



Full wwPDB EM Validation Report ⓘ

Mar 17, 2026 – 03:59 PM UTC

PDB ID : 8GZN / pdb_00008gzn
EMDB ID : EMD-34399
Title : IgM-var2CSA complex
Authors : Akhouri, R.R.; Goel, S.; Skoglund, U.
Deposited on : 2022-09-27
Resolution : 3.60 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

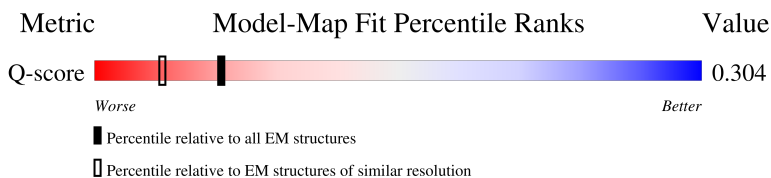
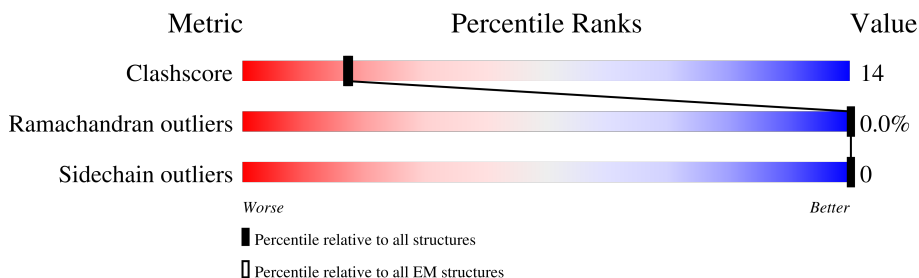
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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	12797 (3.10 - 4.10)

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	453	 19% 10% 71%
1	B	453	 32% 18% 50%
1	C	453	 34% 16% 50%
1	D	453	 35% 14% 51%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	453	
1	F	453	
1	G	453	
1	H	453	
1	K	453	
1	L	453	
2	I	2680	
2	M	2680	
3	J	136	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 35322 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 Immunoglobulin heavy constant mu.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	132	Total	C	N	O	S	0	0
			1026	648	174	198	6		
1	B	227	Total	C	N	O	S	0	0
			1764	1111	299	346	8		
1	C	225	Total	C	N	O	S	0	0
			1749	1103	297	341	8		
1	D	224	Total	C	N	O	S	0	0
			1743	1100	296	339	8		
1	E	224	Total	C	N	O	S	0	0
			1743	1100	296	339	8		
1	F	221	Total	C	N	O	S	0	0
			1723	1087	292	336	8		
1	G	224	Total	C	N	O	S	0	0
			1743	1100	296	339	8		
1	H	230	Total	C	N	O	S	0	0
			1785	1124	301	351	9		
1	K	230	Total	C	N	O	S	0	0
			1786	1124	302	351	9		
1	L	127	Total	C	N	O	S	0	0
			993	626	168	193	6		

- Molecule 2 is a protein called Erythrocyte membrane protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	1115	Total	C	N	O	S	0	0
			9208	5813	1571	1758	66		
2	M	1115	Total	C	N	O	S	0	0
			9208	5813	1571	1758	66		

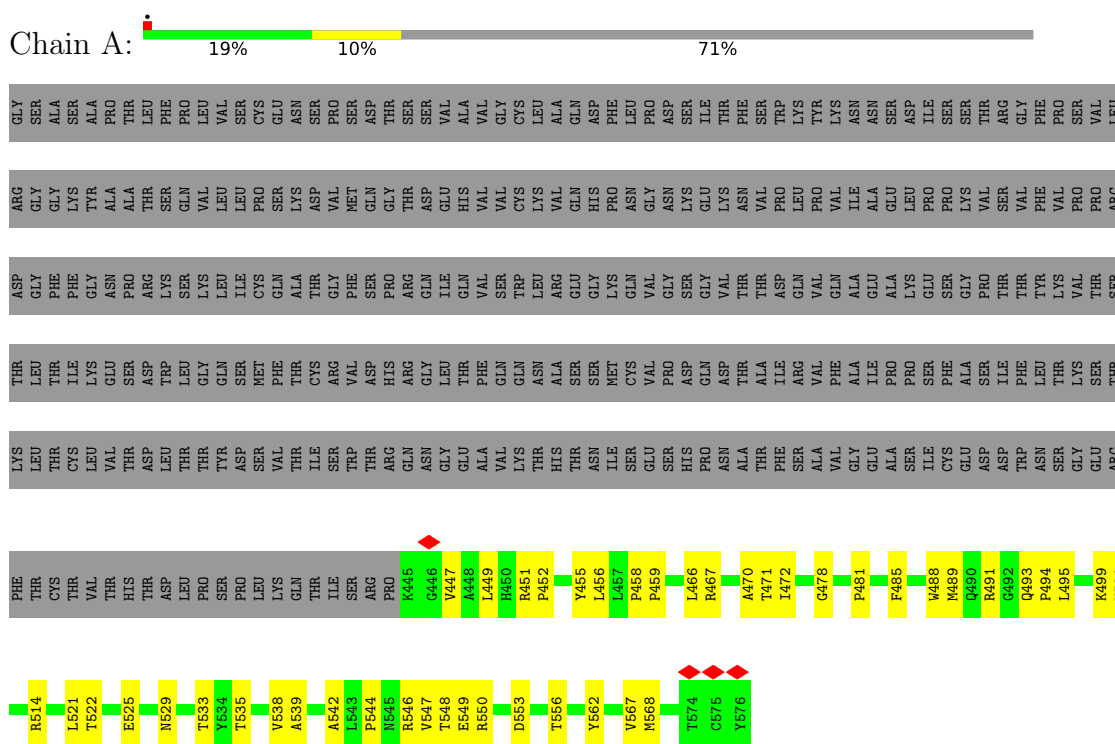
- Molecule 3 is a protein called Immunoglobulin J chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	106	Total	C	N	O	S	0	0
			851	528	150	166	7		

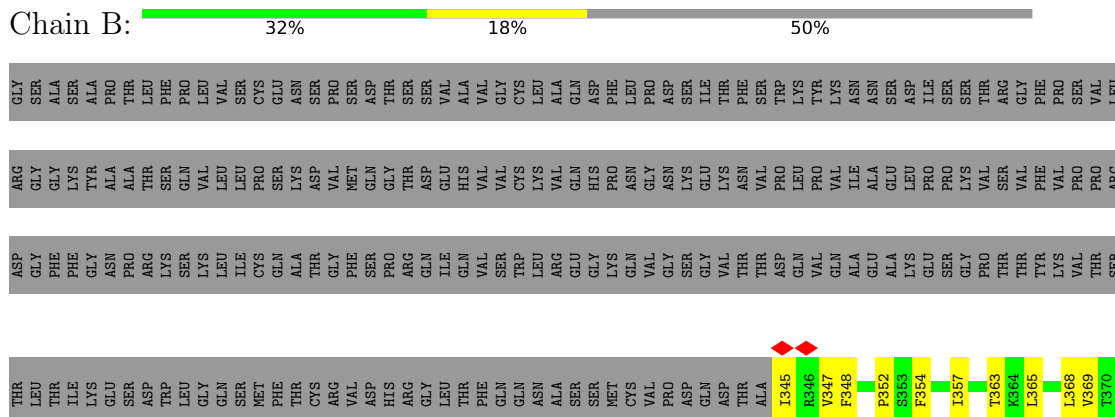
3 Residue-property plots

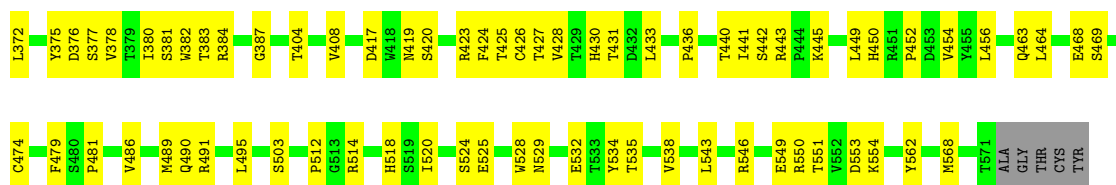
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Immunoglobulin heavy constant mu



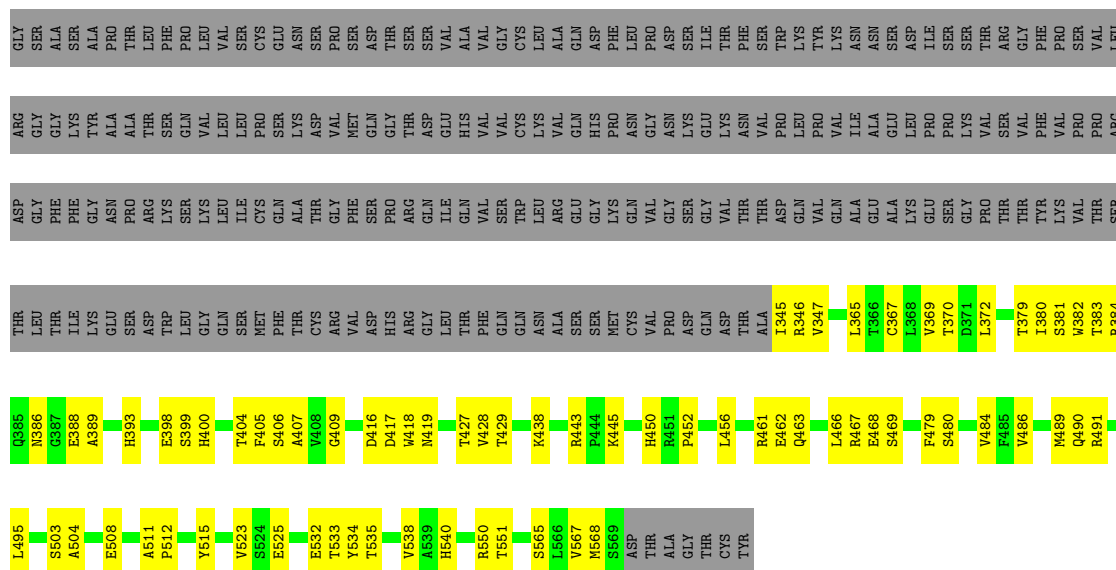
• Molecule 1: Immunoglobulin heavy constant mu





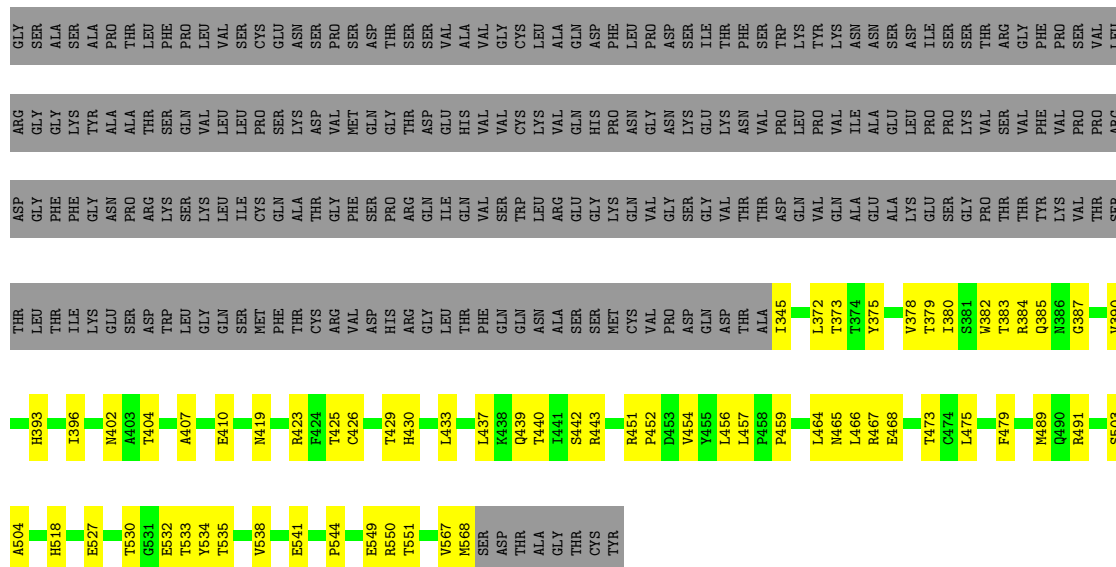
• Molecule 1: Immunoglobulin heavy constant mu

Chain C:

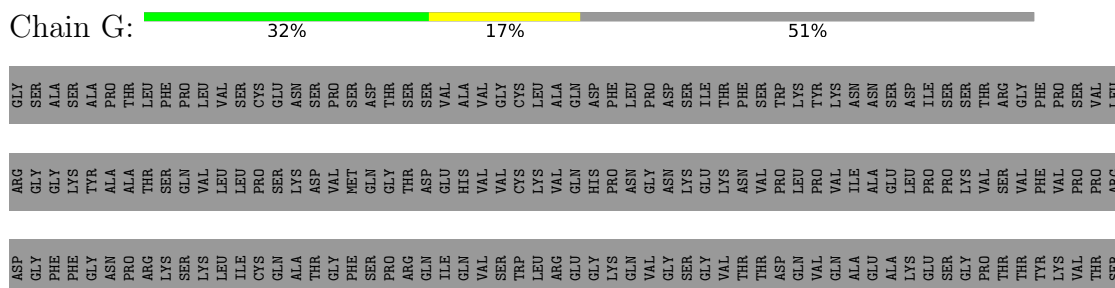


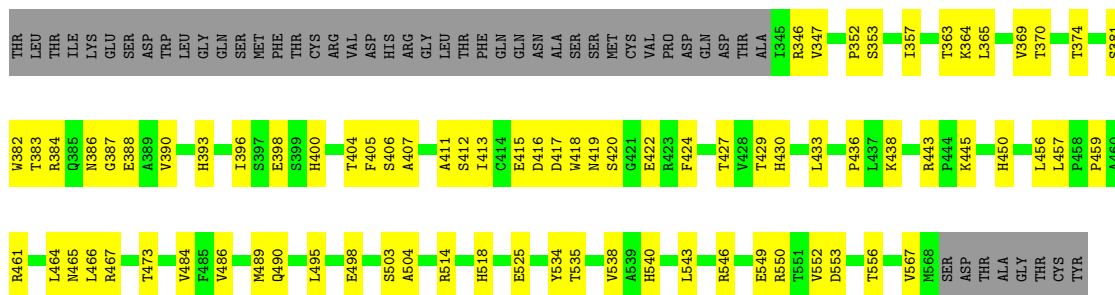
• Molecule 1: Immunoglobulin heavy constant mu

Chain D:

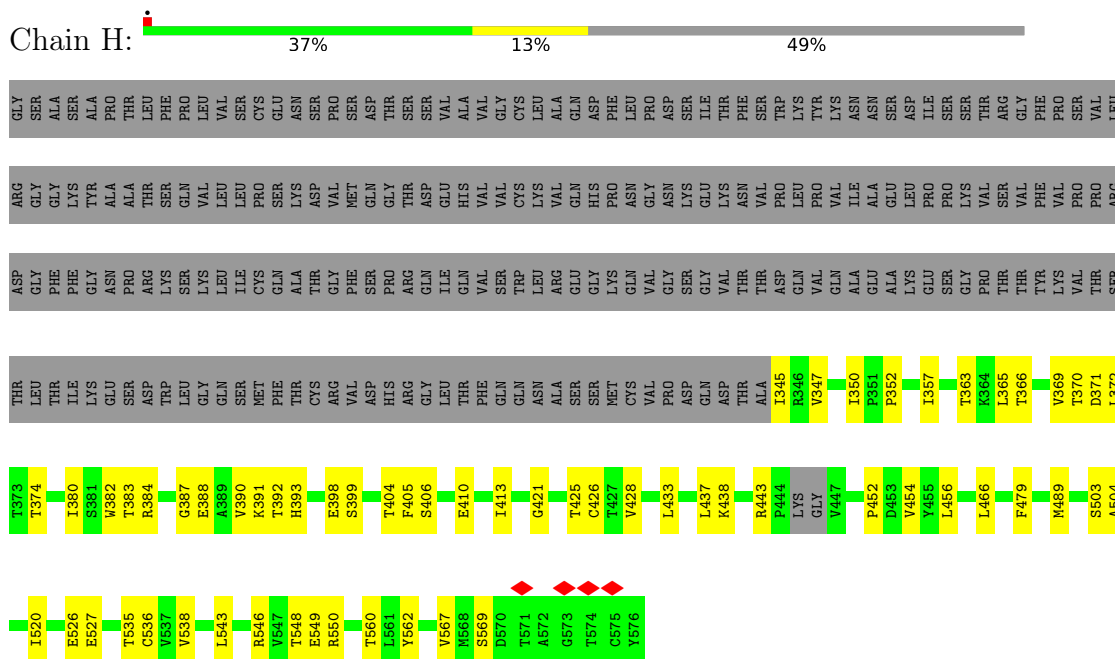


• Molecule 1: Immunoglobulin heavy constant mu

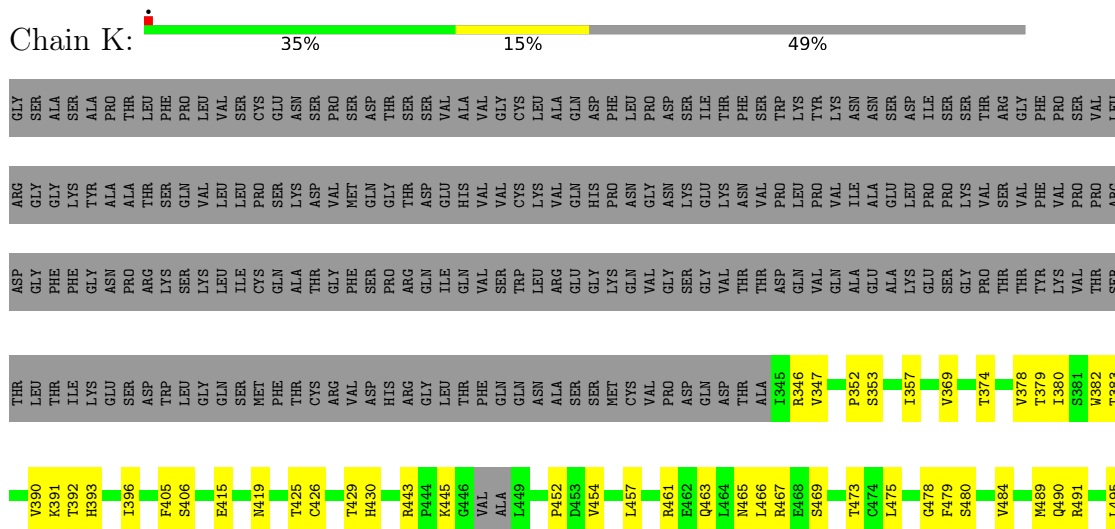


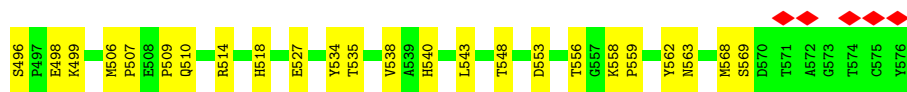


- Molecule 1: Immunoglobulin heavy constant mu



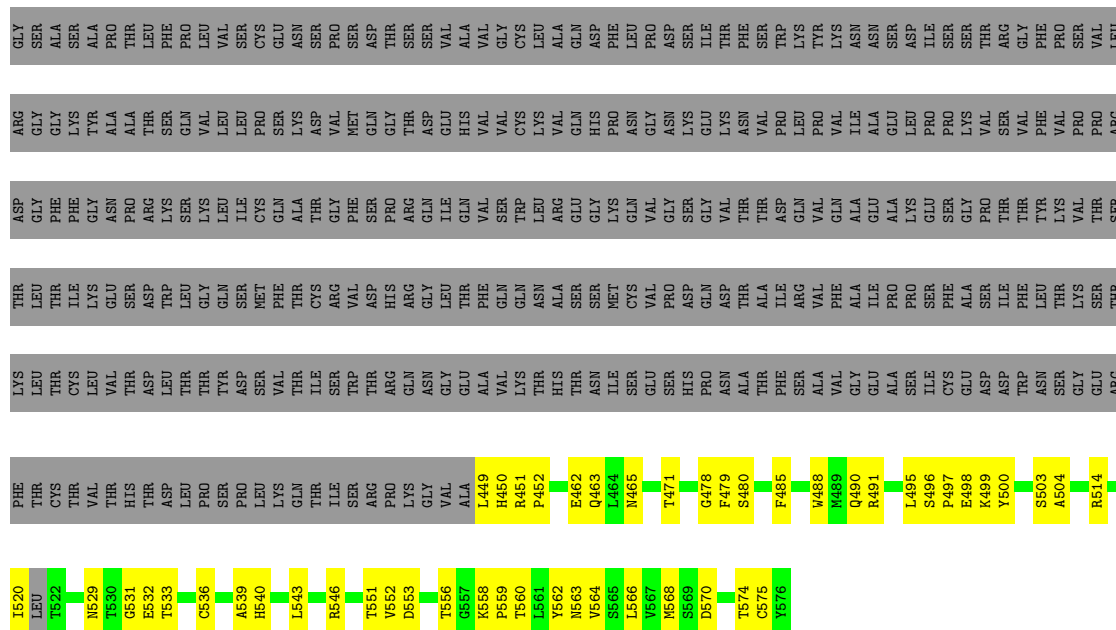
- Molecule 1: Immunoglobulin heavy constant mu





