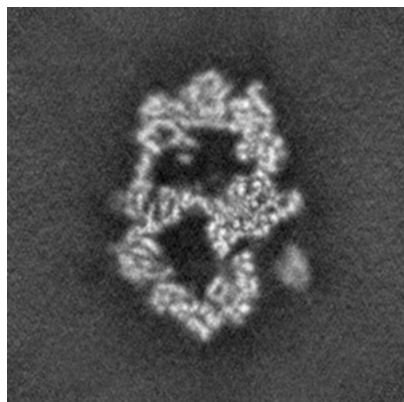


Y Index: 90

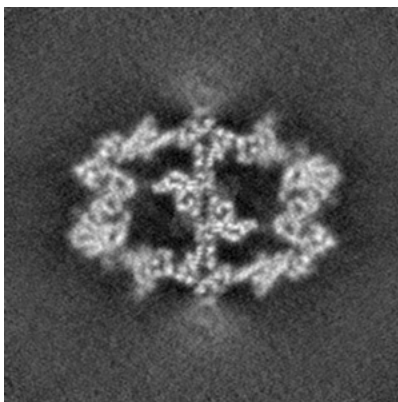


Z Index: 127

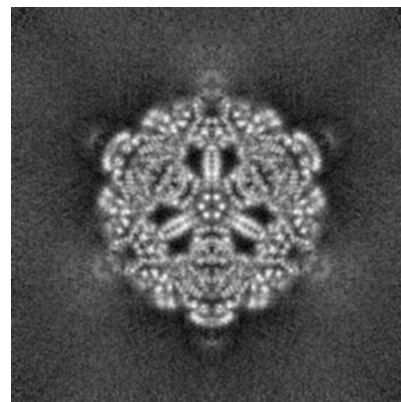
6.3.2 Raw map



X Index: 87



Y Index: 89

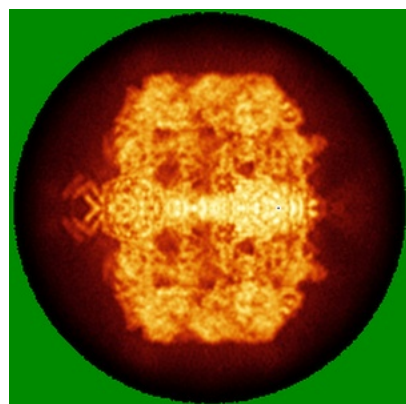


Z Index: 128

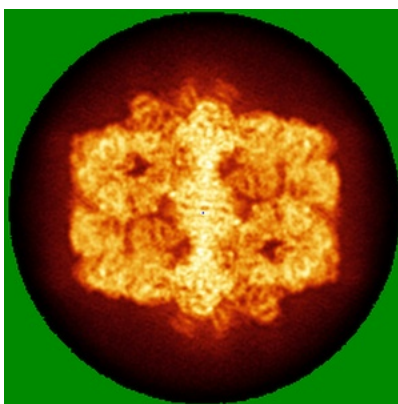
The images above show the largest variance slices of the map in three orthogonal directions.