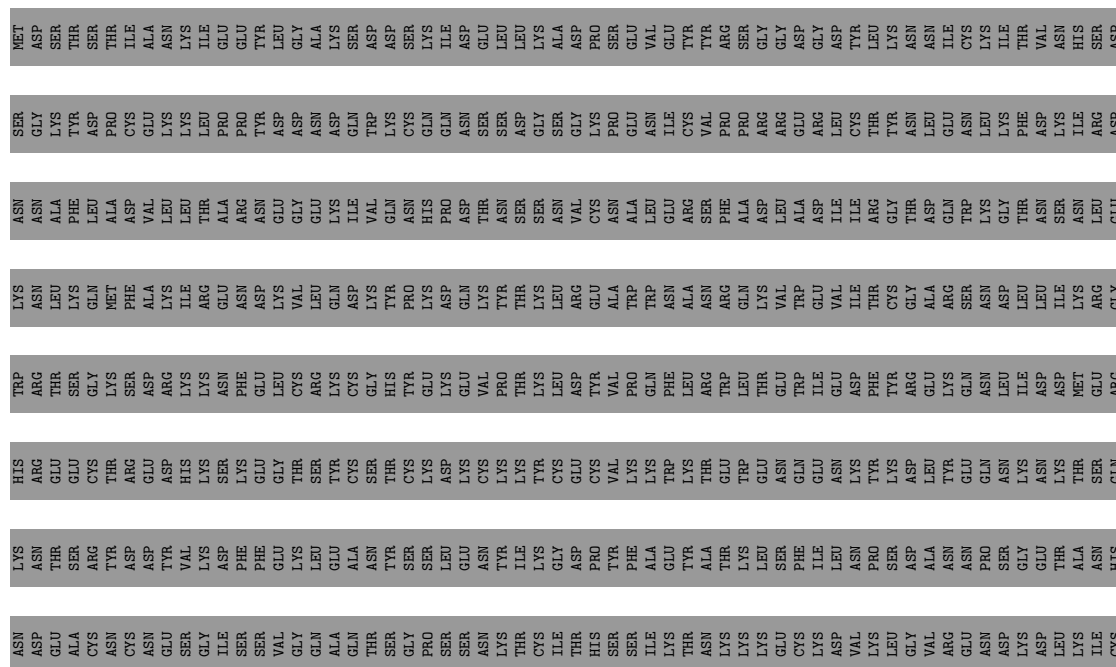
• Molecule 1: Immunoglobulin heavy constant mu

Chain L: 17% 11% 72%

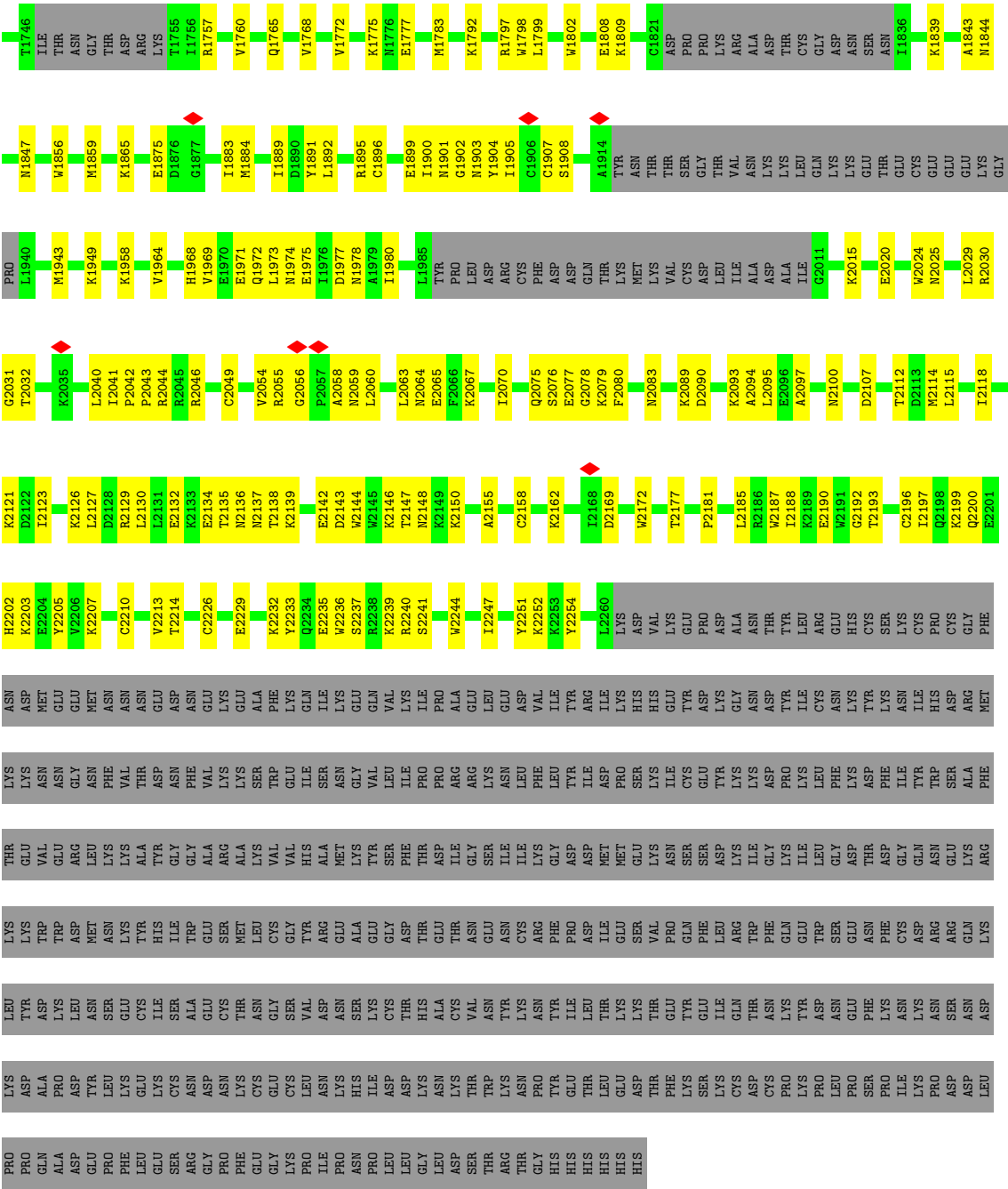


• Molecule 2: Erythrocyte membrane protein 1

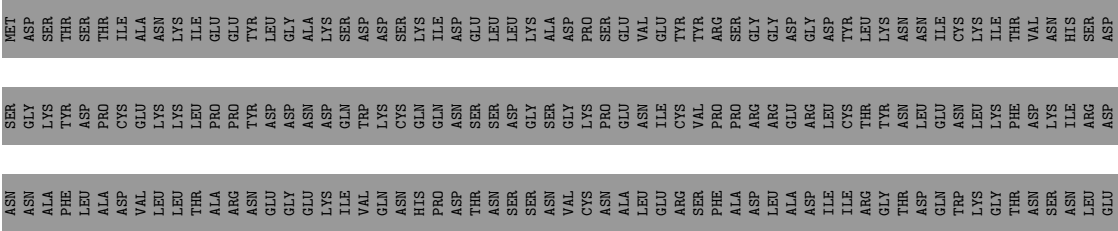
Chain I: 28% 13% 58%



R1627	R1628	Q1629	I1639	N1643	E1644	G1646	K1649	L1655	E1656	T1657	L1658	Q1659	I1660	V1661	R1664	K1671	Q1672	Y1673	T1676	G1677	K1678	D1681	K1685	I1691	R1692	D1697	V1708	H1709	T1713	K1714	Y1715	K1719	S1726	S1727	N1728	D1731	K1735	R1738	W1742									
A1535	P1544	E1545	C1546	I1547	F1551	F1553	I1554	F1555	N1558	I1559	E1560	Y1561	K1562	T1563	Y1564	Y1565	S1570	S1571	S1572	I1573	K1580	Y1581	Y1582	K1583	Y1584	N1585	N1586	A1587	K1590	N1591	N1592	L1595	K1599	D1600	N1601	D1602	W1605	K1611	E1614	N1615	G1616	R1617	S1618					
G1434	D1435	E1436	C1437	P1441	G1444	E1447	D1448	Q1449	S1452	W1453	F1454	K1455	E1456	W1457	F1461	C1462	I1463	E1464	T1478	ASN	GLY	LYS	ASN	GLY	LYS	C1486	S1491	GLY	GLN	G1494	I1497	Q1498	K1504	C1505	E1506	K1507	K1510	E1514	K1515	K1516	Q1517	E1518	W1519	D1520	K1521	K1525		
N1334	L1339	H1345	A1346	V1347	Q1348	R1349	Y1354	K1355	N1356	I1365	Y1366	E1367	H1368	K1371	I1379	I1380	E1381	K1382	P1385	GLN	GLN	LYS	ASN	GLY	LYS	C1486	S1491	GLY	GLN	SER	THR	E1399	N1400	V1401	N1402	R1410	E1411	W1412	W1413	I1420	T1421	K1422	I1423	N1424	K1425	T1431	F1432	N1433
K1106	Q1114	N1117	R1122	Q1125	I1126	Y1127	ALA	ASN	ALA	LYS	GLY	SER	GLN	ASN	LYS	VAL	V1139	S1142	N1143	F1147	E1151	I1154	N1159	GLY	ASP	TRP	S1163	K1164	I1177	K1178	K1179	C1180	N1183	H1186	G1187	E1188	E1189	I1190	F1191	S1192	E1193	K1194	L1195	K1196	E1199			
K1040	E1041	I1042	Q1043	Y1044	Q1045	Q1048	A1053	ASN	ILE	SER	CYS	ILE	CYS	ILE	ASP	VAL	ASP	VAL	GLY	GLY	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY			
LYS	TYR	ALA	CYS	GLN	CYS	LYS	ILE	PRO	T970	N971	E972	T974	R978	K979	E980	Y981	M982	C987	G988	SER	ALA	ARG	ALA	ARG	GLY	ASP	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY			
LEU	SER	VAL	ASN	LEU	ASP	ASN	ILE	CYS	ALA	ASP	LYS	LYS	ALA	PRO	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR		
ARG	TYR	SER	LYS	HIS	ILE	GLY	ASP	ALA	ASN	ASN	LYS	LYS	ALA	PRO	THR	LYS	ASN	CYS	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR		
THR	ALA	MET	LYS	HIS	GLY	ALA	GLY	MET	ILE	LYS	THR	THR	CYS	ASN	VAL	PHE	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY			
GLY	THR	SER	LYS	TRP	ILE	ASP	ASN	PHE	LEU	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR		
ASP	VAL	LYS	ASP	ILE	ASN	PHE	LEU	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR		
VAL	ILE	THR	ASN	CYS	GLY	THR	LYS	GLY	ASN	GLY	ASN	GLY	ASN	GLY	ASN	GLY	ASN	GLY	ASN	GLY	ASN	GLY	ASN	GLY	ASN	GLY	ASN	GLY	ASN	GLY	ASN	GLY	ASN	GLY	ASN	GLY	ASN	GLY	ASN	GLY	ASN	GLY	ASN	GLY	ASN			

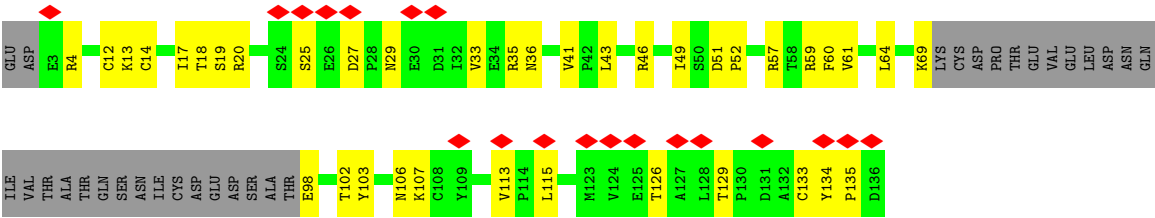


• Molecule 2: Erythrocyte membrane protein 1





- Molecule 3: Immunoglobulin J chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	371049	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 ($e^-/\text{\AA}^2$)	51	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.047	Depositor
Minimum map value	-0.018	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00805	Depositor
Map size (Å)	594.0, 594.0, 594.0	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	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	0.09	0/1053	0.29	0/1442
1	B	0.12	0/1809	0.36	0/2478
1	C	0.11	0/1794	0.34	0/2457
1	D	0.11	0/1788	0.33	0/2449
1	E	0.11	0/1788	0.36	0/2449
1	F	0.12	0/1767	0.34	0/2420
1	G	0.11	0/1788	0.33	0/2449
1	H	0.11	0/1830	0.32	0/2507
1	K	0.11	0/1831	0.35	0/2506
1	L	0.13	0/1019	0.40	0/1395
2	I	0.11	0/9392	0.33	0/12593
2	M	0.12	0/9392	0.36	0/12593
3	J	0.12	0/864	0.36	0/1173
All	All	0.11	0/36115	0.34	0/48911

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1026	0	1001	35	0
1	B	1764	0	1724	65	0
1	C	1749	0	1713	49	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1743	0	1709	41	0
1	E	1743	0	1709	48	0
1	F	1723	0	1682	41	0
1	G	1743	0	1708	56	0
1	H	1785	0	1735	43	0
1	K	1786	0	1737	46	0
1	L	993	0	959	38	0
2	I	9208	0	8976	245	0
2	M	9208	0	8974	246	0
3	J	851	0	843	38	0
All	All	35322	0	34470	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 14.