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

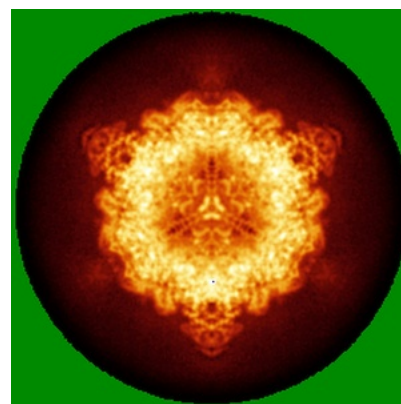
6.4.1 Primary map



X

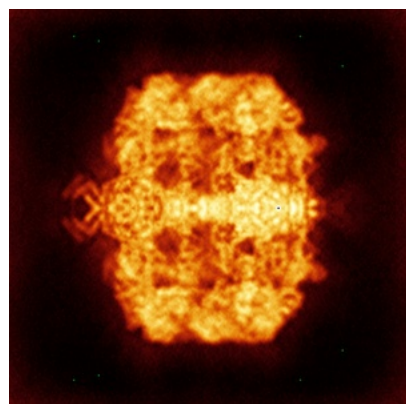


Y

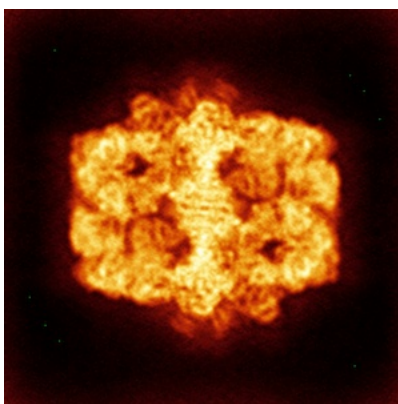


Z

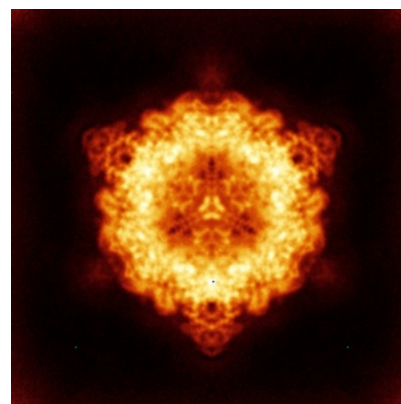
6.4.2 Raw map



X



Y

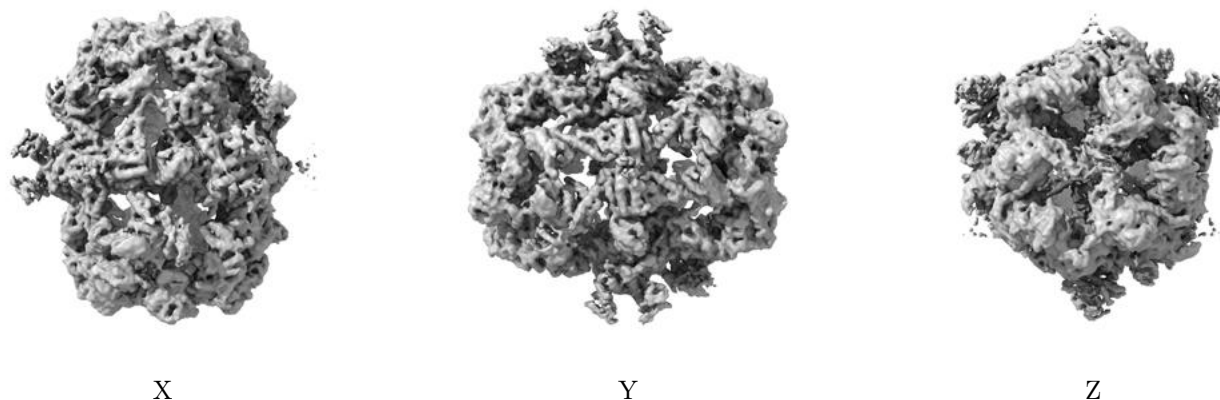


Z

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.

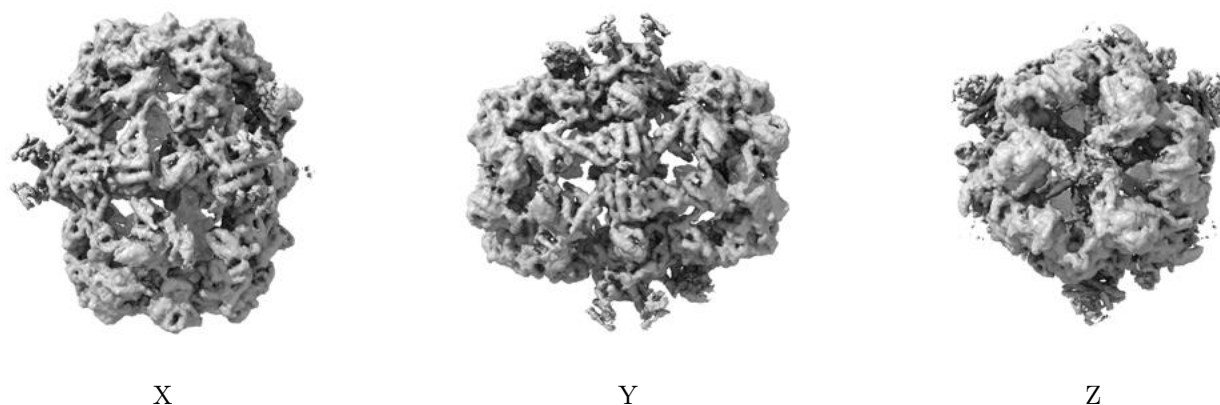
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.7. 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.