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:K:369:VAL:O	1:K:406:SER:HA	1.58	1.04
2:I:1191:PHE:O	2:I:1194:LYS:HB2	1.66	0.93
3:J:4:ARG:HH22	3:J:36:ASN:H	1.23	0.87
1:B:490:GLN:HG2	1:B:491:ARG:HG2	1.60	0.83
1:C:452:PRO:HB3	1:C:479:PHE:HB3	1.61	0.81
1:H:347:VAL:HG22	1:H:369:VAL:HG12	1.64	0.80
2:M:1367:GLU:CD	2:M:1368:HIS:H	1.90	0.80
1:B:452:PRO:HB3	1:B:479:PHE:HB3	1.62	0.79
2:M:2075:GLN:NE2	2:M:2155:ALA:O	2.16	0.79
1:B:428:VAL:O	1:B:436:PRO:HA	1.84	0.78
1:D:426:CYS:HB3	1:D:439:GLN:HB2	1.67	0.77
1:D:527:GLU:OE1	1:D:534:TYR:OH	2.02	0.77
3:J:4:ARG:HH21	3:J:18:THR:HG23	1.49	0.77
2:I:2067:LYS:HA	2:I:2070:ILE:HG12	1.69	0.73
1:K:452:PRO:HB3	1:K:479:PHE:HB3	1.70	0.73
2:I:2129:ARG:NH1	2:I:2132:GLU:O	2.21	0.73
2:M:2139:LYS:HD3	2:M:2142:GLU:HB3	1.71	0.73
2:I:1900:ILE:HB	2:I:1908:SER:HB2	1.71	0.72
2:M:2125:ILE:HG22	2:M:2129:ARG:HH11	1.54	0.72
3:J:4:ARG:HH11	3:J:20:ARG:HB2	1.53	0.71
1:B:454:VAL:HG21	1:B:538:VAL:HG11	1.70	0.71
1:D:425:THR:HG22	1:D:440:THR:HG22	1.73	0.70
2:I:1626:PRO:HA	2:I:1629:GLN:HE21	1.57	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2060:LEU:HD11	2:I:2064:ASN:HA	1.73	0.70
1:F:535:THR:HG22	1:F:551:THR:HB	1.74	0.70
1:K:378:VAL:HG12	1:K:430:HIS:HD2	1.56	0.69
2:I:1293:LYS:HE3	2:I:1380:ILE:HD13	1.74	0.69
1:D:489:MET:HB3	1:D:535:THR:HG23	1.75	0.69
2:I:2213:VAL:HG12	2:I:2214:THR:HG23	1.73	0.69
1:G:467:ARG:O	2:I:2059:ASN:ND2	2.26	0.69
2:M:1365:ILE:H	2:M:1369:ILE:HD11	1.57	0.69
1:L:478:GLY:O	1:L:514:ARG:NH2	2.27	0.68
2:M:1497:ILE:HG22	2:M:1499:GLY:H	1.57	0.68
1:C:463:GLN:NE2	1:C:469:SER:O	2.27	0.68
1:B:489:MET:O	1:B:535:THR:OG1	2.08	0.68
1:D:452:PRO:HB3	1:D:479:PHE:HB3	1.74	0.68
2:I:1122:ARG:NH1	2:I:1125:GLN:O	2.27	0.68
1:C:380:ILE:HG21	1:C:407:ALA:HB1	1.76	0.68
1:A:458:PRO:HA	1:A:472:ILE:HD12	1.76	0.68
2:I:1226:TYR:HE2	2:I:1228:ARG:HH12	1.42	0.68
1:D:393:HIS:HD2	1:D:396:ILE:HD11	1.58	0.68
2:I:2029:LEU:O	2:I:2032:THR:OG1	2.11	0.68
2:M:2054:VAL:HG12	2:M:2056:GLY:H	1.59	0.67
2:I:987:CYS:HA	2:I:1005:CYS:HA	1.76	0.67
2:M:1028:ASP:OD2	2:M:1125:GLN:NE2	2.27	0.67
1:G:383:THR:HB	1:G:387:GLY:HA2	1.74	0.67
1:G:567:VAL:HB	1:H:567:VAL:HG12	1.75	0.67
1:C:384:ARG:HB2	1:C:388:GLU:HB2	1.77	0.67
1:H:369:VAL:O	1:H:406:SER:HA	1.94	0.67
1:E:454:VAL:HG22	1:E:476:VAL:HG22	1.77	0.67
1:C:347:VAL:HG22	1:C:369:VAL:HG13	1.77	0.67
1:C:347:VAL:HG13	1:C:369:VAL:HG22	1.77	0.67
2:M:1869:LYS:HD3	2:M:1874:SER:HA	1.77	0.66
2:M:978:ARG:NH2	2:M:1099:CYS:SG	2.68	0.66
1:B:382:TRP:HB3	1:B:384:ARG:HH22	1.60	0.66
1:F:357:ILE:HD13	1:F:363:THR:HB	1.77	0.66
1:F:532:GLU:HB3	1:F:534:TYR:CZ	2.31	0.66
1:D:451:ARG:HH12	1:D:544:PRO:HD3	1.61	0.66
2:M:1572:SER:O	2:M:1575:SER:N	2.26	0.66
1:G:461:ARG:O	1:G:465:ASN:ND2	2.27	0.66
2:I:1757:ARG:HA	2:I:1760:VAL:HG22	1.78	0.66
1:G:427:THR:HG22	1:G:438:LYS:HG2	1.78	0.66
2:I:2079:LYS:HD2	2:I:2094:ALA:HB1	1.78	0.66
2:M:1348:GLN:NE2	2:M:1437:CYS:SG	2.69	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:1736:ARG:HH22	2:M:1740:ASP:HB3	1.60	0.66
1:B:383:THR:HB	1:B:387:GLY:HA2	1.78	0.65
1:E:465:ASN:O	1:E:467:ARG:NH1	2.29	0.65
1:G:357:ILE:HD12	1:G:363:THR:HG22	1.76	0.65
1:B:456:LEU:HD13	1:B:474:CYS:HB3	1.77	0.65
1:H:384:ARG:HG3	1:H:388:GLU:HB2	1.78	0.65
1:K:465:ASN:HA	1:K:467:ARG:HH11	1.62	0.65
1:C:379:THR:HB	1:C:429:THR:HB	1.78	0.65
2:I:1420:ILE:O	2:I:1424:ASN:ND2	2.30	0.65
2:M:1346:ALA:HA	2:M:1349:ARG:HD2	1.78	0.65
1:G:384:ARG:NH1	1:G:388:GLU:OE1	2.29	0.65
1:A:548:THR:HB	1:A:550:ARG:HH12	1.61	0.65
1:G:489:MET:HB3	1:G:535:THR:OG1	1.97	0.65
2:I:2076:SER:HB3	2:I:2158:CYS:HB2	1.79	0.64
2:I:1515:LYS:NZ	2:I:1518:GLU:OE1	2.25	0.64
2:M:1226:TYR:O	2:M:1228:ARG:NH1	2.29	0.64
1:F:426:CYS:SG	1:F:439:GLN:NE2	2.70	0.64
2:I:1348:GLN:NE2	2:I:1437:CYS:SG	2.71	0.64
2:M:1032:PHE:O	2:M:1035:PHE:HB3	1.97	0.64
1:C:533:THR:HG1	1:C:551:THR:HG1	1.44	0.64
2:I:1004:LEU:HA	2:I:1031:PHE:HE1	1.62	0.64
2:I:1045:GLN:OE1	2:I:1048:GLN:NE2	2.31	0.64
2:I:1964:VAL:O	2:I:1968:HIS:ND1	2.30	0.64
2:M:1669:LEU:O	2:M:1673:TYR:HB2	1.97	0.64
1:G:369:VAL:HB	1:G:407:ALA:HB3	1.80	0.63
1:A:478:GLY:HA2	1:A:514:ARG:HB3	1.80	0.63
2:M:2247:ILE:HA	2:M:2250:ARG:HE	1.63	0.63
2:I:1100:TYR:HA	2:I:1103:TRP:CD1	2.32	0.63
2:I:2236:TRP:HA	2:I:2239:LYS:HD2	1.81	0.63
2:I:2148:ASN:HB3	2:I:2177:THR:HB	1.81	0.63
2:M:2150:LYS:O	2:M:2154:ASN:ND2	2.31	0.63
2:M:2236:TRP:HE3	2:M:2240:ARG:HH11	1.47	0.62
2:M:2248:SER:HA	2:M:2254:TYR:HB2	1.81	0.62
1:A:544:PRO:O	1:A:546:ARG:NH1	2.32	0.62
1:C:416:ASP:OD2	1:C:417:ASP:N	2.32	0.62
2:I:2144:TRP:O	2:I:2148:ASN:ND2	2.32	0.62
1:F:374:THR:HA	1:F:405:PHE:HB2	1.81	0.62
1:F:393:HIS:HB3	1:F:410:GLU:H	1.64	0.62
1:A:493:GLN:NE2	1:A:494:PRO:O	2.33	0.62
2:I:1293:LYS:NZ	2:I:1379:ILE:O	2.32	0.62
1:L:449:LEU:N	1:L:480:SER:O	2.31	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:369:VAL:HG11	1:E:428:VAL:HG11	1.81	0.62
1:F:345:ILE:HD12	1:F:372:LEU:HD11	1.82	0.62
1:K:380:ILE:O	1:K:393:HIS:ND1	2.31	0.62
1:B:491:ARG:HH21	2:M:2055:ARG:CZ	2.12	0.62
1:E:380:ILE:HG12	1:E:428:VAL:HG22	1.82	0.62
2:M:2083:ASN:HB3	2:M:2086:LYS:HB3	1.80	0.61
1:C:486:VAL:HG12	1:C:538:VAL:HG23	1.81	0.61
2:M:1357:MET:HA	2:M:1363:VAL:HG21	1.81	0.61
1:H:352:PRO:HB2	1:H:357:ILE:HD11	1.81	0.61
2:I:2044:ARG:NH2	2:I:2097:ALA:O	2.33	0.61
2:M:1257:HIS:ND1	2:M:1365:ILE:O	2.33	0.61
1:B:535:THR:HB	1:B:549:GLU:OE2	2.01	0.61
1:C:398:GLU:O	1:C:406:SER:OG	2.18	0.61
1:F:484:VAL:HG23	1:F:540:HIS:HB2	1.81	0.61
2:I:1262:GLY:HA2	2:I:1525:LYS:HE2	1.83	0.61
1:A:491:ARG:NH1	1:A:533:THR:O	2.30	0.61
1:G:352:PRO:HB2	1:G:357:ILE:HD11	1.83	0.61
1:L:452:PRO:HB3	1:L:479:PHE:HB3	1.83	0.61
2:M:1857:ASN:O	2:M:1861:ASN:ND2	2.33	0.61
1:L:451:ARG:HD3	1:L:452:PRO:HD2	1.83	0.60
2:M:1142:SER:OG	2:M:1188:GLU:OE1	2.19	0.60
2:M:2029:LEU:O	2:M:2032:THR:OG1	2.19	0.60
2:M:1017:VAL:HG21	2:M:1959:MET:HG3	1.83	0.60
2:M:1121:PHE:O	2:M:1125:GLN:NE2	2.33	0.60
2:M:2249:LYS:NZ	2:M:2250:ARG:O	2.33	0.60
1:K:346:ARG:NH1	1:K:347:VAL:O	2.35	0.60
2:M:1016:THR:HG22	2:M:1026:GLY:HA2	1.83	0.60
2:M:1420:ILE:O	2:M:1424:ASN:ND2	2.35	0.60
2:M:2052:ARG:HE	2:M:2057:PRO:HG3	1.66	0.60
1:G:413:ILE:HD13	1:G:424:PHE:HE2	1.65	0.60
1:C:427:THR:HG22	1:C:438:LYS:HD3	1.83	0.60
2:M:1673:TYR:HE2	2:M:1686:LYS:HG3	1.65	0.60
1:B:442:SER:OG	1:B:445:LYS:NZ	2.35	0.60
1:E:467:ARG:NH2	2:I:1281:SER:O	2.29	0.60
1:H:382:TRP:CD2	1:H:426:CYS:HB3	2.36	0.60
3:J:14:CYS:HB2	3:J:102:THR:HG21	1.84	0.60
2:I:1093:CYS:SG	2:I:1094:LYS:N	2.73	0.60
1:K:391:LYS:NZ	1:K:392:THR:O	2.35	0.60
1:L:533:THR:O	1:L:551:THR:OG1	2.19	0.60
2:M:1046:ILE:HG13	2:M:1050:MET:HE3	1.83	0.60
1:G:461:ARG:HD3	1:G:465:ASN:HD21	1.67	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:36:ASN:ND2	1:L:563:ASN:OD1	2.35	0.59
1:L:450:HIS:ND1	1:L:480:SER:OG	2.30	0.59
2:M:1417:ARG:NH2	2:M:1439:VAL:O	2.34	0.59
2:M:2023:GLU:OE2	2:M:2046:ARG:NH2	2.34	0.59
1:G:346:ARG:NE	1:G:370:THR:OG1	2.35	0.59
1:H:345:ILE:HG21	1:H:433:LEU:HD12	1.84	0.59
1:H:489:MET:O	1:H:535:THR:OG1	2.17	0.59
2:I:1516:LYS:HD2	2:I:1555:PHE:HB3	1.83	0.59
2:I:2030:ARG:HE	2:I:2031:GLY:H	1.49	0.59
1:G:374:THR:HA	1:G:405:PHE:HB2	1.84	0.59
3:J:129:THR:OG1	3:J:133:CYS:SG	2.59	0.59
2:M:2241:SER:HA	2:M:2244:TRP:NE1	2.18	0.59
1:B:381:SER:OG	1:B:427:THR:OG1	2.19	0.59
1:K:443:ARG:HH12	1:K:445:LYS:HD3	1.68	0.59
1:L:496:SER:OG	1:L:498:GLU:OE1	2.20	0.59
1:F:452:PRO:HB3	1:F:479:PHE:HB3	1.84	0.59
2:I:1514:GLU:O	2:I:1517:GLN:NE2	2.36	0.59
2:I:2107:ASP:HB2	2:I:2112:THR:HB	1.83	0.59
2:M:1413:TRP:NE1	2:M:1439:VAL:O	2.33	0.59
1:G:553:ASP:OD1	1:G:556:THR:OG1	2.17	0.59
2:I:2147:THR:HG23	2:I:2150:LYS:HE2	1.85	0.59
1:D:383:THR:HB	1:D:387:GLY:HA2	1.85	0.59
2:M:2076:SER:HB3	2:M:2158:CYS:HB2	1.85	0.58
2:I:1334:ASN:ND2	2:I:1339:LEU:O	2.36	0.58
1:A:547:VAL:HG11	3:J:113:VAL:HG21	1.85	0.58
1:C:419:ASN:O	1:C:443:ARG:NH2	2.35	0.58
1:F:457:LEU:HB2	1:F:473:THR:HB	1.85	0.58
3:J:103:TYR:HB2	1:L:574:THR:HA	1.84	0.58
2:M:1100:TYR:HA	2:M:1103:TRP:HD1	1.68	0.58
2:M:1724:PHE:HD2	2:M:1738:ARG:HG2	1.69	0.58
2:I:2055:ARG:NH2	2:I:2059:ASN:OD1	2.36	0.58
1:H:370:THR:HG22	1:H:406:SER:HB2	1.85	0.58
1:H:391:LYS:NZ	1:H:392:THR:O	2.34	0.58
2:M:1702:ILE:O	2:M:1738:ARG:NH1	2.37	0.58
1:G:384:ARG:NE	1:G:386:ASN:OD1	2.36	0.58
1:L:562:TYR:HB3	1:L:564:VAL:HG23	1.86	0.58
1:G:459:PRO:HG2	1:G:464:LEU:HD11	1.86	0.58
2:I:2041:ILE:O	2:I:2046:ARG:NH2	2.37	0.58
2:M:981:TYR:HE2	2:M:1099:CYS:HB3	1.68	0.58
1:C:381:SER:HA	1:C:393:HIS:HE1	1.68	0.58
1:C:491:ARG:NH2	1:C:532:GLU:OE1	2.36	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:2075:GLN:HE22	2:M:2156:MET:HA	1.69	0.58
1:B:549:GLU:O	1:B:550:ARG:NH1	2.30	0.57
1:G:398:GLU:O	1:G:406:SER:OG	2.21	0.57
2:I:2029:LEU:HD22	2:I:2115:LEU:HD12	1.85	0.57
2:I:1345:HIS:C	2:I:1349:ARG:HE	2.13	0.57
2:I:2015:LYS:HB3	2:I:2078:GLY:HA2	1.87	0.57
1:K:454:VAL:HG21	1:K:538:VAL:HG11	1.86	0.57
2:I:1305:HIS:HE1	2:I:1422:LYS:HD2	1.69	0.57
2:M:1038:TRP:O	2:M:1041:GLU:HG3	2.03	0.57
2:I:1033:ASN:HB3	2:I:1949:LYS:HD2	1.86	0.57
2:M:1036:GLU:O	2:M:1039:ASN:HB3	2.03	0.57
2:M:1765:GLN:HG2	2:M:1783:MET:HE2	1.86	0.57
2:M:2143:ASP:OD1	2:M:2144:TRP:N	2.38	0.57
2:M:2145:TRP:HE1	2:M:2178:THR:HA	1.68	0.57
1:F:393:HIS:ND1	1:F:408:VAL:O	2.38	0.57
2:I:1799:LEU:HD13	2:I:1859:MET:HG3	1.87	0.57
2:M:1219:CYS:N	2:M:1418:CYS:SG	2.78	0.57
2:M:2200:GLN:HA	2:M:2203:LYS:HZ3	1.70	0.57
1:A:500:TYR:HB3	1:A:521:LEU:HD13	1.87	0.57
1:B:450:HIS:CE1	1:B:514:ARG:HH21	2.23	0.57
2:I:979:LYS:HA	2:I:982:MET:HE3	1.86	0.57
1:A:451:ARG:NH2	1:A:542:ALA:O	2.38	0.57
1:F:454:VAL:HG22	1:F:476:VAL:HG22	1.86	0.57
2:M:1293:LYS:NZ	2:M:1379:ILE:O	2.36	0.57
2:M:1757:ARG:HA	2:M:1760:VAL:HG22	1.87	0.56
2:M:2026:ASP:OD2	2:M:2030:ARG:NH2	2.37	0.56
1:D:527:GLU:O	1:D:530:THR:OG1	2.18	0.56
1:E:399:SER:HA	1:E:405:PHE:HA	1.86	0.56
2:I:1356:ASN:HD22	2:I:1449:GLN:HG2	1.69	0.56
2:I:2024:TRP:CD1	2:I:2043:PRO:HD3	2.40	0.56
2:M:1113:LYS:O	2:M:1117:ASN:ND2	2.38	0.56
1:E:452:PRO:HB3	1:E:479:PHE:HB3	1.86	0.56
1:H:536:CYS:N	1:H:549:GLU:OE2	2.37	0.56
2:I:1452:SER:O	2:I:1456:GLU:HG2	2.05	0.56
3:J:33:VAL:HB	1:L:559:PRO:HA	1.85	0.56
1:G:430:HIS:HB3	1:G:433:LEU:HD13	1.87	0.56
1:H:452:PRO:HB3	1:H:479:PHE:HB3	1.88	0.56
2:I:2181:PRO:HB3	2:I:2185:LEU:HD22	1.86	0.56
1:L:558:LYS:HZ3	1:L:560:THR:HA	1.70	0.56
2:I:2024:TRP:HD1	2:I:2042:PRO:HA	1.70	0.56
2:M:2077:GLU:HA	2:M:2080:PHE:HB3	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:2236:TRP:O	2:M:2240:ARG:NH1	2.39	0.56
1:C:565:SER:O	1:C:567:VAL:HG23	2.06	0.56
1:E:383:THR:HA	1:E:389:ALA:HA	1.87	0.56
1:E:416:ASP:OD1	1:E:417:ASP:N	2.39	0.56
2:I:1599:LYS:O	2:I:1672:GLN:NE2	2.39	0.56
2:I:1856:TRP:HA	2:I:1859:MET:SD	2.46	0.56
2:M:1043:GLN:O	2:M:1046:ILE:HG22	2.06	0.56
2:I:1122:ARG:NH1	2:I:1125:GLN:OE1	2.39	0.56
1:D:423:ARG:HA	1:D:442:SER:HB3	1.88	0.55
1:G:382:TRP:HB2	1:G:390:VAL:HG21	1.87	0.55
1:G:486:VAL:HG12	1:G:538:VAL:HG23	1.88	0.55
2:M:2213:VAL:HG12	2:M:2214:THR:HG23	1.88	0.55
2:M:1122:ARG:NH1	2:M:1139:VAL:O	2.39	0.55
2:M:1151:GLU:HA	2:M:1154:ILE:HG22	1.88	0.55
2:M:1100:TYR:HA	2:M:1103:TRP:CD1	2.41	0.55
1:E:459:PRO:HD3	1:E:472:ILE:HG13	1.87	0.55
3:J:4:ARG:NH2	3:J:18:THR:O	2.40	0.55
2:M:1421:THR:HA	2:M:1424:ASN:HD21	1.72	0.55
2:M:2075:GLN:HA	2:M:2079:LYS:H	1.72	0.55
2:M:2125:ILE:HG22	2:M:2129:ARG:NH1	2.22	0.55
2:M:2142:GLU:O	2:M:2146:LYS:N	2.34	0.55
2:I:1644:GLU:OE2	2:I:1719:LYS:NZ	2.39	0.55
2:M:1850:ASN:HD22	2:M:1853:ARG:HH12	1.55	0.55
2:I:978:ARG:NH2	2:I:1099:CYS:SG	2.72	0.55
2:M:1701:ILE:HG22	2:M:1706:ASP:HB2	1.88	0.55
2:I:1154:ILE:HG21	2:I:1164:LYS:HE2	1.89	0.55
1:K:465:ASN:HA	1:K:467:ARG:NH1	2.22	0.55
1:D:383:THR:OG1	1:D:425:THR:OG1	2.25	0.55
1:D:402:ASN:OD1	1:D:404:THR:OG1	2.21	0.55
2:M:2095:LEU:HD22	2:M:2172:TRP:HD1	1.72	0.55
1:C:369:VAL:HG11	1:C:428:VAL:HG21	1.88	0.54
2:M:1871:ASN:ND2	2:M:1877:GLY:O	2.38	0.54
2:I:1041:GLU:O	2:I:1045:GLN:N	2.38	0.54
1:K:374:THR:HA	1:K:405:PHE:HB2	1.89	0.54
2:M:1421:THR:HG22	2:M:1433:ASN:HA	1.89	0.54
1:C:400:HIS:CD2	1:C:406:SER:HB3	2.42	0.54
1:C:567:VAL:HG12	1:C:567:VAL:O	2.07	0.54
1:F:489:MET:HB3	1:F:535:THR:OG1	2.08	0.54
2:M:1821:CYS:O	2:M:1957:HIS:NE2	2.40	0.54
2:M:2036:HIS:CE1	2:M:2250:ARG:HH22	2.25	0.54
2:M:2107:ASP:HB3	2:M:2112:THR:HB	1.88	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1151:GLU:HA	2:I:1154:ILE:HG22	1.89	0.54
1:K:353:SER:O	1:K:357:ILE:HG12	2.08	0.54
2:M:2015:LYS:HB3	2:M:2078:GLY:HA2	1.88	0.54
1:A:459:PRO:HG3	1:A:470:ALA:HB1	1.89	0.54
3:J:57:ARG:NH2	3:J:59:ARG:O	2.40	0.54
2:M:1719:LYS:O	2:M:1723:ILE:HG12	2.06	0.54
2:I:1183:ASN:HB2	2:I:1186:HIS:HB3	1.90	0.54
2:M:1473:ARG:O	2:M:1477:THR:OG1	2.19	0.54
2:I:971:ASN:OD1	2:I:974:THR:OG1	2.26	0.54
2:I:1792:LYS:O	2:I:1797:ARG:NH1	2.41	0.54
2:M:1227:ILE:HD11	2:M:1302:ASN:HB3	1.90	0.54
2:M:2016:THR:HG21	2:M:2081:LEU:HD22	1.90	0.54
1:E:489:MET:HB3	1:E:535:THR:OG1	2.08	0.54
2:I:1605:TRP:CE2	2:I:1626:PRO:HD3	2.43	0.54
2:M:978:ARG:HH12	2:M:1095:GLU:HB2	1.73	0.54
1:E:393:HIS:HB3	1:E:410:GLU:H	1.73	0.54
1:H:393:HIS:HB2	1:H:410:GLU:HG3	1.88	0.54
2:I:1895:ARG:NH2	2:I:1904:TYR:O	2.40	0.53
2:I:1949:LYS:O	2:I:1958:LYS:NZ	2.34	0.53
2:M:1985:LEU:HB2	2:M:2149:LYS:HE3	1.90	0.53
2:I:1349:ARG:NH1	2:I:1456:GLU:OE1	2.41	0.53
2:M:1955:SER:HA	2:M:1958:LYS:HD3	1.89	0.53
1:B:535:THR:HG22	1:B:551:THR:HG23	1.89	0.53
1:E:391:LYS:NZ	1:E:392:THR:O	2.36	0.53
1:H:345:ILE:N	1:H:371:ASP:O	2.42	0.53
2:I:2044:ARG:HH12	2:I:2100:ASN:HB2	1.72	0.53
2:I:2241:SER:HA	2:I:2244:TRP:CH2	2.44	0.53
1:L:503:SER:OG	1:L:504:ALA:N	2.41	0.53
2:M:1786:GLU:OE2	2:M:1787:HIS:ND1	2.41	0.53
1:B:383:THR:OG1	1:B:425:THR:OG1	2.26	0.53
2:I:1399:GLU:HG2	2:I:1401:VAL:HG22	1.89	0.53
2:I:2025:ASN:HA	2:I:2040:LEU:HD22	1.91	0.53
1:A:499:LYS:NZ	1:A:522:THR:O	2.41	0.53
1:D:380:ILE:HD13	1:D:407:ALA:HB1	1.89	0.53
1:D:433:LEU:HD21	1:D:437:LEU:HB2	1.90	0.53
2:I:1114:GLN:HA	2:I:1117:ASN:HD21	1.73	0.53
1:F:347:VAL:HG22	1:F:369:VAL:HG13	1.91	0.53
1:H:543:LEU:HD13	1:H:548:THR:HG23	1.91	0.53
2:I:2064:ASN:HB3	2:I:2067:LYS:HE3	1.90	0.53
3:J:46:ARG:NH1	3:J:51:ASP:O	2.30	0.53
1:K:480:SER:HB3	1:K:514:ARG:HE	1.74	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:ILE:HG23	1:B:428:VAL:HG12	1.91	0.53
2:M:1853:ARG:HE	2:M:1948:ASN:HA	1.72	0.53
1:C:450:HIS:HB2	1:C:480:SER:HB3	1.89	0.53
1:F:380:ILE:HG21	1:F:409:GLY:HA3	1.90	0.53
2:I:1497:ILE:O	2:I:1498:GLN:NE2	2.34	0.53
2:I:2134:GLU:HG2	2:I:2136:ASN:H	1.74	0.53
3:J:4:ARG:HE	3:J:18:THR:HG23	1.74	0.53
1:B:532:GLU:HB3	1:B:534:TYR:CZ	2.44	0.53
1:H:393:HIS:HB3	1:H:410:GLU:H	1.73	0.53
2:I:1143:ASN:HB3	2:I:1973:LEU:HD21	1.91	0.53
2:I:1425:LYS:HA	2:I:1431:ILE:HG12	1.91	0.53
2:M:1516:LYS:NZ	2:M:1555:PHE:O	2.35	0.53
1:B:543:LEU:HB2	1:B:546:ARG:HA	1.91	0.52
2:I:2233:TYR:HA	2:I:2236:TRP:NE1	2.24	0.52
1:K:489:MET:HB3	1:K:535:THR:OG1	2.08	0.52
2:M:1143:ASN:HB3	2:M:1973:LEU:HD11	1.91	0.52
2:M:1681:ASP:OD1	2:M:1682:ASP:N	2.40	0.52
2:I:1570:TYR:C	2:I:1572:SER:H	2.15	0.52
1:E:396:ILE:HG23	1:E:407:ALA:HA	1.91	0.52
1:G:503:SER:OG	1:G:504:ALA:N	2.42	0.52
2:I:1580:LYS:O	2:I:1590:LYS:NZ	2.42	0.52
2:M:1154:ILE:HG21	2:M:1164:LYS:HE2	1.91	0.52
2:M:1740:ASP:OD1	2:M:1741:TRP:N	2.42	0.52
2:M:2247:ILE:HA	2:M:2250:ARG:NE	2.24	0.52
2:I:2137:ASN:OD1	2:I:2139:LYS:NZ	2.42	0.52
3:J:4:ARG:NH2	3:J:36:ASN:HB2	2.24	0.52
1:B:503:SER:HG	1:B:518:HIS:H	1.58	0.52
1:H:503:SER:OG	1:H:504:ALA:N	2.40	0.52
2:M:2017:LYS:HE3	2:M:2047:GLN:HB3	1.92	0.52
2:M:1838:CYS:SG	2:M:1960:LYS:NZ	2.82	0.52
1:G:365:LEU:HB2	1:G:411:ALA:HB3	1.92	0.52
1:K:463:GLN:NE2	1:K:469:SER:O	2.43	0.52
2:M:1147:PHE:CE1	2:M:1969:VAL:HG22	2.44	0.52
2:M:1193:GLU:O	2:M:1197:ASN:ND2	2.42	0.52
1:C:393:HIS:CD2	1:C:409:GLY:HA2	2.45	0.52
1:D:475:LEU:HD12	1:D:518:HIS:HE2	1.75	0.52
1:F:347:VAL:HG13	1:F:369:VAL:HG22	1.92	0.52
2:I:1681:ASP:O	2:I:1685:LYS:HG2	2.10	0.52
1:H:383:THR:HB	1:H:387:GLY:HA2	1.92	0.52
2:I:1639:ILE:O	2:I:1643:ASN:ND2	2.43	0.52
2:I:1655:LEU:HD12	2:I:1658:LEU:HD11	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:1354:TYR:O	2:M:1358:ILE:HG23	2.09	0.52
1:F:530:THR:OG1	2:M:1238:LYS:NZ	2.41	0.51
2:I:2015:LYS:HG3	2:I:2077:GLU:HB3	1.91	0.51
2:M:1356:ASN:HD22	2:M:1449:GLN:HG2	1.73	0.51
2:I:2060:LEU:HB2	2:I:2127:LEU:HD12	1.92	0.51
2:I:2095:LEU:HD13	2:I:2172:TRP:CD1	2.44	0.51
2:M:1381:GLU:OE1	2:M:1400:ASN:ND2	2.44	0.51
2:I:1627:ARG:NH1	2:I:1697:ASP:OD2	2.43	0.51
2:M:1981:LYS:HD3	2:M:1984:LYS:HZ3	1.75	0.51
1:H:569:SER:O	1:H:569:SER:OG	2.29	0.51
2:I:1399:GLU:N	2:I:1402:ASN:OD1	2.44	0.51
2:M:1254:THR:OG1	2:M:1258:GLY:O	2.25	0.51
2:M:2080:PHE:HB2	2:M:2162:LYS:HG3	1.93	0.51
2:M:2175:ILE:HD12	2:M:2176:PRO:HD2	1.92	0.51
1:L:488:TRP:HB3	1:L:495:LEU:HD12	1.93	0.51
2:M:1710:ASP:OD1	2:M:1713:THR:OG1	2.27	0.51
1:C:367:CYS:HB2	1:C:382:TRP:CZ2	2.46	0.51
1:D:503:SER:OG	1:D:504:ALA:N	2.43	0.51
2:I:1421:THR:HA	2:I:1424:ASN:HD21	1.76	0.51
2:I:1457:TRP:NE1	2:I:1518:GLU:OE1	2.36	0.51
2:I:2118:ILE:HA	2:I:2121:LYS:HZ3	1.74	0.51
2:I:2129:ARG:NH2	2:I:2135:THR:HG22	2.25	0.51
2:M:2244:TRP:O	2:M:2247:ILE:HG22	2.11	0.51
1:G:416:ASP:OD1	1:G:417:ASP:N	2.44	0.51
1:G:466:LEU:HD11	2:I:2056:GLY:HA3	1.92	0.51
3:J:4:ARG:NH2	3:J:18:THR:HG23	2.21	0.51
3:J:29:ASN:HD22	1:L:529:ASN:HD22	1.57	0.51
1:C:346:ARG:NE	1:C:370:THR:OG1	2.42	0.51
1:C:489:MET:HB3	1:C:535:THR:HG23	1.92	0.51
2:I:1147:PHE:CE2	2:I:1969:VAL:HG22	2.46	0.51
2:I:1975:GLU:HA	2:I:1978:ASN:HD21	1.75	0.51
1:B:486:VAL:HG12	1:B:538:VAL:HG23	1.92	0.51
1:K:568:MET:HA	1:L:568:MET:SD	2.51	0.51
2:M:1443:THR:OG1	2:M:1445:ASN:OD1	2.20	0.51
1:A:467:ARG:HD2	1:A:525:GLU:HG3	1.92	0.51
1:E:384:ARG:HD2	1:E:388:GLU:HB2	1.93	0.51
1:H:380:ILE:HG13	1:H:428:VAL:HG22	1.92	0.51
1:K:489:MET:HE2	1:K:489:MET:HA	1.93	0.51
1:K:563:ASN:HB3	1:L:563:ASN:HA	1.93	0.51
1:K:383:THR:HG22	1:K:390:VAL:HG11	1.93	0.50
2:M:1582:TYR:HB2	2:M:1590:LYS:HD3	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:489:MET:HE2	1:B:489:MET:HA	1.94	0.50
1:G:467:ARG:HA	1:G:525:GLU:HG3	1.93	0.50
2:I:1305:HIS:CE1	2:I:1422:LYS:HD2	2.46	0.50
2:I:1249:TRP:HB3	2:I:1264:CYS:HB3	1.92	0.50
1:K:352:PRO:HB2	1:K:357:ILE:HD11	1.92	0.50
2:M:1723:ILE:HG13	2:M:1724:PHE:N	2.27	0.50
2:M:2169:ASP:OD1	2:M:2169:ASP:N	2.44	0.50
1:A:459:PRO:HB3	1:A:471:THR:H	1.76	0.50
2:I:2015:LYS:HE2	2:I:2077:GLU:HB2	1.92	0.50
1:A:553:ASP:H	1:A:556:THR:HG22	1.77	0.50
1:F:467:ARG:HB2	1:F:467:ARG:NH1	2.25	0.50
1:G:484:VAL:HG12	1:G:540:HIS:CD2	2.47	0.50
2:I:1772:VAL:HG13	2:I:1777:GLU:HG3	1.94	0.50
1:K:496:SER:HB3	1:K:499:LYS:HD3	1.93	0.50
2:M:1723:ILE:HG13	2:M:1724:PHE:H	1.77	0.50
2:I:1671:LYS:HD3	2:I:1775:LYS:HE2	1.94	0.50
2:I:2169:ASP:N	2:I:2169:ASP:OD1	2.44	0.50
2:M:1452:SER:O	2:M:1456:GLU:HG2	2.11	0.50
2:M:2123:ILE:O	2:M:2127:LEU:HD23	2.12	0.50
1:E:443:ARG:O	1:E:445:LYS:NZ	2.45	0.50
2:I:1839:LYS:HB2	2:I:1964:VAL:HG21	1.93	0.50
1:D:384:ARG:HG2	1:D:385:GLN:H	1.75	0.50
2:I:1097:CYS:SG	2:I:1101:LYS:NZ	2.84	0.50
2:M:2183:GLN:HA	2:M:2186:ARG:HB3	1.92	0.50
1:D:382:TRP:HB2	1:D:390:VAL:HG21	1.94	0.50
1:K:465:ASN:OD1	1:K:466:LEU:HD12	2.11	0.50
1:B:491:ARG:NH2	2:M:2055:ARG:HG2	2.27	0.49
1:D:466:LEU:HG	1:D:468:GLU:OE1	2.12	0.49
1:G:347:VAL:HG23	1:G:369:VAL:HG22	1.94	0.49
2:I:1768:VAL:O	2:I:1772:VAL:HG23	2.12	0.49
2:I:2188:ILE:O	2:I:2192:GLY:N	2.41	0.49
1:K:553:ASP:O	1:K:556:THR:OG1	2.26	0.49
2:M:2222:GLU:HG3	2:M:2224:ASN:H	1.77	0.49
1:F:454:VAL:HG21	1:F:538:VAL:HG11	1.92	0.49
1:K:378:VAL:HG12	1:K:430:HIS:CD2	2.41	0.49
2:M:1349:ARG:NE	2:M:1456:GLU:OE2	2.45	0.49
1:G:457:LEU:HB2	1:G:473:THR:OG1	2.13	0.49
2:I:1896:CYS:O	2:I:1907:CYS:HB2	2.13	0.49
1:K:484:VAL:HG12	1:K:540:HIS:CD2	2.47	0.49
2:M:2186:ARG:NH1	2:M:2190:GLU:HB2	2.28	0.49
1:B:463:GLN:NE2	1:B:469:SER:O	2.46	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1177:ILE:HD11	2:I:1980:ILE:HD11	1.93	0.49
2:I:1411:GLU:N	2:I:1411:GLU:OE1	2.41	0.49
1:K:461:ARG:NH1	1:K:465:ASN:HB3	2.28	0.49
1:E:345:ILE:HG13	1:E:372:LEU:HG	1.95	0.49
2:M:1345:HIS:HB3	2:M:1349:ARG:CZ	2.43	0.49
2:M:2152:ILE:HG12	2:M:2175:ILE:HG22	1.94	0.49
1:H:454:VAL:HG21	1:H:538:VAL:HG11	1.95	0.49
2:I:1365:ILE:HG13	2:I:1366:TYR:N	2.28	0.49
2:I:1457:TRP:CH2	2:I:1519:TRP:HB2	2.48	0.49
2:M:1497:ILE:HB	2:M:1502:LYS:HB3	1.95	0.49
1:A:535:THR:OG1	1:A:549:GLU:OE1	2.22	0.49
1:F:416:ASP:N	1:F:416:ASP:OD1	2.46	0.49
1:L:485:PHE:HB2	1:L:539:ALA:HB3	1.93	0.49
2:M:2188:ILE:O	2:M:2192:GLY:N	2.42	0.49
1:F:430:HIS:CD2	1:F:432:ASP:H	2.31	0.49
2:I:1673:TYR:O	2:I:1676:THR:OG1	2.28	0.49
2:I:2076:SER:OG	2:I:2077:GLU:N	2.46	0.49
1:L:540:HIS:H	1:L:543:LEU:HD12	1.77	0.49
2:M:1045:GLN:HB3	2:M:1049:TYR:CE2	2.47	0.49
2:I:2075:GLN:NE2	2:I:2155:ALA:O	2.46	0.49
2:I:2126:LYS:NZ	2:I:2130:LEU:HD11	2.27	0.49
2:I:2196:CYS:O	2:I:2199:LYS:HG2	2.13	0.49
2:M:1570:TYR:C	2:M:1572:SER:H	2.20	0.49
1:C:503:SER:OG	1:C:504:ALA:N	2.46	0.49
1:G:490:GLN:HE22	1:G:534:TYR:HE1	1.58	0.49
2:I:1601:ASN:OD1	2:I:1672:GLN:NE2	2.45	0.49
2:M:1444:GLY:HA2	2:M:1447:GLU:HG3	1.95	0.49
2:M:2193:THR:HA	2:M:2196:CYS:SG	2.53	0.49
1:A:452:PRO:HD3	1:A:542:ALA:HB3	1.95	0.48
2:I:1572:SER:OG	2:I:1573:ILE:N	2.32	0.48
1:L:488:TRP:CZ3	1:L:536:CYS:HB3	2.47	0.48
1:L:531:GLY:C	1:L:533:THR:H	2.20	0.48
1:D:491:ARG:HH21	1:D:532:GLU:HG2	1.78	0.48
1:E:524:SER:OG	1:E:526:GLU:OE1	2.26	0.48
1:H:382:TRP:HB2	1:H:390:VAL:HG21	1.94	0.48
2:I:1681:ASP:N	2:I:1681:ASP:OD1	2.44	0.48
2:I:1883:ILE:C	2:I:1884:MET:HE2	2.38	0.48
2:I:2049:CYS:O	2:I:2070:ILE:HD12	2.14	0.48
2:M:2064:ASN:HB3	2:M:2067:LYS:HD3	1.95	0.48
1:E:531:GLY:C	1:E:533:THR:H	2.20	0.48
2:I:1193:GLU:O	2:I:1196:LYS:HB2	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:491:ARG:NH1	1:L:532:GLU:O	2.46	0.48
2:M:2251:TYR:O	2:M:2252:LYS:HE2	2.13	0.48
1:H:357:ILE:HG12	1:H:363:THR:HB	1.96	0.48
2:M:1972:GLN:O	2:M:1975:GLU:HG3	2.13	0.48
1:E:475:LEU:HD13	1:E:518:HIS:CD2	2.49	0.48
1:H:560:THR:HG22	1:K:559:PRO:HA	1.95	0.48
2:I:1114:GLN:HA	2:I:1117:ASN:ND2	2.29	0.48
2:I:1943:MET:N	2:I:1943:MET:HE2	2.28	0.48
2:I:2210:CYS:HB3	2:I:2226:CYS:HB3	1.71	0.48
3:J:43:LEU:HD22	1:L:570:ASP:HB2	1.94	0.48
1:L:532:GLU:O	1:L:533:THR:HG22	2.14	0.48
2:M:1182:ASN:HB3	2:M:1186:HIS:HE1	1.77	0.48
2:M:1977:ASP:HA	2:M:1980:ILE:HG22	1.96	0.48
1:A:447:VAL:HG21	1:A:481:PRO:HB3	1.96	0.48
1:E:425:THR:OG1	1:E:440:THR:HG22	2.13	0.48
1:G:381:SER:HA	1:G:393:HIS:HE1	1.77	0.48
2:I:1658:LEU:HA	2:I:1661:VAL:HG12	1.96	0.48
2:I:1735:LYS:HE2	2:I:1738:ARG:HD3	1.95	0.48
2:I:2132:GLU:HG2	2:I:2138:THR:HA	1.95	0.48
2:M:1029:VAL:O	2:M:1032:PHE:HB3	2.14	0.48
2:M:1154:ILE:HD12	2:M:1158:PHE:HD2	1.79	0.48
2:I:1356:ASN:ND2	2:I:1449:GLN:HG2	2.29	0.48
2:M:2103:TYR:HB3	2:M:2186:ARG:HE	1.77	0.48
1:B:525:GLU:O	1:B:529:ASN:ND2	2.46	0.48
1:G:429:THR:HG23	1:G:436:PRO:HG3	1.95	0.48
1:E:496:SER:OG	1:E:498:GLU:OE1	2.26	0.48
3:J:43:LEU:HB3	1:L:570:ASP:HA	1.95	0.48
3:J:106:ASN:OD1	3:J:107:LYS:N	2.47	0.48
1:K:415:GLU:O	1:K:419:ASN:ND2	2.47	0.48
2:M:1611:LYS:HB3	2:M:1709:HIS:CG	2.48	0.48
1:B:382:TRP:CZ2	1:B:426:CYS:HB2	2.49	0.47
1:D:379:THR:HB	1:D:429:THR:HB	1.96	0.47
1:E:461:ARG:O	1:E:461:ARG:NH1	2.46	0.47
2:I:1102:LEU:HD23	2:I:1106:LYS:HD3	1.95	0.47
2:I:1269:THR:O	2:I:1272:LEU:HB2	2.14	0.47
2:M:1844:ASN:HA	2:M:1847:ASN:HD21	1.79	0.47
2:M:1853:ARG:NE	2:M:1947:LEU:O	2.47	0.47
1:B:425:THR:HG22	1:B:440:THR:HG22	1.96	0.47
1:C:467:ARG:HA	1:C:525:GLU:OE2	2.14	0.47
1:E:348:PHE:O	1:E:367:CYS:HA	2.14	0.47
1:G:413:ILE:HD12	1:G:417:ASP:HB2	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:2124:LYS:NZ	2:M:2125:ILE:HG12	2.28	0.47
2:I:1506:GLU:HB3	2:I:1510:LYS:NZ	2.29	0.47
1:K:393:HIS:CD2	1:K:396:ILE:HD11	2.50	0.47
2:M:2079:LYS:NZ	2:M:2098:MET:SD	2.88	0.47
1:G:400:HIS:HB2	1:G:404:THR:HB	1.96	0.47
2:M:1590:LYS:HB2	2:M:1664:ARG:HH22	1.79	0.47
1:B:423:ARG:HA	1:B:441:ILE:O	2.14	0.47
1:C:533:THR:OG1	1:C:551:THR:OG1	2.14	0.47
1:G:466:LEU:HD12	2:I:2058:ALA:H	1.79	0.47
1:G:552:VAL:HG23	1:G:556:THR:HG21	1.97	0.47
2:I:1027:ASN:O	2:I:1030:THR:OG1	2.26	0.47
2:I:1381:GLU:O	2:I:1382:LYS:NZ	2.33	0.47
2:I:1581:TYR:HB2	2:I:1660:ILE:HD11	1.97	0.47
2:I:2232:LYS:O	2:I:2235:GLU:HG2	2.15	0.47
2:M:1292:THR:H	2:M:1295:LEU:HD12	1.80	0.47
2:M:1843:ALA:O	2:M:1847:ASN:ND2	2.48	0.47
2:M:2063:LEU:HB2	2:M:2065:GLU:OE2	2.15	0.47
1:B:449:LEU:HD22	1:B:481:PRO:HD3	1.97	0.47
1:B:514:ARG:HD3	1:B:514:ARG:HA	1.71	0.47
1:B:518:HIS:HD2	1:B:520:ILE:HD11	1.80	0.47
1:F:384:ARG:NH1	1:F:388:GLU:OE1	2.47	0.47
1:G:413:ILE:HD13	1:G:424:PHE:CE2	2.49	0.47
2:I:1977:ASP:OD1	2:I:1978:ASN:N	2.48	0.47
2:M:1639:ILE:HD13	2:M:1657:THR:HG21	1.96	0.47
2:I:1504:LYS:HA	2:I:1507:LYS:HD2	1.97	0.47
2:I:1506:GLU:HB3	2:I:1510:LYS:HZ3	1.80	0.47
3:J:69:LYS:NZ	3:J:98:GLU:OE2	2.39	0.47
3:J:113:VAL:HG13	3:J:126:THR:HG21	1.97	0.47
2:M:1497:ILE:HD13	2:M:1501:CYS:HB3	1.97	0.47
2:M:2240:ARG:HA	2:M:2243:GLN:HG3	1.96	0.47
1:B:417:ASP:O	1:B:420:SER:OG	2.33	0.47
1:C:466:LEU:HB2	1:C:468:GLU:OE1	2.14	0.47
1:F:456:LEU:HD11	1:F:536:CYS:SG	2.55	0.47
1:H:456:LEU:HD13	1:H:550:ARG:HB2	1.97	0.47
2:I:1602:ASP:N	2:I:1602:ASP:OD1	2.48	0.47
1:D:457:LEU:HB2	1:D:473:THR:OG1	2.15	0.47
1:F:417:ASP:OD1	1:F:418:TRP:N	2.47	0.47
2:M:1868:ARG:HA	2:M:1881:SER:HA	1.97	0.47
2:M:1869:LYS:NZ	2:M:1873:GLU:O	2.38	0.47
1:K:379:THR:HB	1:K:429:THR:OG1	2.15	0.46
1:A:488:TRP:O	1:A:489:MET:HE2	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:MET:HE1	3:J:64:LEU:HD13	1.97	0.46
1:G:384:ARG:HE	1:G:386:ASN:CG	2.20	0.46
1:H:345:ILE:HG12	1:H:372:LEU:HD23	1.97	0.46
2:I:1592:ASN:HB3	2:I:1595:LEU:HB2	1.97	0.46
2:M:2066:PHE:CE2	2:M:2070:ILE:HD11	2.50	0.46
1:E:356:SER:O	1:E:360:THR:OG1	2.25	0.46
2:I:2205:TYR:OH	2:I:2229:GLU:OE1	2.33	0.46
2:M:1572:SER:OG	2:M:1573:ILE:N	2.41	0.46
2:M:1960:LYS:O	2:M:1963:GLU:HG3	2.15	0.46
1:A:451:ARG:HH22	1:A:544:PRO:HD3	1.80	0.46
1:F:419:ASN:O	1:F:443:ARG:NH2	2.43	0.46
2:I:1260:THR:HG22	2:I:1262:GLY:H	1.81	0.46
2:I:2041:ILE:HD12	2:I:2042:PRO:HD2	1.98	0.46
1:K:383:THR:N	1:K:425:THR:O	2.42	0.46
2:M:987:CYS:HA	2:M:1005:CYS:HA	1.98	0.46
2:M:1556:ASN:ND2	2:M:1561:TYR:HB3	2.30	0.46
2:M:2045:ARG:NE	2:M:2113:ASP:OD2	2.48	0.46
1:B:512:PRO:O	1:B:514:ARG:N	2.39	0.46
1:D:541:GLU:OE1	1:D:541:GLU:N	2.46	0.46
1:E:423:ARG:HA	1:E:442:SER:HB3	1.97	0.46
1:F:456:LEU:HD23	1:F:552:VAL:HG12	1.96	0.46
2:M:1506:GLU:HB3	2:M:1510:LYS:NZ	2.31	0.46
1:E:457:LEU:HB2	1:E:473:THR:OG1	2.15	0.46
2:I:1291:ASP:OD1	2:I:1292:THR:N	2.48	0.46
2:I:2126:LYS:HZ3	2:I:2130:LEU:HD11	1.80	0.46
1:L:462:GLU:HA	1:L:465:ASN:ND2	2.31	0.46
2:M:1278:TRP:HB2	2:M:1372:LEU:HD21	1.97	0.46
1:B:375:TYR:HE2	1:B:431:THR:HB	1.81	0.46
1:C:384:ARG:HH21	1:C:386:ASN:HB2	1.79	0.46
1:H:366:THR:HG23	1:H:410:GLU:HB3	1.97	0.46
2:I:1038:TRP:O	2:I:1041:GLU:HG3	2.15	0.46
2:I:1971:GLU:OE1	2:I:1972:GLN:NE2	2.46	0.46
1:L:552:VAL:HG13	1:L:556:THR:HB	1.97	0.46
2:I:970:THR:OG1	2:I:971:ASN:N	2.49	0.46
2:M:2218:ALA:O	2:M:2223:SER:OG	2.28	0.46
1:B:525:GLU:HA	1:B:528:TRP:HB3	1.97	0.46
1:D:465:ASN:O	1:D:467:ARG:HG3	2.16	0.46
1:K:383:THR:OG1	1:K:425:THR:O	2.31	0.46
2:M:1420:ILE:HA	2:M:1423:ILE:HG22	1.98	0.46
2:M:2189:LYS:O	2:M:2193:THR:N	2.32	0.46
1:G:418:TRP:O	1:G:443:ARG:HD3	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1559:ILE:O	2:I:1563:THR:HG22	2.16	0.45
2:M:1664:ARG:HD2	2:M:1668:TYR:CZ	2.51	0.45
1:B:348:PHE:HD2	1:B:368:LEU:HD11	1.81	0.45
2:M:2202:HIS:HA	2:M:2205:TYR:CD2	2.50	0.45
1:B:378:VAL:HG22	1:B:430:HIS:ND1	2.31	0.45
1:C:490:GLN:HB2	1:C:495:LEU:HD11	1.97	0.45
1:G:450:HIS:CD2	1:G:514:ARG:HH21	2.34	0.45
2:I:1189:GLU:O	2:I:1192:SER:HB3	2.17	0.45
2:I:1346:ALA:N	2:I:1349:ARG:HH21	2.14	0.45
2:I:1420:ILE:HA	2:I:1423:ILE:HG22	1.98	0.45
2:I:2114:MET:SD	2:I:2114:MET:N	2.87	0.45
3:J:46:ARG:CZ	3:J:52:PRO:HA	2.47	0.45
1:A:538:VAL:HG12	1:A:548:THR:H	1.82	0.45
2:I:2193:THR:HA	2:I:2196:CYS:SG	2.56	0.45
1:A:449:LEU:HB3	1:A:542:ALA:HA	1.98	0.45
1:D:489:MET:HE2	1:D:489:MET:HA	1.97	0.45
1:F:348:PHE:HE1	1:F:370:THR:HG22	1.82	0.45
1:H:421:GLY:HA2	1:H:443:ARG:HD2	1.97	0.45
2:I:1349:ARG:HH11	2:I:1456:GLU:HG3	1.82	0.45
2:I:1691:ILE:HD11	2:I:1783:MET:HG3	1.98	0.45
2:I:1715:TYR:O	2:I:1719:LYS:HG2	2.17	0.45
3:J:57:ARG:HB3	3:J:60:PHE:CE2	2.51	0.45
2:M:1376:ILE:HA	2:M:1379:ILE:HG22	1.98	0.45
2:M:2181:PRO:HB2	2:M:2186:ARG:HB2	1.98	0.45
1:A:549:GLU:O	1:A:550:ARG:NH1	2.43	0.45
1:C:484:VAL:HG12	1:C:540:HIS:CD2	2.51	0.45
1:F:364:LYS:NZ	1:F:412:SER:OG	2.35	0.45
1:G:400:HIS:NE2	1:G:406:SER:HB3	2.32	0.45
2:I:2129:ARG:HH22	2:I:2135:THR:HG22	1.82	0.45
2:M:1027:ASN:O	2:M:1030:THR:OG1	2.28	0.45
2:M:1039:ASN:OD1	2:M:1043:GLN:NE2	2.46	0.45
2:M:1949:LYS:HB2	2:M:1954:TYR:CE2	2.51	0.45
1:C:399:SER:HA	1:C:405:PHE:HA	1.97	0.45
1:D:378:VAL:HG22	1:D:430:HIS:CE1	2.51	0.45
1:D:530:THR:OG1	1:D:532:GLU:OE2	2.34	0.45
1:G:384:ARG:HB2	1:G:422:GLU:HG2	1.99	0.45
1:H:466:LEU:HD23	1:H:466:LEU:H	1.82	0.45
2:M:1768:VAL:HB	2:M:1783:MET:HE1	1.99	0.45
2:M:2051:SER:OG	2:M:2052:ARG:NH1	2.50	0.45
1:B:347:VAL:HG22	1:B:369:VAL:HG13	1.99	0.45
1:C:400:HIS:N	1:C:404:THR:O	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:535:THR:OG1	1:C:550:ARG:O	2.26	0.45
1:D:456:LEU:HD23	1:D:550:ARG:HB2	1.99	0.45
1:D:535:THR:HB	1:D:551:THR:HG22	1.99	0.45
1:G:549:GLU:OE1	1:G:549:GLU:N	2.50	0.45
2:I:1039:ASN:O	2:I:1043:GLN:NE2	2.50	0.45
2:I:1583:LYS:HG3	2:I:1584:TYR:H	1.82	0.45
2:M:1965:TYR:O	2:M:1969:VAL:HG23	2.17	0.45
1:D:568:MET:SD	1:D:568:MET:N	2.86	0.45