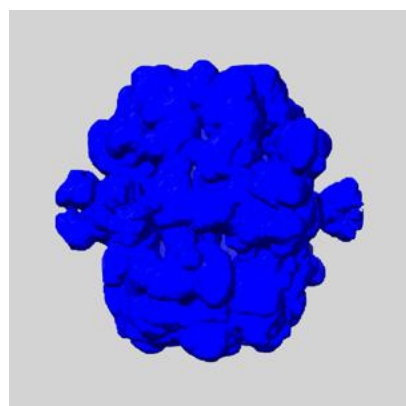
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

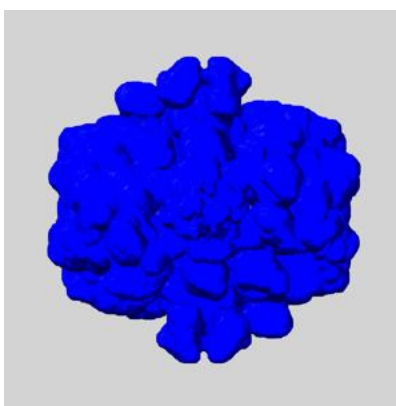
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

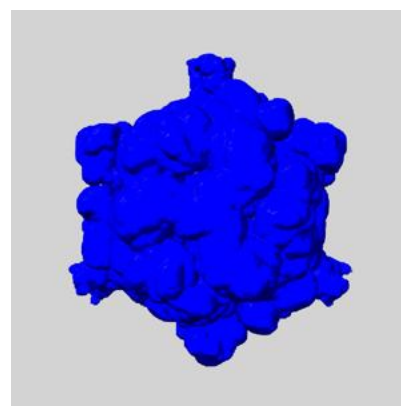
6.6.1 emd_13846_msk_1.map [i](#)