1:E:535:THR:HG22	1:E:551:THR:HB	1.98	0.45
3:J:134:TYR:HD1	3:J:135:PRO:HD2	1.81	0.45
1:B:384:ARG:HA	1:B:424:PHE:HD1	1.83	0.45
1:E:423:ARG:HB3	1:E:440:THR:HB	1.98	0.45
1:E:509:PRO:HD3	1:F:501:VAL:HG21	1.99	0.45
1:G:489:MET:HE2	1:G:489:MET:HA	1.98	0.45
2:I:1544:PRO:HA	2:I:1547:ILE:HD11	1.99	0.45
1:K:478:GLY:HA2	1:K:514:ARG:HB3	1.99	0.45
2:M:1100:TYR:OH	2:M:1198:ALA:O	2.29	0.45
2:M:1783:MET:O	2:M:1783:MET:HG2	2.17	0.45
1:B:382:TRP:HB3	1:B:384:ARG:NH2	2.28	0.44
1:C:523:VAL:HG11	1:C:534:TYR:CE2	2.52	0.44
2:I:979:LYS:HD3	2:I:1865:LYS:HD2	1.98	0.44
2:M:1352:ILE:HD11	2:M:1442:PRO:HB2	1.98	0.44
2:M:1515:LYS:HA	2:M:1518:GLU:HG3	1.99	0.44
2:M:1515:LYS:HD2	2:M:1518:GLU:OE2	2.16	0.44
2:M:2035:LYS:HG3	2:M:2036:HIS:H	1.82	0.44
1:A:467:ARG:HH12	1:A:529:ASN:HD21	1.64	0.44
1:B:490:GLN:C	1:B:491:ARG:HG2	2.43	0.44
1:D:393:HIS:HA	1:D:410:GLU:HG2	1.98	0.44
1:D:491:ARG:HA	1:D:533:THR:HG21	2.00	0.44
1:E:374:THR:OG1	1:E:403:ALA:O	2.35	0.44
2:I:1692:ARG:NH1	2:I:1902:GLY:O	2.51	0.44
2:I:1843:ALA:O	2:I:1847:ASN:ND2	2.50	0.44
1:L:566:LEU:HD23	1:L:566:LEU:H	1.82	0.44
2:M:1603:MET:HE1	2:M:1629:GLN:HB2	1.98	0.44
1:B:376:ASP:CG	1:B:377:SER:H	2.26	0.44
2:I:1611:LYS:HD2	2:I:1709:HIS:HE1	1.82	0.44
2:I:2054:VAL:HG23	2:I:2123:ILE:HD12	1.98	0.44
2:M:1362:SER:O	2:M:1362:SER:OG	2.33	0.44
2:M:2124:LYS:HG3	2:M:2125:ILE:N	2.32	0.44
1:B:345:ILE:HA	1:B:371:ASP:HB3	2.00	0.44
1:B:433:LEU:O	1:B:433:LEU:HD12	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1367:GLU:OE1	2:I:1368:HIS:ND1	2.51	0.44
2:I:1742:TRP:CE2	2:I:1757:ARG:HB3	2.52	0.44
1:K:558:LYS:HE2	1:K:558:LYS:HA	1.99	0.44
2:M:1454:PHE:HD1	2:M:1522:GLN:HG2	1.82	0.44
2:M:1813:TYR:O	2:M:1817:MET:HG2	2.18	0.44
2:M:2233:TYR:HA	2:M:2236:TRP:CD1	2.52	0.44
1:B:491:ARG:NH1	1:B:532:GLU:OE2	2.51	0.44
1:H:382:TRP:CE2	1:H:426:CYS:HB3	2.52	0.44
2:I:2030:ARG:NE	2:I:2031:GLY:H	2.14	0.44
1:B:372:LEU:HD23	1:B:372:LEU:HA	1.88	0.44
1:C:383:THR:HG22	1:C:389:ALA:HA	2.00	0.44
1:E:385:GLN:HB3	1:E:422:GLU:HG3	1.99	0.44
1:E:512:PRO:HD2	2:M:1226:TYR:CZ	2.53	0.44
1:E:553:ASP:OD1	1:E:556:THR:OG1	2.29	0.44
1:G:415:GLU:HG3	1:G:419:ASN:HD22	1.83	0.44
2:I:1291:ASP:OD1	2:I:1295:LEU:HB2	2.17	0.44
2:I:1625:PRO:HG3	2:I:1798:TRP:CD1	2.52	0.44
2:I:2185:LEU:HA	2:I:2188:ILE:HG12	1.99	0.44
2:M:1583:LYS:HG2	2:M:1584:TYR:H	1.82	0.44
2:M:2124:LYS:HB2	2:M:2124:LYS:HE2	1.80	0.44
1:G:353:SER:O	1:G:357:ILE:HG12	2.17	0.44
1:H:365:LEU:HD22	1:H:413:ILE:HG12	2.00	0.44
2:M:1194:LYS:HA	2:M:1197:ASN:HD21	1.82	0.44
2:M:1544:PRO:HA	2:M:1547:ILE:HD11	2.00	0.44
1:A:455:TYR:CE2	1:B:463:GLN:HB2	2.52	0.44
1:E:400:HIS:CD2	1:E:406:SER:HB3	2.53	0.44
2:I:1708:VAL:HG23	2:I:1713:THR:HG21	1.99	0.44
2:M:1041:GLU:OE1	2:M:1045:GLN:NE2	2.51	0.44
2:M:1365:ILE:HG13	2:M:1366:TYR:N	2.32	0.44
2:M:1561:TYR:O	2:M:1565:TYR:HB2	2.18	0.44
2:M:2062:SER:O	2:M:2131:LEU:HD11	2.18	0.44
2:I:1433:ASN:C	2:I:1435:ASP:H	2.25	0.44
3:J:19:SER:HB2	3:J:35:ARG:HD2	2.00	0.44
1:L:490:GLN:HG2	1:L:491:ARG:HG2	1.99	0.44
1:B:468:GLU:OE1	1:B:468:GLU:N	2.51	0.43
1:F:469:SER:OG	1:F:470:ALA:N	2.51	0.43
2:I:1901:ASN:HD21	2:I:1903:ASN:HB2	1.83	0.43
2:I:2207:LYS:HD3	2:I:2207:LYS:HA	1.70	0.43
3:J:102:THR:HG21	1:L:575:CYS:HB2	1.99	0.43
2:M:1514:GLU:HG2	2:M:1515:LYS:N	2.32	0.43
2:M:2170:PRO:O	2:M:2174:THR:N	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:VAL:HG12	3:J:61:VAL:HA	2.00	0.43
1:C:461:ARG:HD2	1:C:462:GLU:N	2.34	0.43
1:E:484:VAL:HG23	1:E:540:HIS:HB2	1.99	0.43
1:G:456:LEU:HD23	1:G:550:ARG:HB2	1.99	0.43
1:H:372:LEU:O	1:H:404:THR:OG1	2.28	0.43
2:I:1605:TRP:CH2	2:I:1802:TRP:HB2	2.54	0.43
2:I:1646:GLY:HA3	2:I:1649:LYS:HE3	1.99	0.43
2:M:1046:ILE:O	2:M:1050:MET:HG2	2.18	0.43
2:M:1740:ASP:O	2:M:1744:ASN:N	2.52	0.43
2:M:2236:TRP:O	2:M:2240:ARG:HG2	2.18	0.43
1:E:529:ASN:HA	1:E:554:LYS:HD2	1.99	0.43
1:F:552:VAL:HG23	1:F:556:THR:HG21	1.99	0.43
2:I:1038:TRP:CG	2:I:1114:GLN:HE21	2.37	0.43
1:K:506:MET:SD	1:K:507:PRO:HD2	2.59	0.43
2:M:1365:ILE:HG13	2:M:1366:TYR:H	1.82	0.43
2:I:2237:SER:O	2:I:2241:SER:N	2.48	0.43
2:M:1853:ARG:HG2	2:M:1947:LEU:HB3	2.01	0.43
1:C:345:ILE:HG12	1:C:372:LEU:HD23	2.00	0.43
1:C:418:TRP:O	1:C:443:ARG:NH1	2.52	0.43
1:C:443:ARG:O	1:C:445:LYS:NZ	2.46	0.43
1:G:490:GLN:HB2	1:G:495:LEU:HD11	2.00	0.43
2:I:1382:LYS:HA	2:I:1382:LYS:HD3	1.79	0.43
2:I:2090:ASP:HB3	2:I:2093:LYS:HD3	2.00	0.43
1:B:568:MET:HB3	1:C:568:MET:HG2	2.00	0.43
1:E:421:GLY:HA3	1:E:445:LYS:HD3	2.01	0.43
2:I:2247:ILE:O	2:I:2254:TYR:HB2	2.18	0.43
1:K:490:GLN:HG3	1:K:491:ARG:HG2	1.99	0.43
2:M:1514:GLU:HA	2:M:1517:GLN:NE2	2.34	0.43
2:M:2028:ASP:N	2:M:2028:ASP:OD1	2.51	0.43
2:M:2139:LYS:HD2	2:M:2139:LYS:O	2.19	0.43
2:M:2144:TRP:O	2:M:2148:ASN:ND2	2.52	0.43
1:B:354:PHE:HA	1:B:357:ILE:HD12	2.00	0.43
1:C:365:LEU:HD23	1:C:365:LEU:H	1.84	0.43
1:C:567:VAL:HG13	1:D:567:VAL:HG13	2.00	0.43
1:H:425:THR:HG21	1:H:438:LYS:HD3	2.01	0.43
2:I:1413:TRP:CG	2:I:1441:PRO:HD3	2.54	0.43
1:L:497:PRO:HA	1:L:500:TYR:CZ	2.54	0.43
1:A:485:PHE:HB3	1:A:539:ALA:HB3	2.00	0.43
1:E:419:ASN:HA	1:E:443:ARG:NE	2.33	0.43
1:H:543:LEU:HB2	1:H:546:ARG:HA	2.01	0.43
2:I:1272:LEU:HD11	2:I:1354:TYR:CE1	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1808:GLU:HG3	2:I:1809:LYS:HE2	2.00	0.43
2:I:2064:ASN:CB	2:I:2067:LYS:HE3	2.49	0.43
2:M:1227:ILE:HG23	2:M:1276:GLU:OE2	2.19	0.43
2:M:2125:ILE:HA	2:M:2128:ASP:OD2	2.18	0.43
1:A:568:MET:HB3	1:B:568:MET:SD	2.58	0.43
1:B:469:SER:HA	1:B:524:SER:HA	1.99	0.43
2:I:1899:GLU:HG3	2:I:1901:ASN:H	1.84	0.43
1:E:489:MET:HA	1:E:489:MET:HE2	2.01	0.43
2:I:1639:ILE:HG21	2:I:1657:THR:HG21	2.01	0.43
2:I:1660:ILE:O	2:I:1664:ARG:HG2	2.19	0.43
2:I:1844:ASN:HA	2:I:1847:ASN:HD21	1.84	0.43
3:J:4:ARG:HD2	3:J:20:ARG:HB2	2.01	0.43
2:M:1265:ILE:HG12	2:M:1365:ILE:HG21	2.01	0.43
1:A:495:LEU:HD23	1:A:495:LEU:HA	1.84	0.42
1:C:508:GLU:OE2	1:C:511:ALA:HB3	2.19	0.42
1:D:372:LEU:HD23	1:D:430:HIS:CD2	2.54	0.42
2:I:1454:PHE:HE2	2:I:1535:ALA:HB1	1.83	0.42
2:I:2236:TRP:O	2:I:2240:ARG:N	2.46	0.42
2:M:1309:GLU:HG2	2:M:1423:ILE:HD12	2.01	0.42
2:M:1458:GLY:HA3	2:M:1539:LEU:HD11	2.01	0.42
2:M:1719:LYS:O	2:M:1722:GLU:HG3	2.19	0.42
2:M:2075:GLN:NE2	2:M:2156:MET:HA	2.33	0.42
2:M:2182:PRO:O	2:M:2186:ARG:N	2.31	0.42
1:B:419:ASN:O	1:B:443:ARG:NH2	2.52	0.42
1:B:463:GLN:HG3	1:B:464:LEU:HD12	2.01	0.42
1:E:346:ARG:HD2	1:E:348:PHE:CZ	2.54	0.42
1:F:459:PRO:HD3	1:F:472:ILE:HG12	2.01	0.42
1:H:382:TRP:HA	1:H:426:CYS:HA	2.01	0.42
2:I:1142:SER:HB3	2:I:1187:GLY:HA2	2.01	0.42
1:L:533:THR:HA	1:L:553:ASP:HA	2.01	0.42
2:M:1240:PHE:CD1	2:M:1241:PRO:HA	2.54	0.42
2:M:1600:ASP:N	2:M:1630:GLN:OE1	2.52	0.42
2:M:1698:LEU:HA	2:M:1701:ILE:HG12	2.00	0.42
2:M:2024:TRP:CD1	2:M:2046:ARG:HH21	2.37	0.42
2:M:2148:ASN:HA	2:M:2151:SER:HB3	2.02	0.42
1:C:418:TRP:CZ2	1:C:443:ARG:HB3	2.54	0.42
1:F:400:HIS:NE2	1:F:406:SER:OG	2.46	0.42
2:I:1462:CYS:HB3	2:I:1546:CYS:HB3	1.85	0.42
2:M:2107:ASP:OD2	2:M:2187:TRP:NE1	2.52	0.42
1:B:553:ASP:CG	1:B:554:LYS:H	2.27	0.42
1:G:417:ASP:O	1:G:420:SER:OG	2.36	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1903:ASN:O	2:I:1905:ILE:N	2.49	0.42
2:I:2063:LEU:HB3	2:I:2065:GLU:HG3	1.99	0.42
3:J:25:SER:O	3:J:27:ASP:N	2.52	0.42
1:K:490:GLN:HB2	1:K:495:LEU:HD11	2.02	0.42
1:L:558:LYS:HZ3	1:L:560:THR:HG22	1.83	0.42
2:M:1357:MET:O	2:M:1373:GLN:NE2	2.49	0.42
2:M:2024:TRP:HB2	2:M:2040:LEU:HD13	2.01	0.42
1:A:539:ALA:HB2	3:J:115:LEU:HD11	2.01	0.42
1:C:511:ALA:HB1	1:C:512:PRO:HD2	2.01	0.42
2:I:2202:HIS:CE1	2:I:2233:TYR:HB3	2.54	0.42
2:M:2225:ASN:ND2	2:M:2229:GLU:OE2	2.52	0.42
2:I:1617:ARG:NH1	2:I:1875:GLU:OE1	2.53	0.42
2:I:1731:ASP:O	2:I:1735:LYS:HG2	2.19	0.42
2:I:2080:PHE:O	2:I:2083:ASN:N	2.52	0.42
2:I:2200:GLN:HA	2:I:2203:LYS:HZ3	1.84	0.42
1:L:543:LEU:HB2	1:L:546:ARG:HA	2.02	0.42
2:M:2035:LYS:HG3	2:M:2036:HIS:CD2	2.55	0.42
1:A:466:LEU:H	1:A:466:LEU:HD23	1.83	0.42
1:D:549:GLU:N	1:D:549:GLU:OE1	2.53	0.42
1:E:419:ASN:HA	1:E:443:ARG:HE	1.85	0.42
2:I:1311:LEU:HD23	2:I:1311:LEU:HA	1.85	0.42
2:I:2213:VAL:O	2:I:2214:THR:OG1	2.31	0.42
2:M:1025:ASP:OD1	2:M:1025:ASP:N	2.50	0.42
2:M:1029:VAL:HA	2:M:1032:PHE:HB3	2.00	0.42
2:M:1114:GLN:HA	2:M:1117:ASN:HD21	1.84	0.42
1:G:498:GLU:OE1	1:G:498:GLU:N	2.53	0.42
2:I:1042:ILE:HD13	2:I:1042:ILE:HA	1.90	0.42
2:I:1252:LYS:HD3	2:I:1521:LYS:HG2	2.01	0.42
2:I:1974:ASN:HA	2:I:1977:ASP:OD2	2.20	0.42
2:I:2162:LYS:HD3	2:I:2162:LYS:HA	1.86	0.42
2:M:1626:PRO:O	2:M:1630:GLN:HG2	2.19	0.42
1:B:419:ASN:HA	1:B:443:ARG:NH1	2.35	0.42
1:E:396:ILE:HA	1:E:408:VAL:HG22	2.02	0.42
1:E:473:THR:HG22	1:E:520:ILE:HG22	2.02	0.42
1:F:384:ARG:HB2	1:F:388:GLU:HB2	2.01	0.42
1:G:419:ASN:O	1:G:445:LYS:NZ	2.44	0.42
2:I:1410:ARG:HD2	2:I:1410:ARG:HA	1.86	0.42
2:I:1765:GLN:HA	2:I:1768:VAL:HG12	2.01	0.42
1:K:475:LEU:HD13	1:K:518:HIS:CE1	2.55	0.42
2:M:2119:GLU:OE1	2:M:2124:LYS:HB3	2.20	0.42
1:A:455:TYR:CZ	1:B:463:GLN:HB2	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:373:THR:HG23	1:D:375:TYR:HB3	2.01	0.42
1:E:378:VAL:HG22	1:E:430:HIS:CD2	2.55	0.42
1:H:569:SER:N	1:K:569:SER:HB2	2.35	0.42
2:I:1036:GLU:O	2:I:1040:LYS:HG2	2.19	0.42
2:I:2143:ASP:OD1	2:I:2144:TRP:N	2.52	0.42
3:J:17:ILE:HD11	3:J:35:ARG:HH21	1.83	0.42
2:M:1146:PHE:HA	2:M:1149:CYS:SG	2.60	0.42
2:M:1944:ASN:OD1	2:M:1945:GLU:N	2.52	0.42
1:D:419:ASN:O	1:D:443:ARG:NE	2.53	0.41
1:H:428:VAL:HB	1:H:437:LEU:HB2	2.01	0.41
2:I:1457:TRP:HZ2	2:I:1515:LYS:HD2	1.85	0.41
2:I:2197:ILE:HD12	2:I:2197:ILE:HA	1.94	0.41
3:J:49:ILE:HG13	3:J:103:TYR:CE1	2.55	0.41
1:L:463:GLN:HE22	1:L:471:THR:HG23	1.85	0.41
1:B:490:GLN:OE1	1:B:495:LEU:HD21	2.20	0.41
1:B:491:ARG:HH12	2:M:2054:VAL:HG13	1.85	0.41
1:D:475:LEU:HD12	1:D:518:HIS:NE2	2.34	0.41
1:E:364:LYS:HE3	1:E:364:LYS:HB3	1.92	0.41
1:F:475:LEU:HD13	1:F:518:HIS:CD2	2.55	0.41
1:G:364:LYS:HD3	1:G:412:SER:HA	2.02	0.41
2:I:2251:TYR:C	2:I:2252:LYS:HD3	2.45	0.41
1:A:562:TYR:HB2	1:B:562:TYR:HD1	1.85	0.41
2:I:1328:LYS:HD2	2:I:1328:LYS:O	2.20	0.41
1:K:543:LEU:HD13	1:K:548:THR:HG23	2.01	0.41
2:M:1381:GLU:O	2:M:1382:LYS:HE2	2.19	0.41
2:M:1963:GLU:O	2:M:1966:LEU:HG	2.20	0.41
2:I:1444:GLY:HA2	2:I:1447:GLU:HG3	2.01	0.41
2:I:1561:TYR:O	2:I:1565:TYR:HB2	2.20	0.41
2:I:2020:GLU:HG3	2:I:2024:TRP:HZ2	1.84	0.41
2:I:2041:ILE:HG23	2:I:2046:ARG:HH21	1.85	0.41
1:K:527:GLU:OE1	1:K:534:TYR:OH	2.34	0.41
2:M:1356:ASN:ND2	2:M:1449:GLN:HG2	2.35	0.41
2:M:1669:LEU:O	2:M:1673:TYR:CB	2.68	0.41
2:M:2247:ILE:O	2:M:2250:ARG:HG2	2.20	0.41
1:C:479:PHE:CE1	1:C:515:TYR:HB2	2.55	0.41
1:F:382:TRP:CD2	1:F:426:CYS:HB3	2.55	0.41
2:I:2187:TRP:O	2:I:2190:GLU:HG3	2.20	0.41
2:M:1272:LEU:HD12	2:M:1272:LEU:O	2.20	0.41
2:M:1497:ILE:HG21	2:M:1501:CYS:HB3	2.03	0.41
2:M:1529:LYS:HG3	2:M:1530:TYR:HD1	1.85	0.41
2:M:2089:LYS:HD3	2:M:2089:LYS:HA	1.77	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:LEU:HB3	1:B:408:VAL:HA	2.02	0.41
1:G:518:HIS:CE1	1:H:520:ILE:HD11	2.56	0.41
2:I:1272:LEU:O	2:I:1272:LEU:HD12	2.21	0.41
2:I:1300:ILE:O	2:I:1304:ILE:HG12	2.20	0.41
2:I:1368:HIS:CD2	2:I:1371:LYS:HB2	2.56	0.41
2:I:1558:ASN:HB3	2:I:1561:TYR:HD2	1.86	0.41
3:J:41:VAL:HG12	1:L:568:MET:HB2	2.02	0.41
1:G:543:LEU:HB2	1:G:546:ARG:HA	2.02	0.41
1:H:526:GLU:HG2	1:H:527:GLU:N	2.36	0.41
2:I:981:TYR:CE2	2:I:1099:CYS:HB3	2.55	0.41
2:I:1179:LYS:HG2	2:I:1180:CYS:SG	2.61	0.41
2:I:1611:LYS:HD2	2:I:1709:HIS:CE1	2.56	0.41
2:I:2142:GLU:O	2:I:2146:LYS:N	2.37	0.41
1:A:451:ARG:HH12	1:A:544:PRO:HD2	1.86	0.41
1:A:456:LEU:HD23	1:A:550:ARG:HG3	2.01	0.41
1:B:352:PRO:HD3	1:B:365:LEU:HB3	2.03	0.41
1:B:372:LEU:O	1:B:404:THR:HA	2.21	0.41
1:E:443:ARG:HA	1:E:444:PRO:HD3	1.93	0.41
1:F:364:LYS:HE3	1:F:364:LYS:HB3	1.77	0.41
1:F:529:ASN:HA	1:F:554:LYS:HD3	2.02	0.41
1:H:350:ILE:O	1:H:350:ILE:HG13	2.20	0.41
1:H:374:THR:HA	1:H:405:PHE:HB2	2.03	0.41
2:I:1025:ASP:OD1	2:I:1025:ASP:N	2.53	0.41
2:I:1195:LEU:O	2:I:1199:GLU:N	2.54	0.41
2:I:1742:TRP:CZ2	2:I:1757:ARG:HB3	2.56	0.41
2:I:1891:TYR:O	2:I:1895:ARG:HB2	2.21	0.41
2:I:1975:GLU:HA	2:I:1978:ASN:ND2	2.34	0.41
2:I:2089:LYS:HD3	2:I:2089:LYS:HA	1.77	0.41
3:J:4:ARG:HH11	3:J:20:ARG:CB	2.29	0.41
1:K:496:SER:OG	1:K:498:GLU:OE1	2.34	0.41
2:M:1662:ALA:O	2:M:1665:GLU:HG3	2.20	0.41
2:M:1717:ASP:OD1	2:M:1718:SER:N	2.54	0.41
2:M:1874:SER:OG	2:M:1876:ASP:O	2.36	0.41
2:M:2018:LEU:HD21	2:M:2021:LEU:HD13	2.02	0.41
2:M:2071:LEU:HD11	2:M:2154:ASN:OD1	2.21	0.41
1:C:456:LEU:HD13	1:C:550:ARG:HB2	2.03	0.41
1:E:532:GLU:OE2	2:I:1238:LYS:NZ	2.51	0.41
1:H:562:TYR:HB2	1:K:562:TYR:HB2	2.03	0.41
2:I:1042:ILE:O	2:I:1045:GLN:HB3	2.21	0.41
2:I:1515:LYS:HD3	2:I:1515:LYS:HA	1.83	0.41
3:J:59:ARG:HD2	3:J:60:PHE:N	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:509:PRO:HG2	1:K:510:GLN:OE1	2.21	0.41
2:M:1613:LEU:HD11	2:M:1617:ARG:HG3	2.03	0.41
2:M:1724:PHE:CD2	2:M:1738:ARG:HG2	2.53	0.41
1:G:396:ILE:HD11	1:G:407:ALA:HA	2.03	0.40
2:I:1899:GLU:O	2:I:1905:ILE:HG12	2.20	0.40
1:D:345:ILE:HD12	1:D:372:LEU:HG	2.02	0.40
1:D:454:VAL:HG21	1:D:538:VAL:HG11	2.03	0.40
1:F:511:ALA:HB3	1:F:514:ARG:HB2	2.03	0.40
1:H:398:GLU:HG2	1:H:399:SER:H	1.87	0.40
3:J:106:ASN:OD1	3:J:107:LYS:HG3	2.21	0.40
1:K:382:TRP:CE2	1:K:426:CYS:HB2	2.57	0.40
2:M:1242:GLY:O	2:M:1243:LYS:NZ	2.45	0.40
2:M:1868:ARG:NH2	2:M:1884:MET:SD	2.94	0.40
1:F:508:GLU:OE1	1:F:510:GLN:N	2.54	0.40
1:G:364:LYS:HE2	1:G:364:LYS:HB2	1.90	0.40
2:I:2043:PRO:HA	2:I:2046:ARG:NE	2.36	0.40
1:K:457:LEU:HB2	1:K:473:THR:CG2	2.52	0.40
1:L:471:THR:HB	1:L:520:ILE:HD11	2.03	0.40
1:L:496:SER:H	1:L:499:LYS:HZ2	1.70	0.40
1:B:357:ILE:HG12	1:B:363:THR:HG22	2.03	0.40
1:B:568:MET:HB3	1:C:568:MET:CG	2.52	0.40
1:F:514:ARG:NH1	2:I:1226:TYR:OH	2.55	0.40
2:I:1461:PHE:O	2:I:1464:GLU:HG3	2.21	0.40
2:I:1889:ILE:HD12	2:I:1892:LEU:HD11	2.02	0.40
3:J:12:CYS:SG	3:J:13:LYS:N	2.94	0.40
2:M:1038:TRP:O	2:M:1039:ASN:C	2.65	0.40
1:D:459:PRO:HG2	1:D:464:LEU:HD11	2.04	0.40
2:I:1178:LYS:HB3	2:I:1178:LYS:HE2	1.86	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	130/453 (29%)	123 (95%)	7 (5%)	0	100	100
1	B	225/453 (50%)	206 (92%)	19 (8%)	0	100	100
1	C	223/453 (49%)	195 (87%)	28 (13%)	0	100	100
1	D	222/453 (49%)	204 (92%)	18 (8%)	0	100	100
1	E	222/453 (49%)	206 (93%)	16 (7%)	0	100	100
1	F	217/453 (48%)	198 (91%)	19 (9%)	0	100	100
1	G	222/453 (49%)	203 (91%)	19 (9%)	0	100	100
1	H	226/453 (50%)	206 (91%)	20 (9%)	0	100	100
1	K	226/453 (50%)	206 (91%)	20 (9%)	0	100	100
1	L	123/453 (27%)	112 (91%)	11 (9%)	0	100	100
2	I	1085/2680 (40%)	991 (91%)	94 (9%)	0	100	100
2	M	1085/2680 (40%)	976 (90%)	108 (10%)	1 (0%)	48	79
3	J	102/136 (75%)	89 (87%)	13 (13%)	0	100	100
All	All	4308/10026 (43%)	3915 (91%)	392 (9%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	1367	GLU

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	115/399 (29%)	115 (100%)	0	100	100
1	B	203/399 (51%)	203 (100%)	0	100	100
1	C	201/399 (50%)	201 (100%)	0	100	100
1	D	200/399 (50%)	200 (100%)	0	100	100
1	E	200/399 (50%)	200 (100%)	0	100	100
1	F	198/399 (50%)	198 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	200/399 (50%)	200 (100%)	0	100	100
1	H	205/399 (51%)	205 (100%)	0	100	100
1	K	205/399 (51%)	205 (100%)	0	100	100
1	L	112/399 (28%)	112 (100%)	0	100	100
2	I	1013/2431 (42%)	1013 (100%)	0	100	100
2	M	1013/2431 (42%)	1013 (100%)	0	100	100
3	J	100/128 (78%)	100 (100%)	0	100	100
All	All	3965/8980 (44%)	3965 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	529	ASN
1	B	529	ASN
1	B	540	HIS
1	C	393	HIS
1	C	439	GLN
1	D	430	HIS
1	F	430	HIS
1	G	463	GLN
1	G	465	ASN
1	H	490	GLN
2	I	1001	ASN
2	I	1043	GLN
2	I	1197	ASN
2	I	1271	ASN
2	I	1302	ASN
2	I	1305	HIS
2	I	1400	ASN
2	I	1402	ASN
2	I	1615	ASN
2	I	1629	GLN
2	I	1776	ASN
2	I	1778	ASN
2	I	1844	ASN
2	I	1861	ASN
2	I	1901	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	I	1957	HIS
2	I	2100	ASN
2	I	2148	ASN
2	I	2194	ASN
2	I	2202	HIS
1	K	518	HIS
2	M	1045	GLN
2	M	1197	ASN
2	M	1368	HIS
2	M	1400	ASN
2	M	1402	ASN
2	M	1424	ASN
2	M	1488	ASN
2	M	1744	ASN
2	M	1758	GLN
2	M	1850	ASN
2	M	1972	GLN
2	M	1974	ASN
2	M	2036	HIS
2	M	2075	GLN
2	M	2148	ASN
2	M	2200	GLN
2	M	2212	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.