X



Y

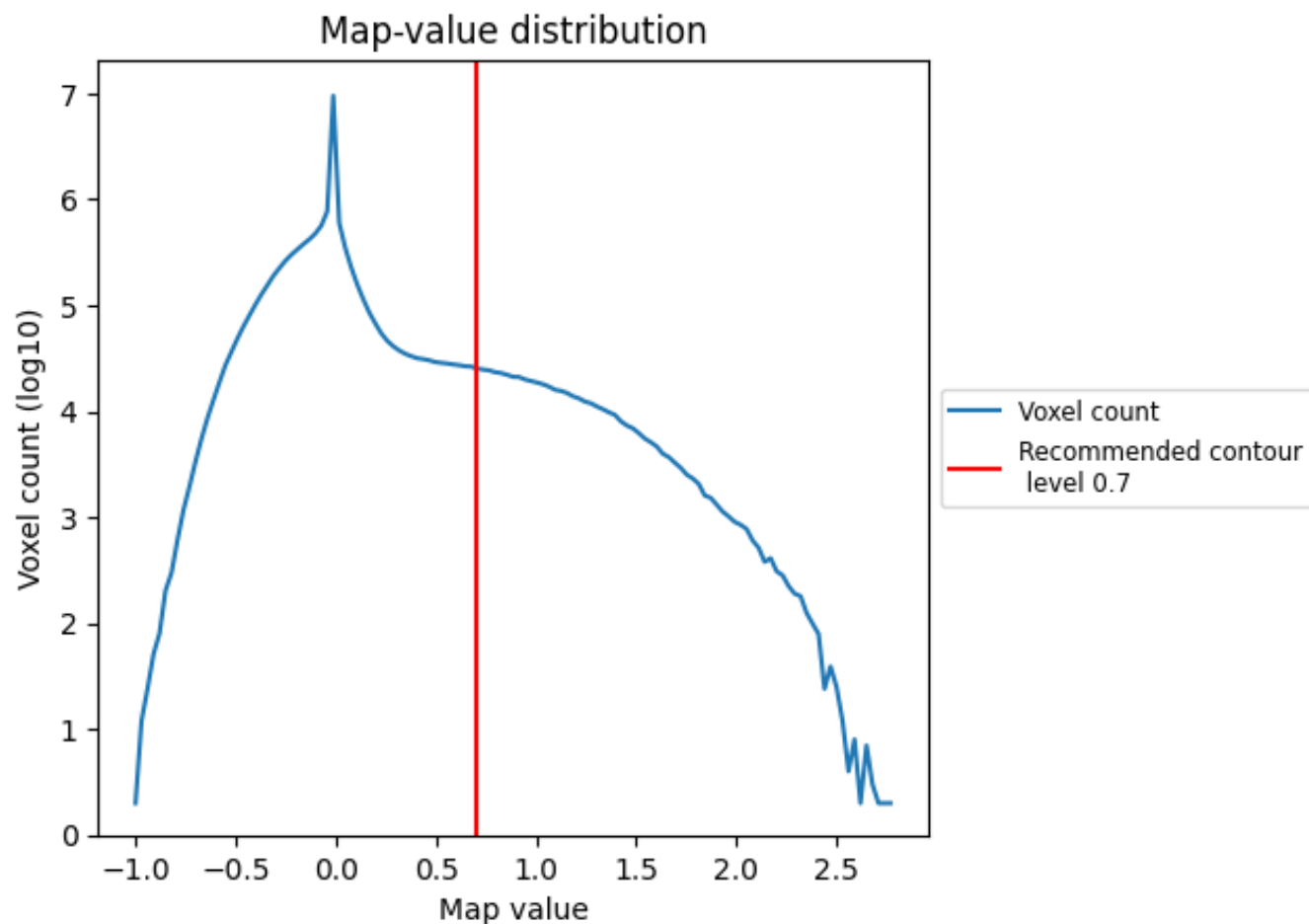


Z

7 Map analysis [i](#)

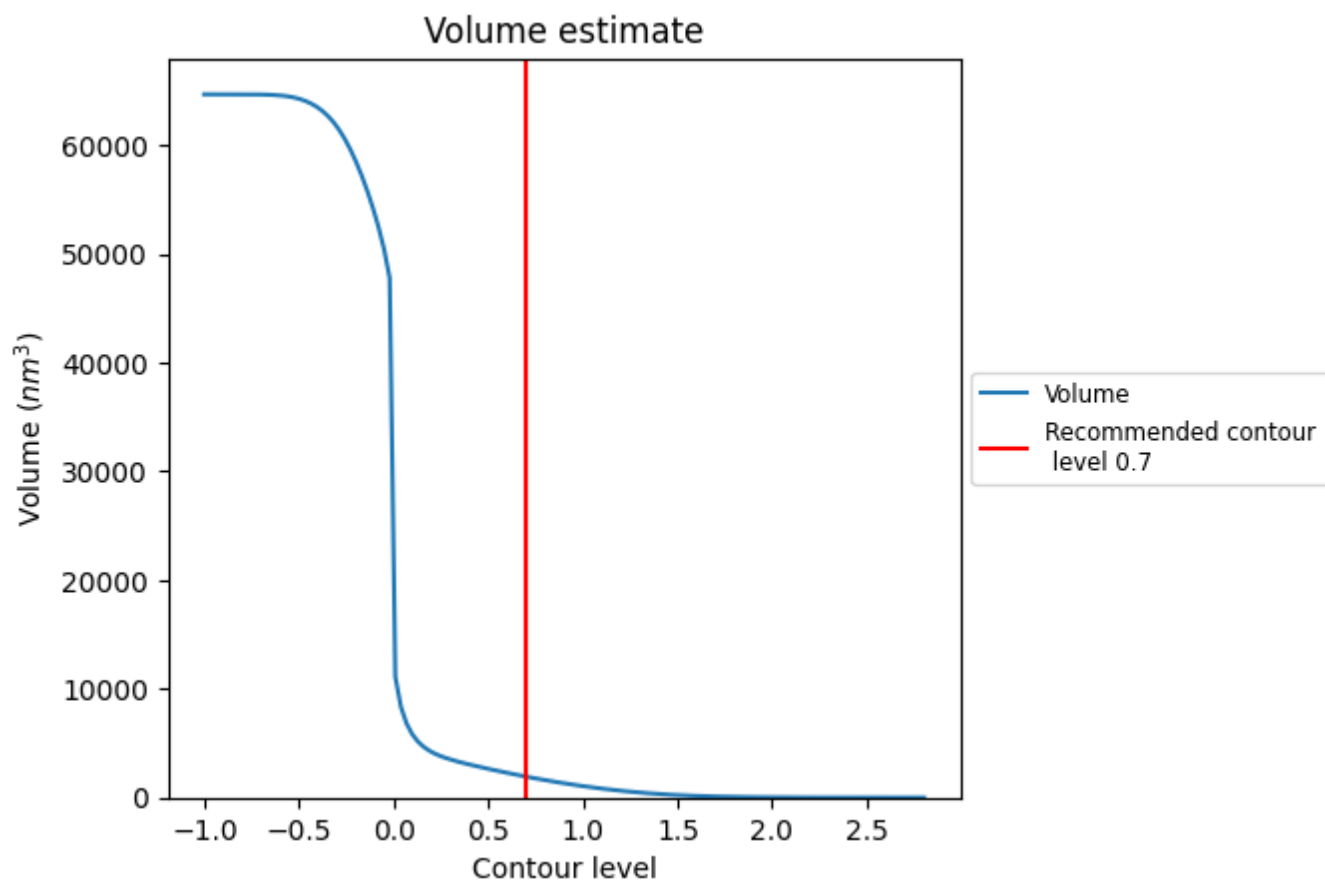
This section contains the results of statistical analysis of the map.

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.

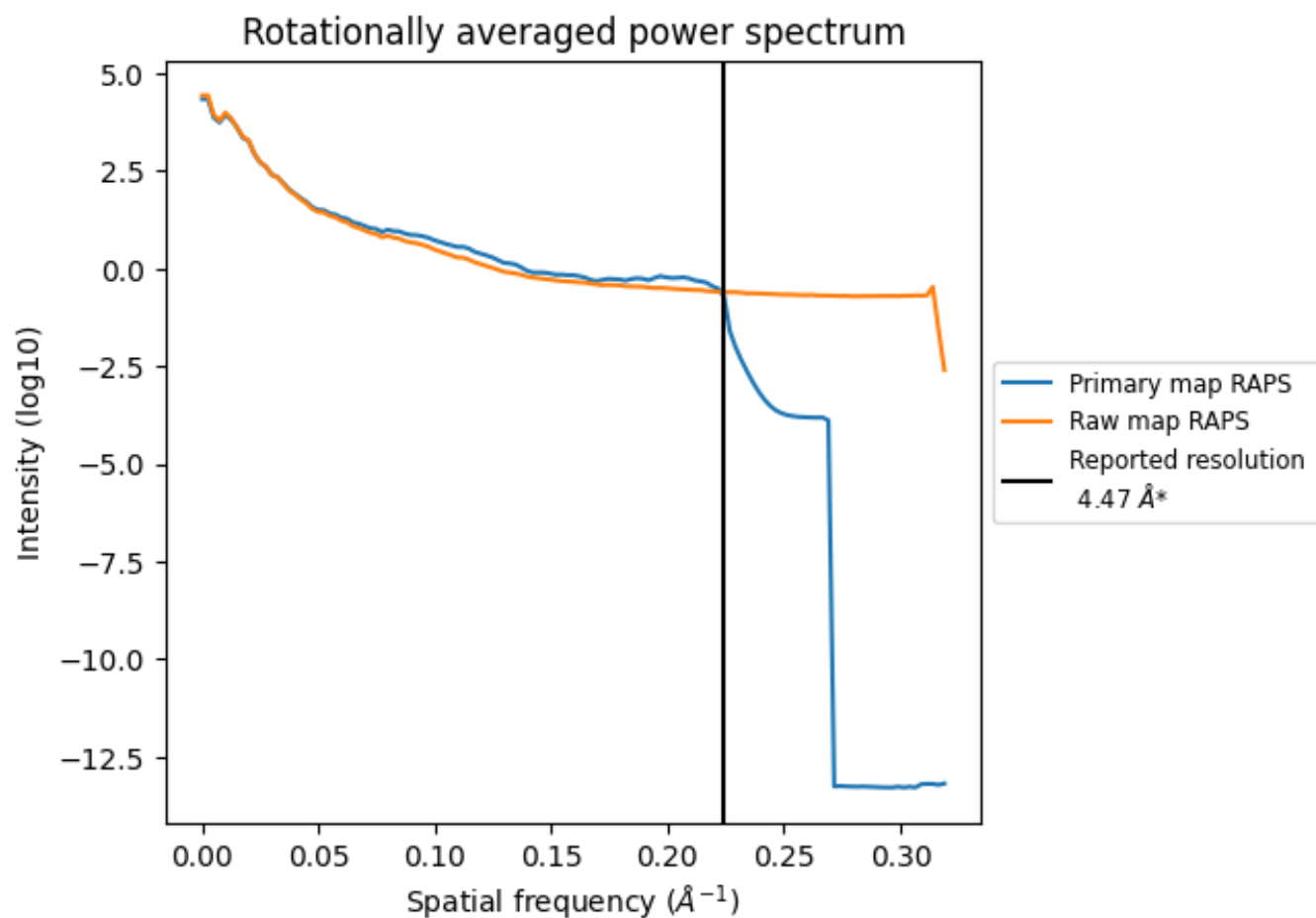
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1924 nm³; this corresponds to an approximate mass of 1738 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 ⓘ