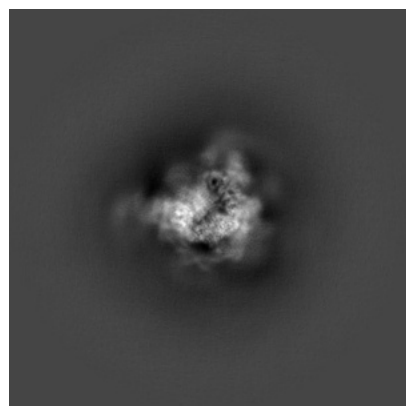
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34399. These allow visual inspection of the internal detail of the map and identification of artifacts.

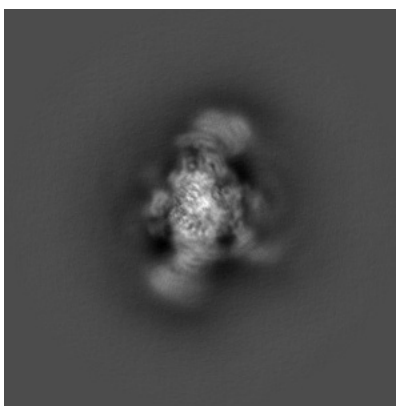
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

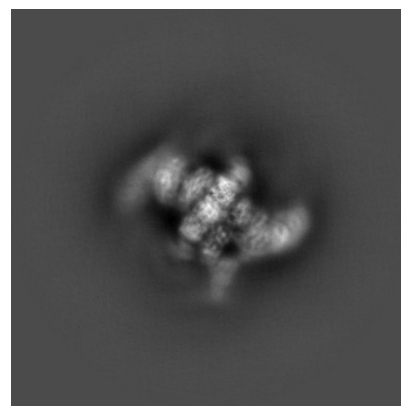
6.1.1 Primary map



X

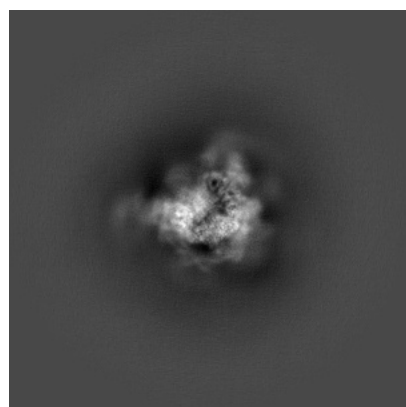


Y

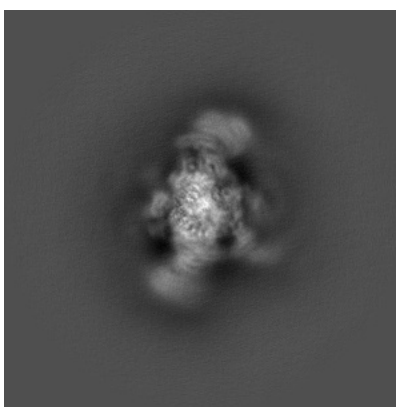


Z

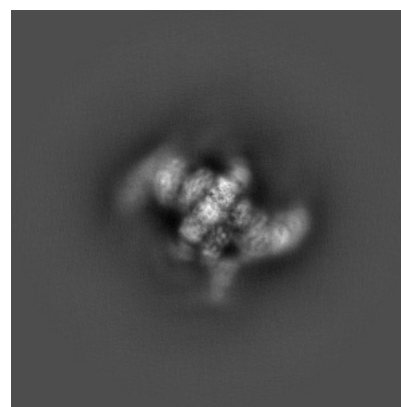
6.1.2 Raw map



X



Y

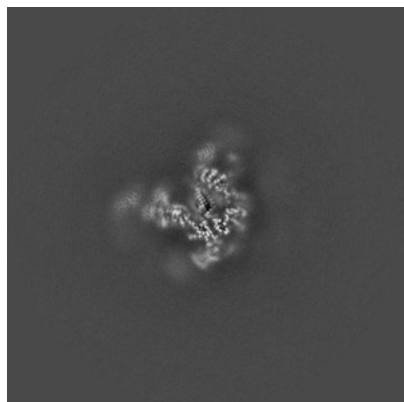


Z

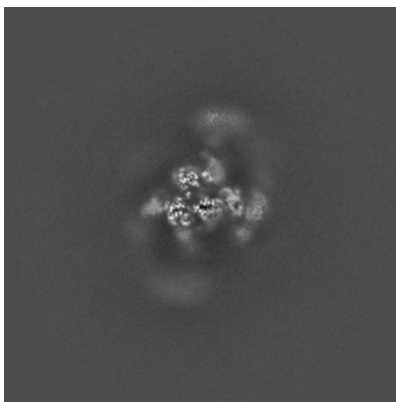
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

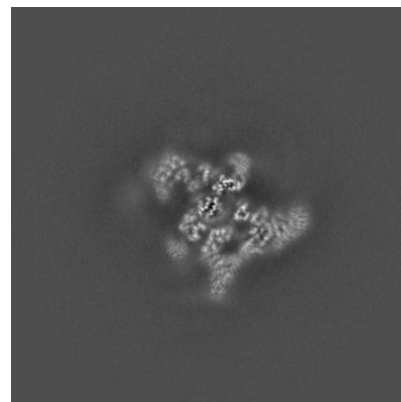
6.2.1 Primary map



X Index: 270

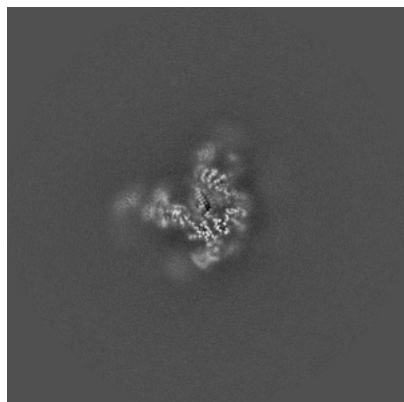


Y Index: 270

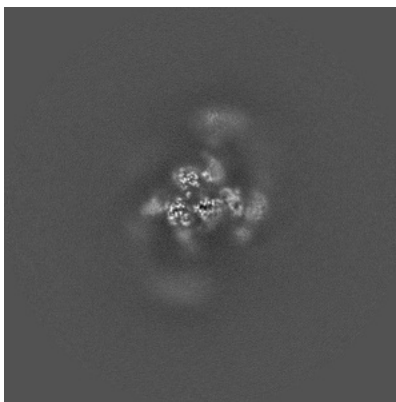


Z Index: 270

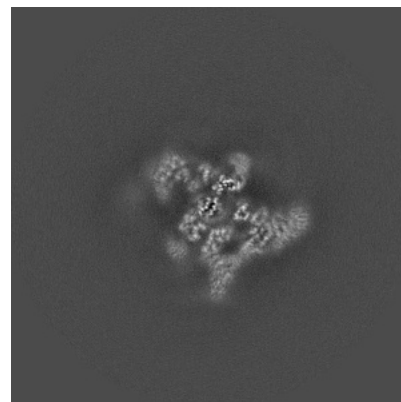
6.2.2 Raw map



X Index: 270



Y Index: 270

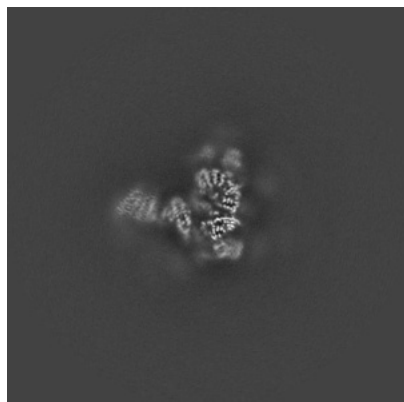


Z Index: 270

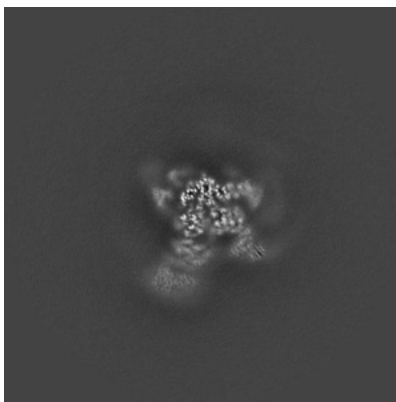
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

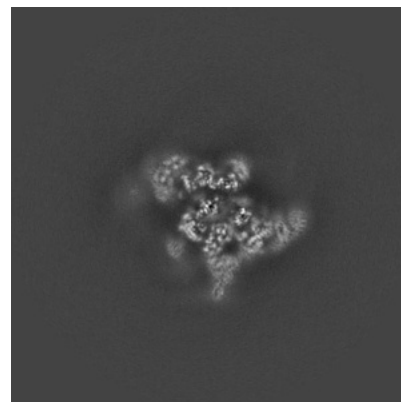
6.3.1 Primary map



X Index: 283

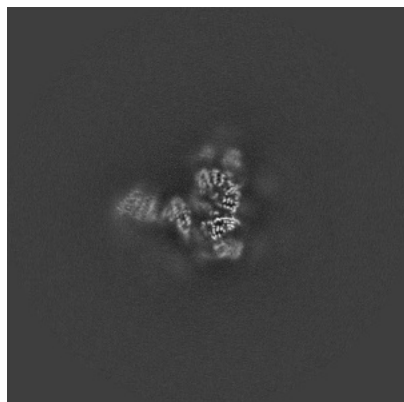


Y Index: 301

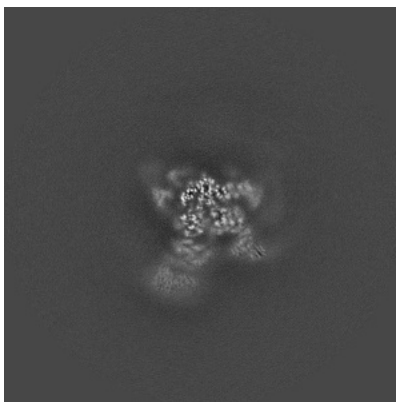


Z Index: 265

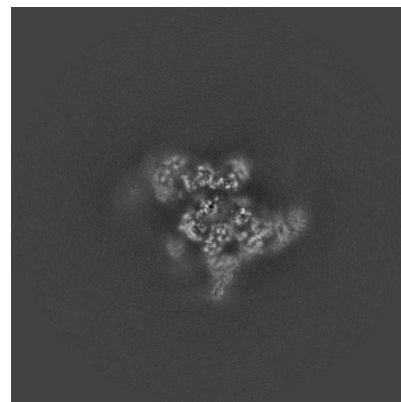
6.3.2 Raw map



X Index: 283



Y Index: 301

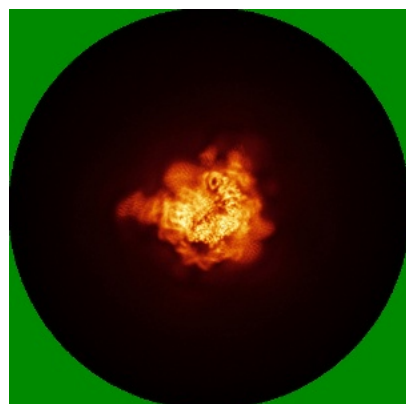


Z Index: 265

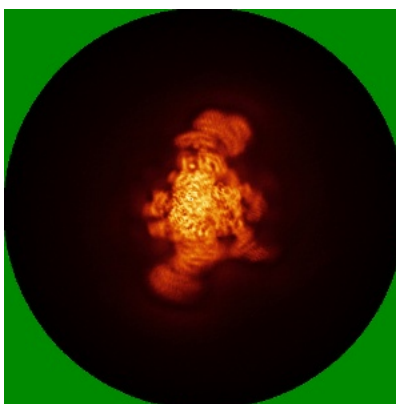
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

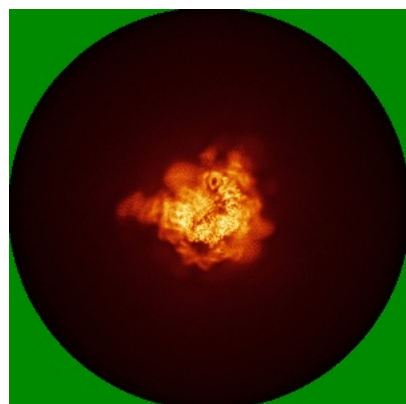


Y

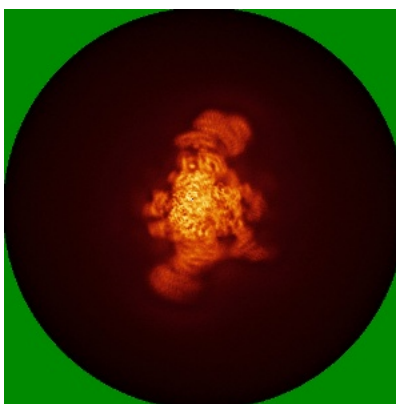


Z

6.4.2 Raw map



X



Y

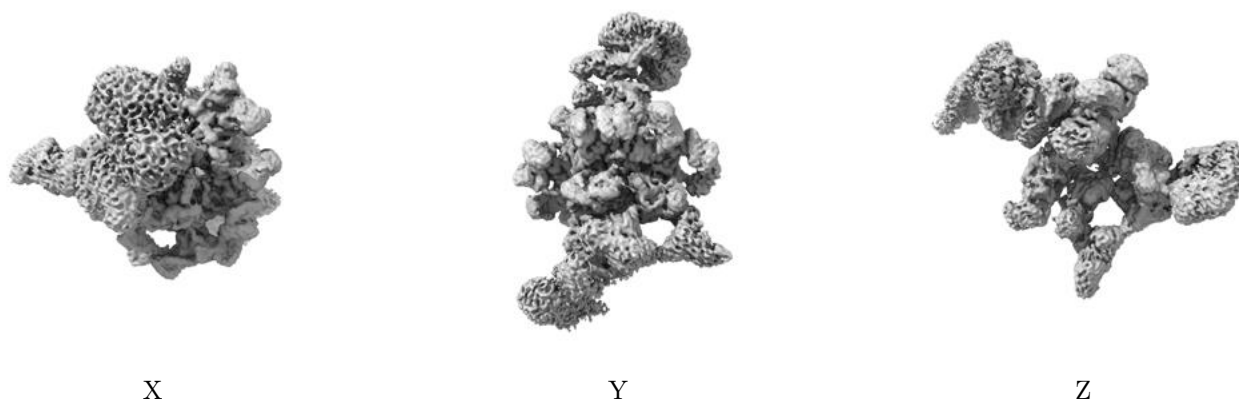


Z

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.

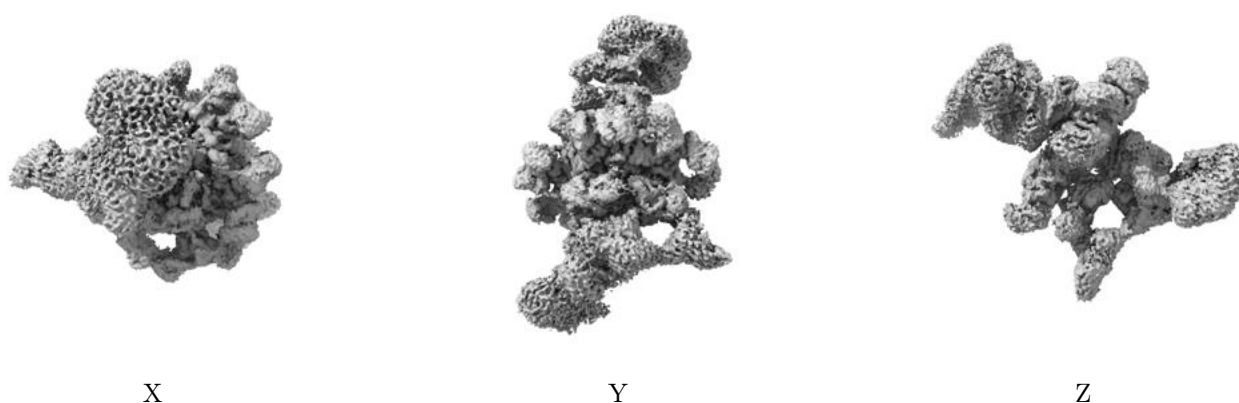
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00805. 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.

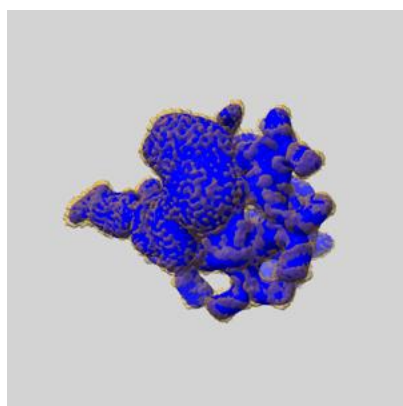
6.6 Mask visualisation [i](#)

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

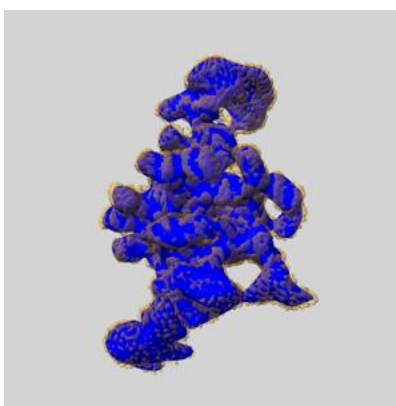
A mask typically either:

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

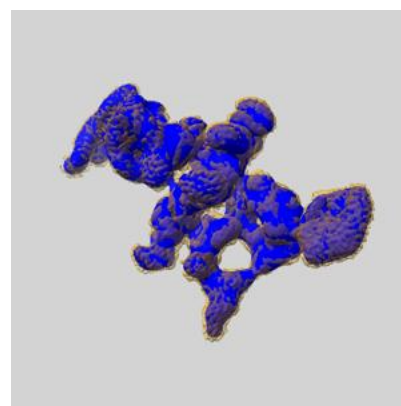
6.6.1 emd_34399_msk_1.map [i](#)



X



Y

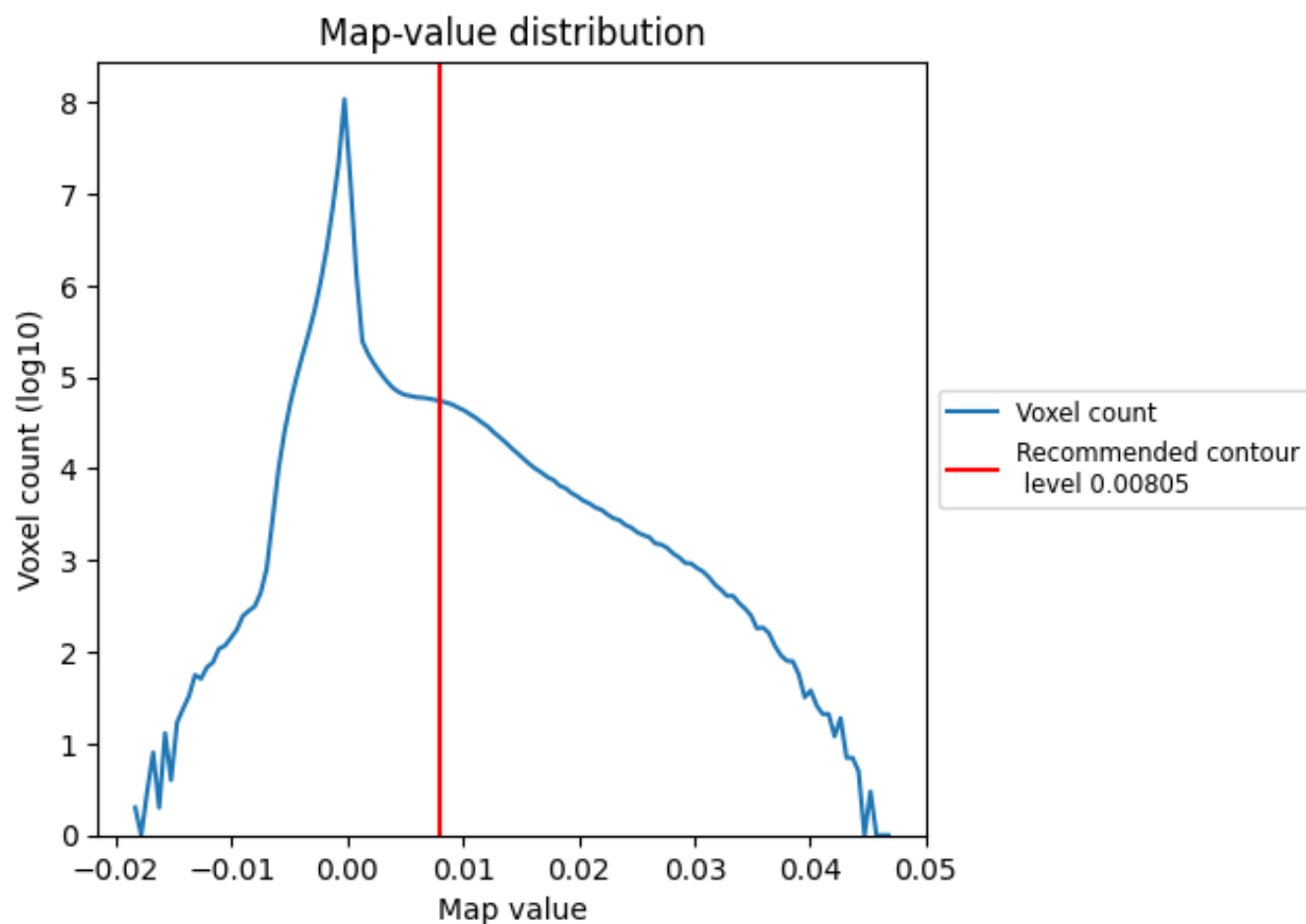


Z

7 Map analysis [i](#)

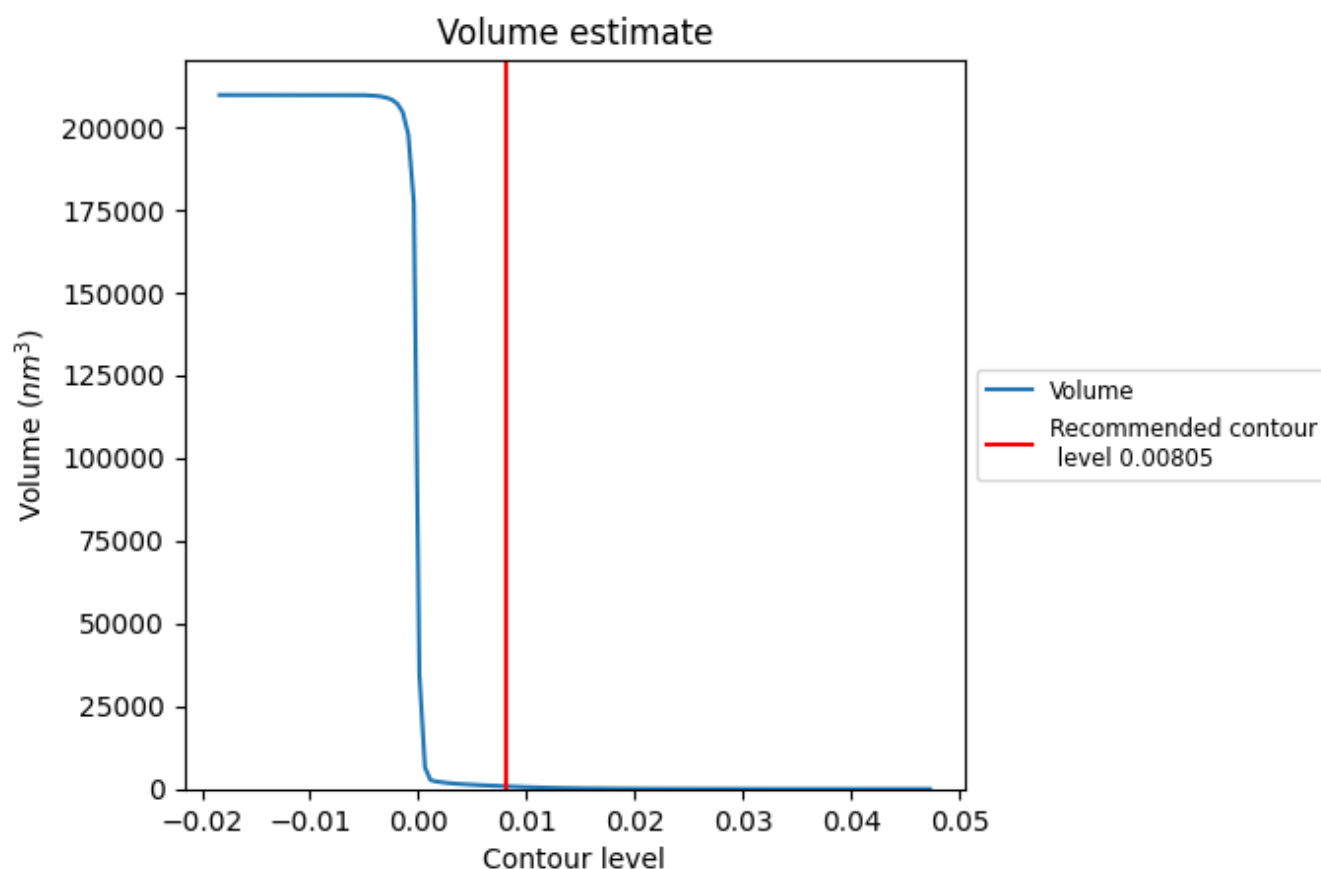
This section contains the results of statistical analysis of the map.

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.

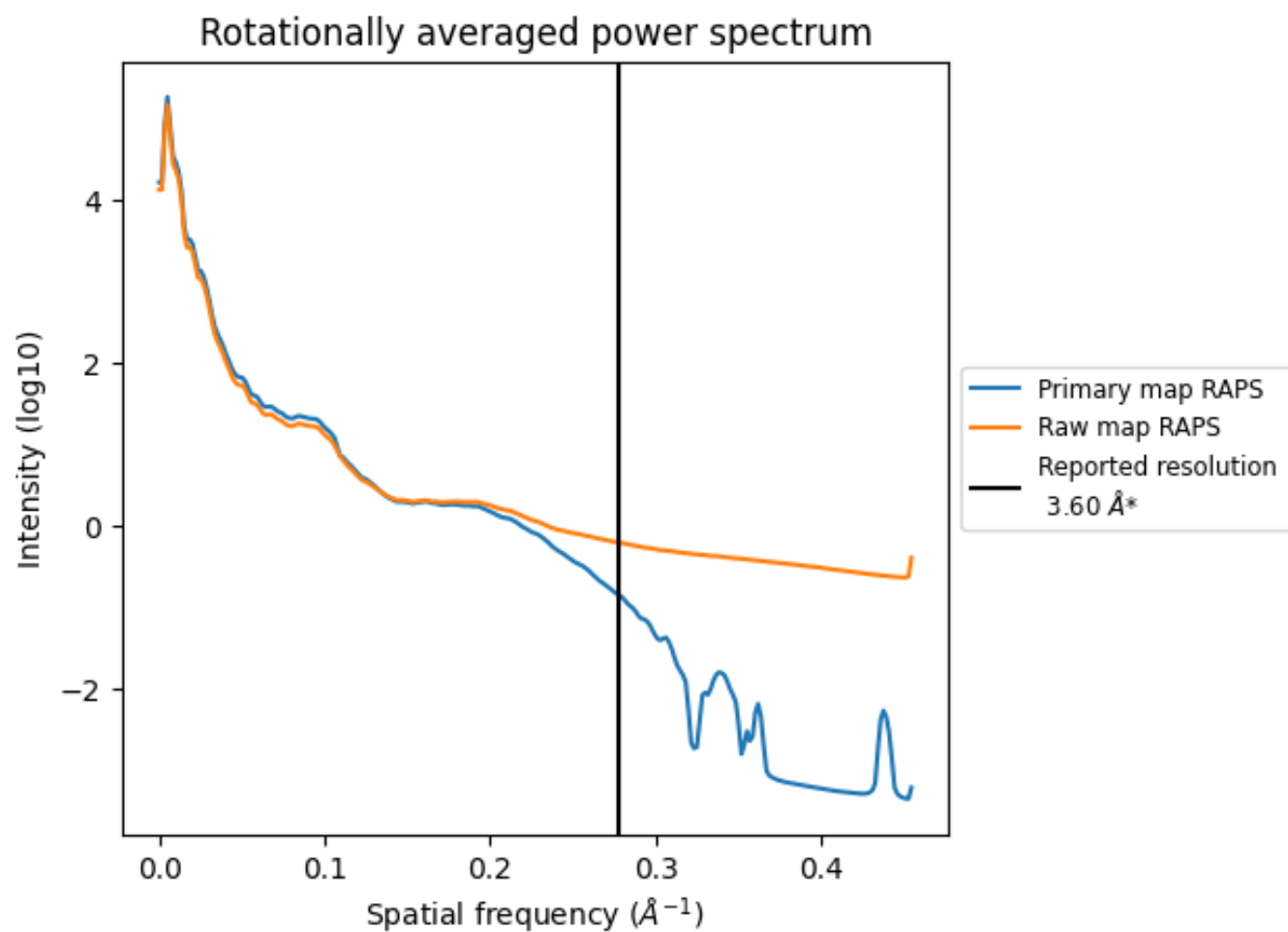
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 809 nm^3 ; this corresponds to an approximate mass of 731 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 ⓘ

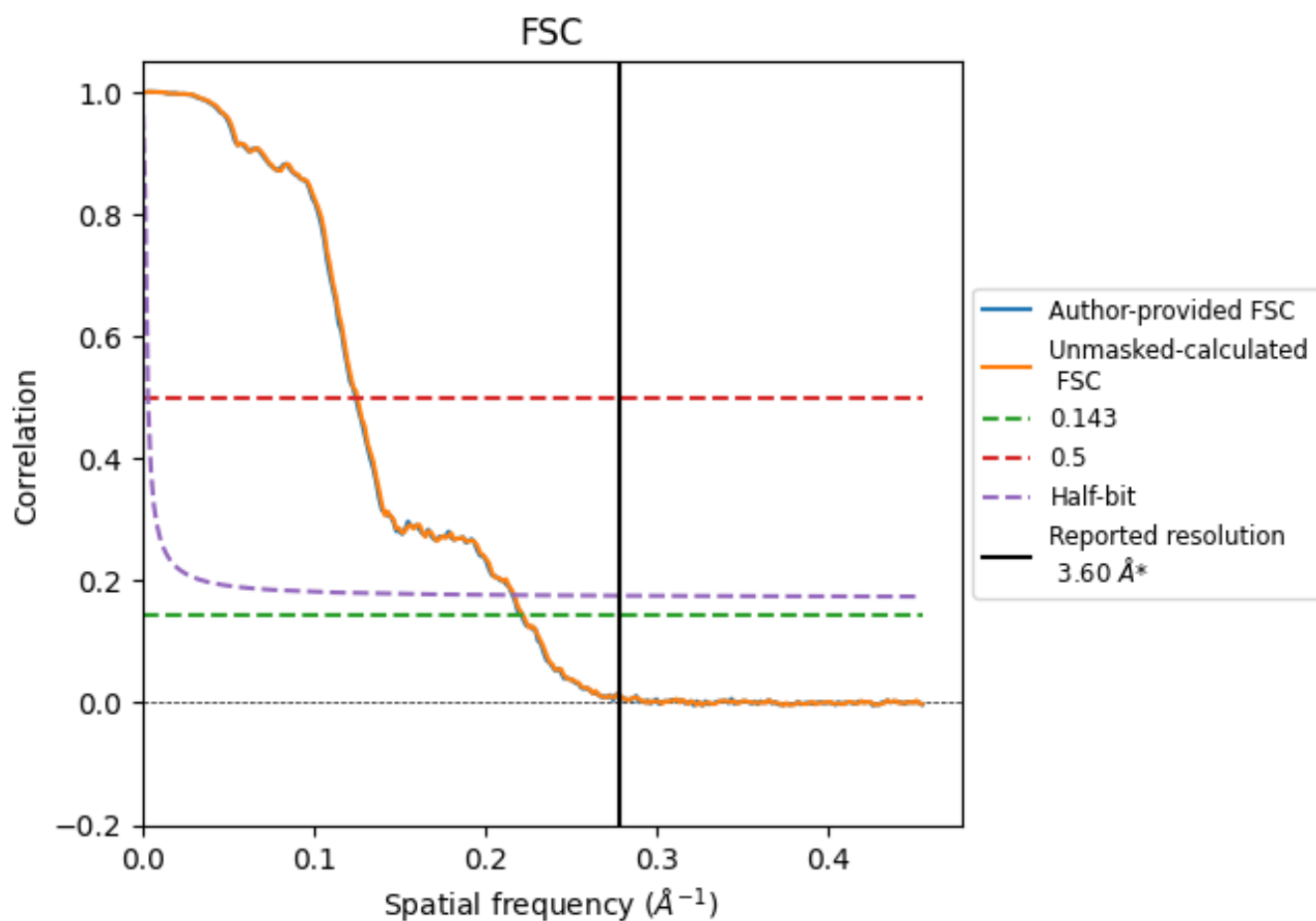


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 $0.278 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	4.52	8.05	4.63
Unmasked-calculated*	4.50	7.98	4.61

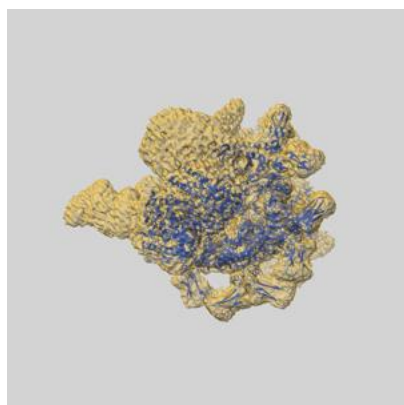
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.52 differs from the reported value 3.6 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.50 differs from the reported value 3.6 by more than 10 %

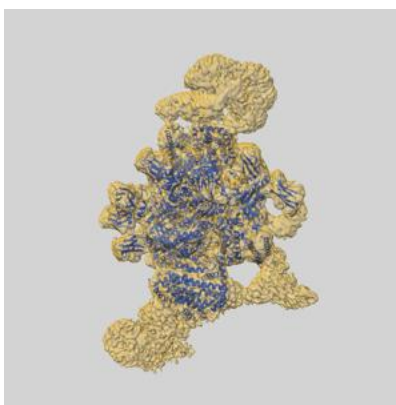
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-34399 and PDB model 8GZN. Per-residue inclusion information can be found in section 3 on page 5.

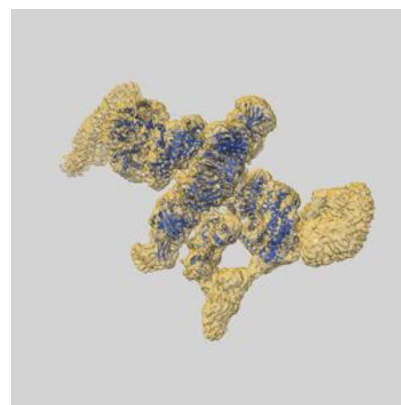
9.1 Map-model overlay [i](#)



X



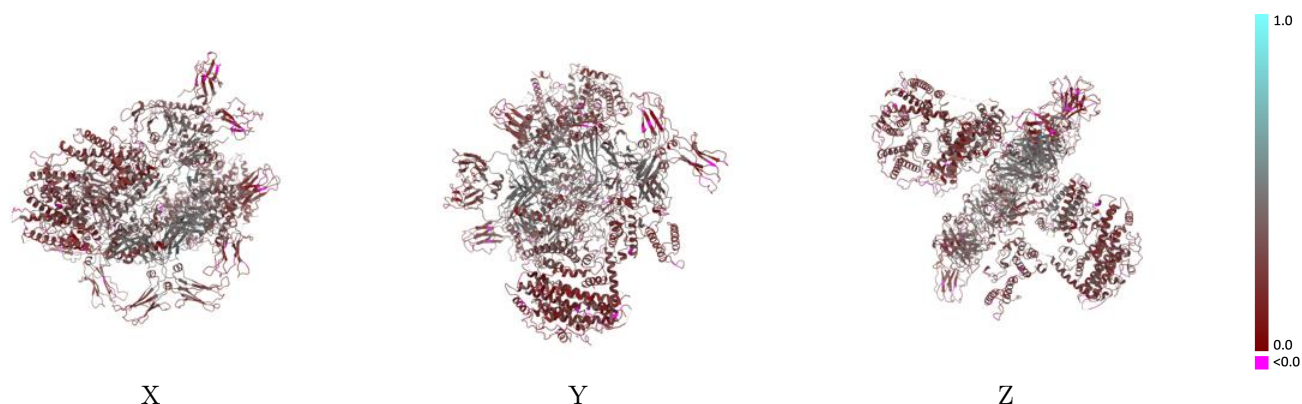
Y



Z

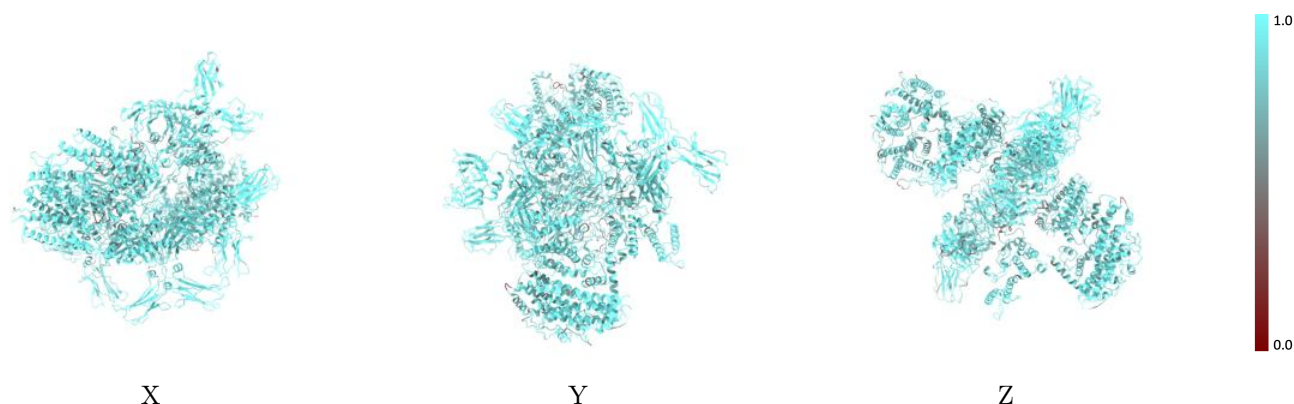
The images above show the 3D surface view of the map at the recommended contour level 0.00805 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



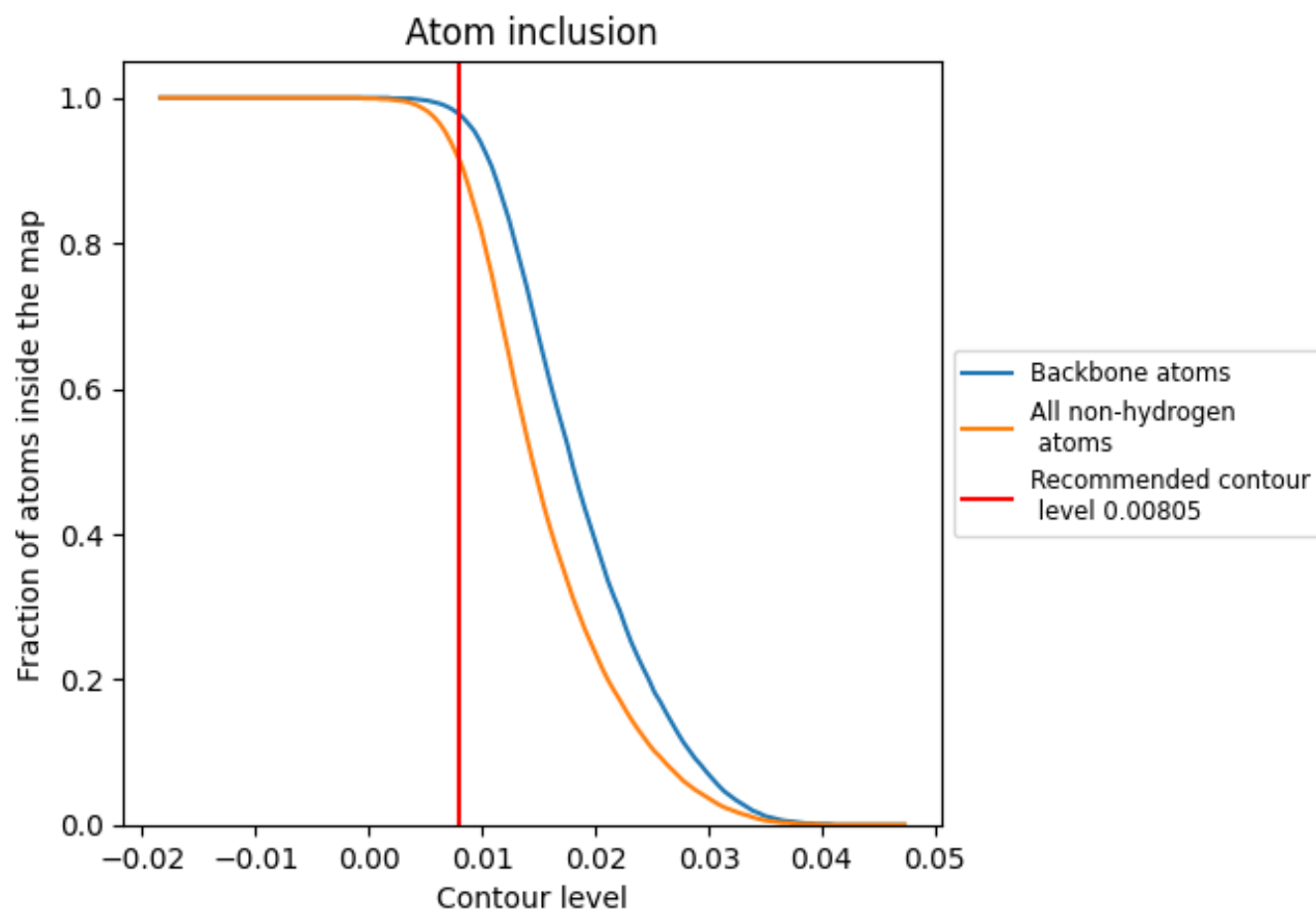
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00805).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 91% 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 (0.00805) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9130	 0.3040
A	 0.9120	 0.3280
B	 0.9120	 0.3300
C	 0.9560	 0.3410
D	 0.9550	 0.3630
E	 0.9590	 0.3830
F	 0.9510	 0.3730
G	 0.9400	 0.3620
H	 0.9450	 0.3300
I	 0.8870	 0.2540
J	 0.7250	 0.2720
K	 0.9210	 0.3080
L	 0.9550	 0.3170
M	 0.9070	 0.2840