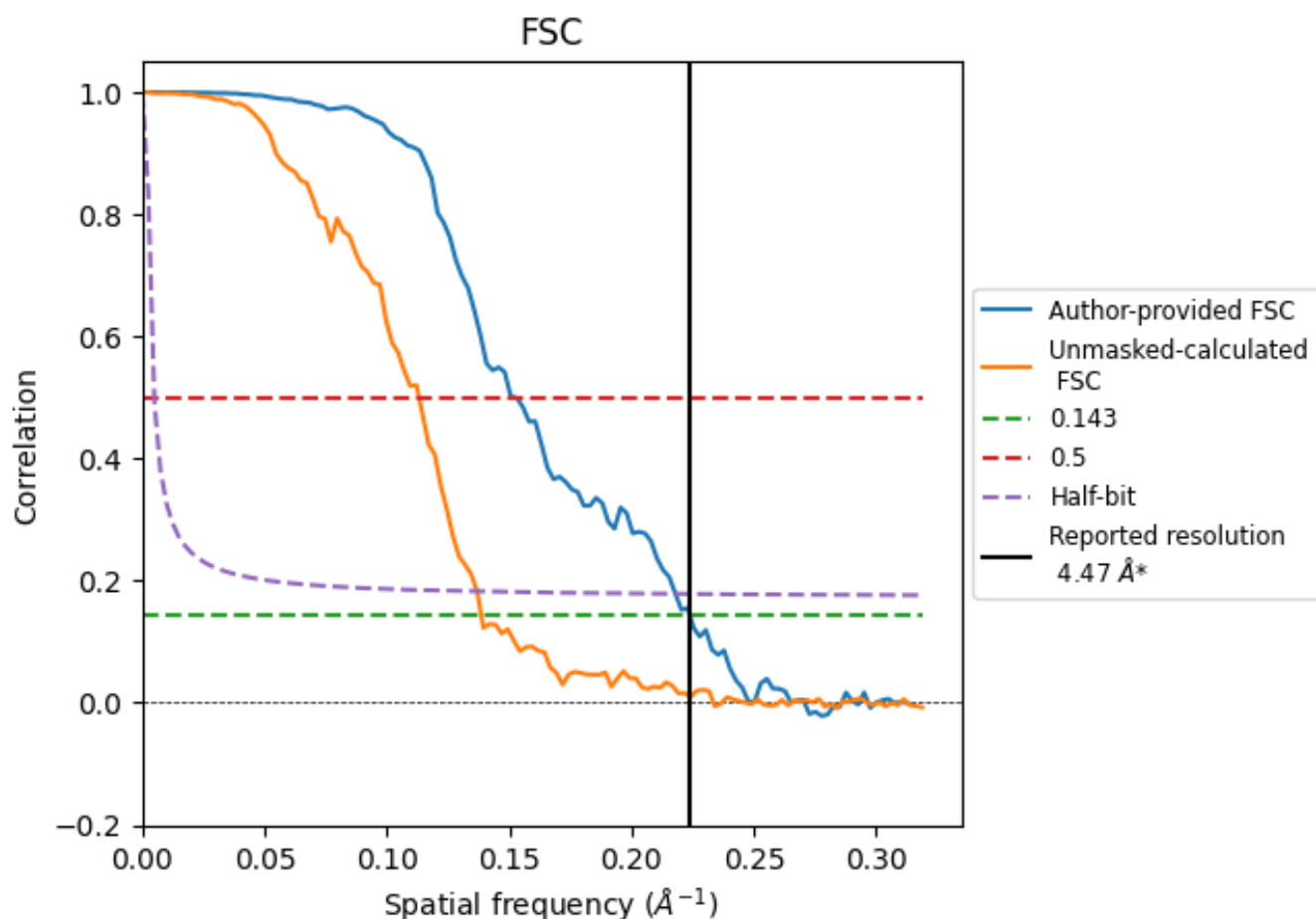


*Reported resolution corresponds to spatial frequency of 0.224 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.224 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

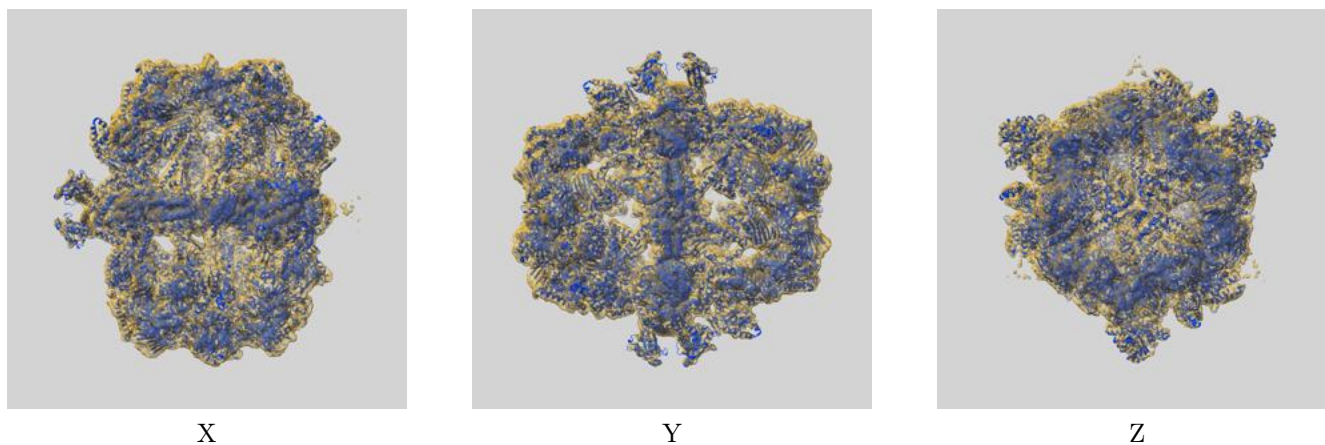
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.47	-	-
Author-provided FSC curve	4.47	6.55	4.59
Unmasked-calculated*	7.21	8.83	7.30

*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 7.21 differs from the reported value 4.47 by more than 10 %

9 Map-model fit [i](#)

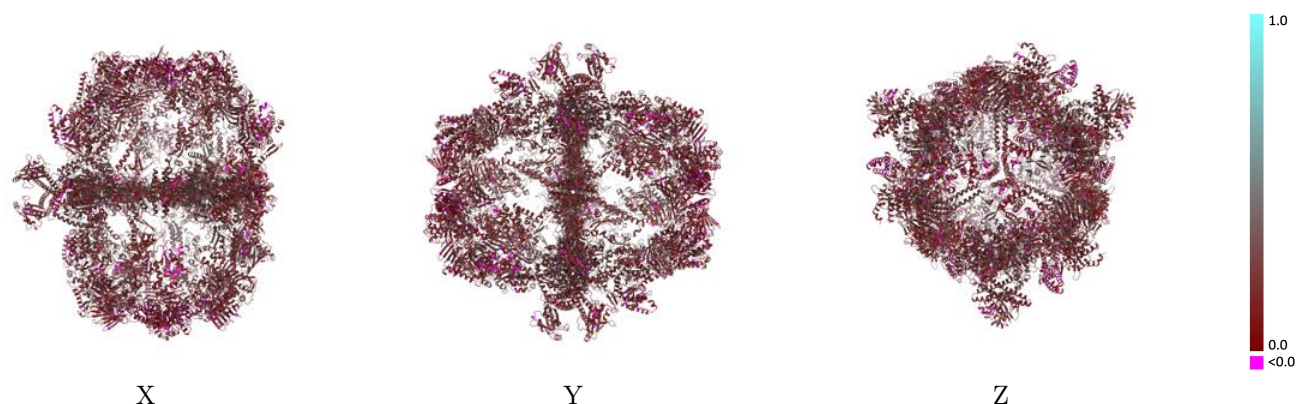
This section contains information regarding the fit between EMDB map EMD-13846 and PDB model 7Q5S. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



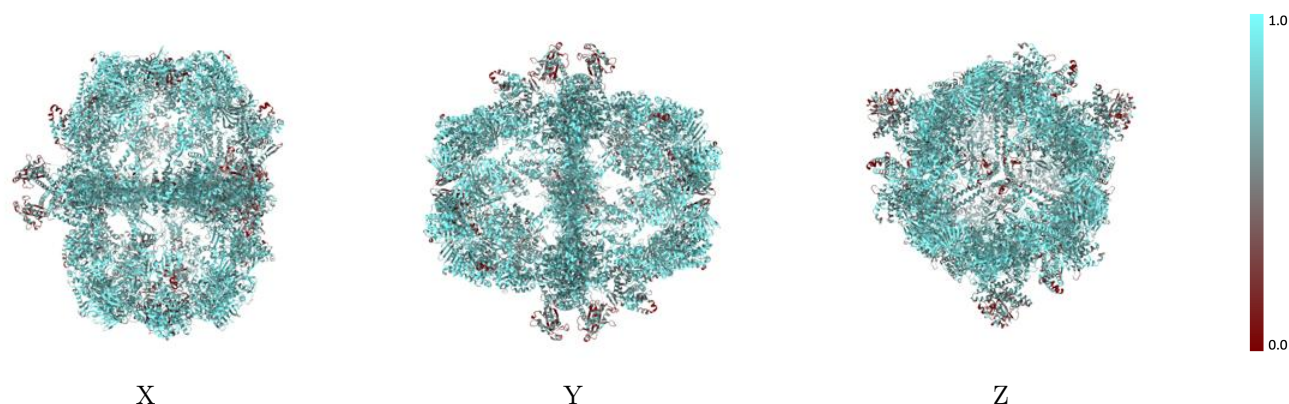
The images above show the 3D surface view of the map at the recommended contour level 0.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



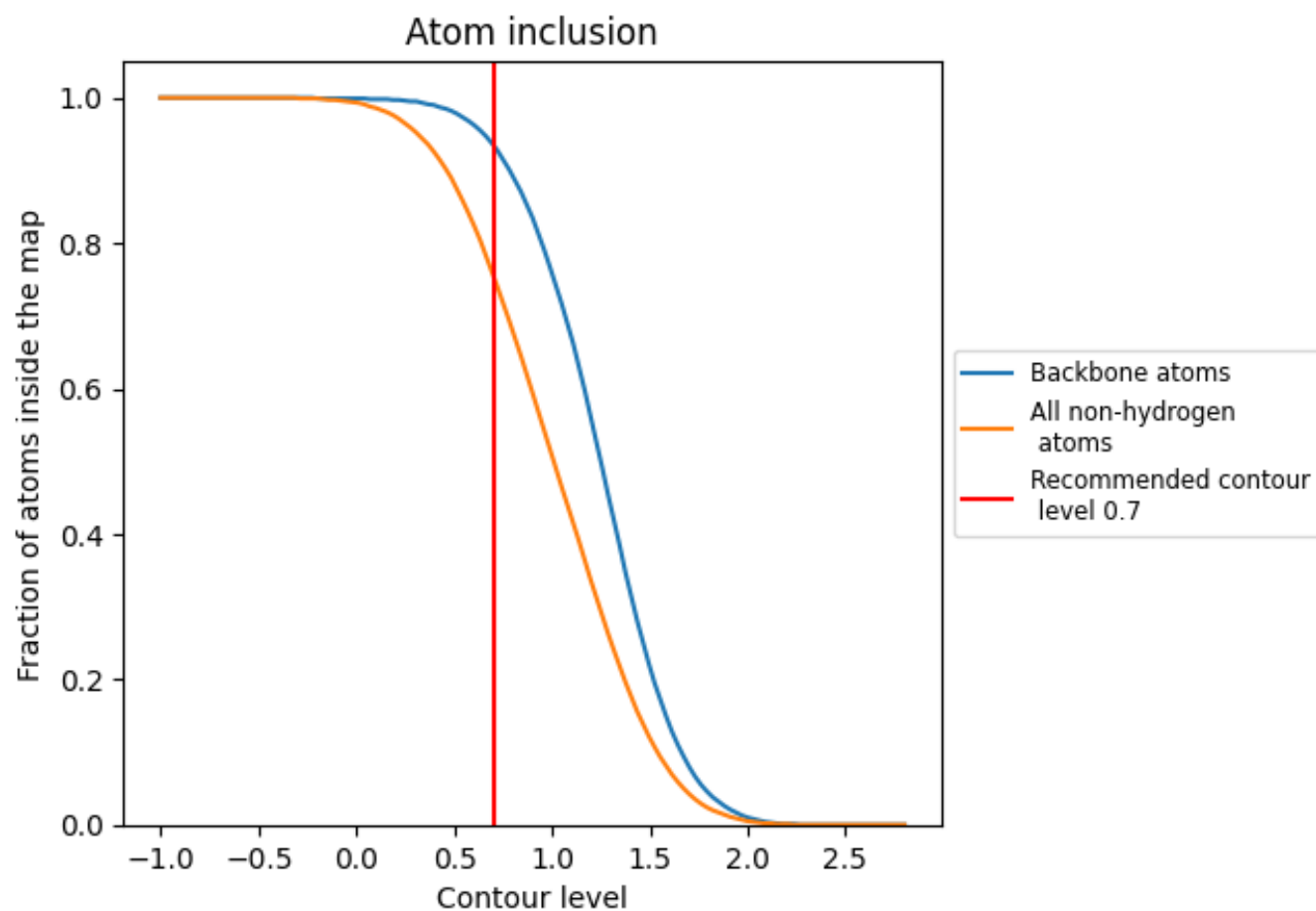
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.7).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 76% 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 (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7550	0.2270
A	0.7370	0.2570
B	0.7700	0.2050
C	0.7690	0.2040
D	0.7330	0.2560
E	0.7700	0.2050
F	0.7360	0.2560
G	0.7680	0.2040
H	0.7360	0.2560
I	0.7710	0.2050
J	0.7360	0.2550
K	0.7700	0.2060
L	0.7360	0.2560

