



Full wwPDB EM Validation Report ⓘ

Nov 3, 2024 – 03:37 am GMT

PDB ID : 7B52
EMDB ID : EMD-12017
Title : VAR2CSA full ectodomain
Authors : Wang, K.T.; Gourdon, P.E.; Dagil, R.; Salanti, A.
Deposited on : 2020-12-03
Resolution : 3.80 Å (reported)
Based on initial models : 2Y8D, 4P1T

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.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

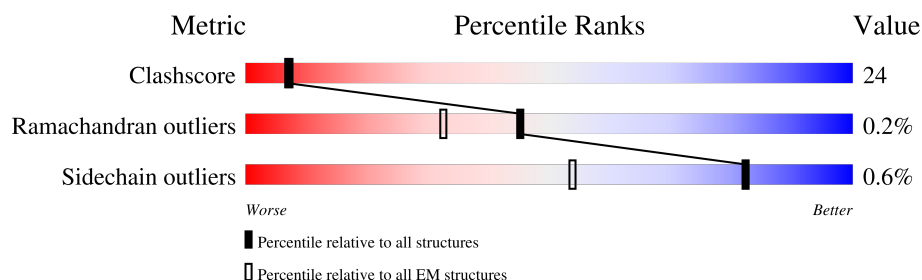
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	2649	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 13186 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 Erythrocyte membrane protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1638	Total	C	N	O	S	1	0
			13186	8294	2229	2576	87		

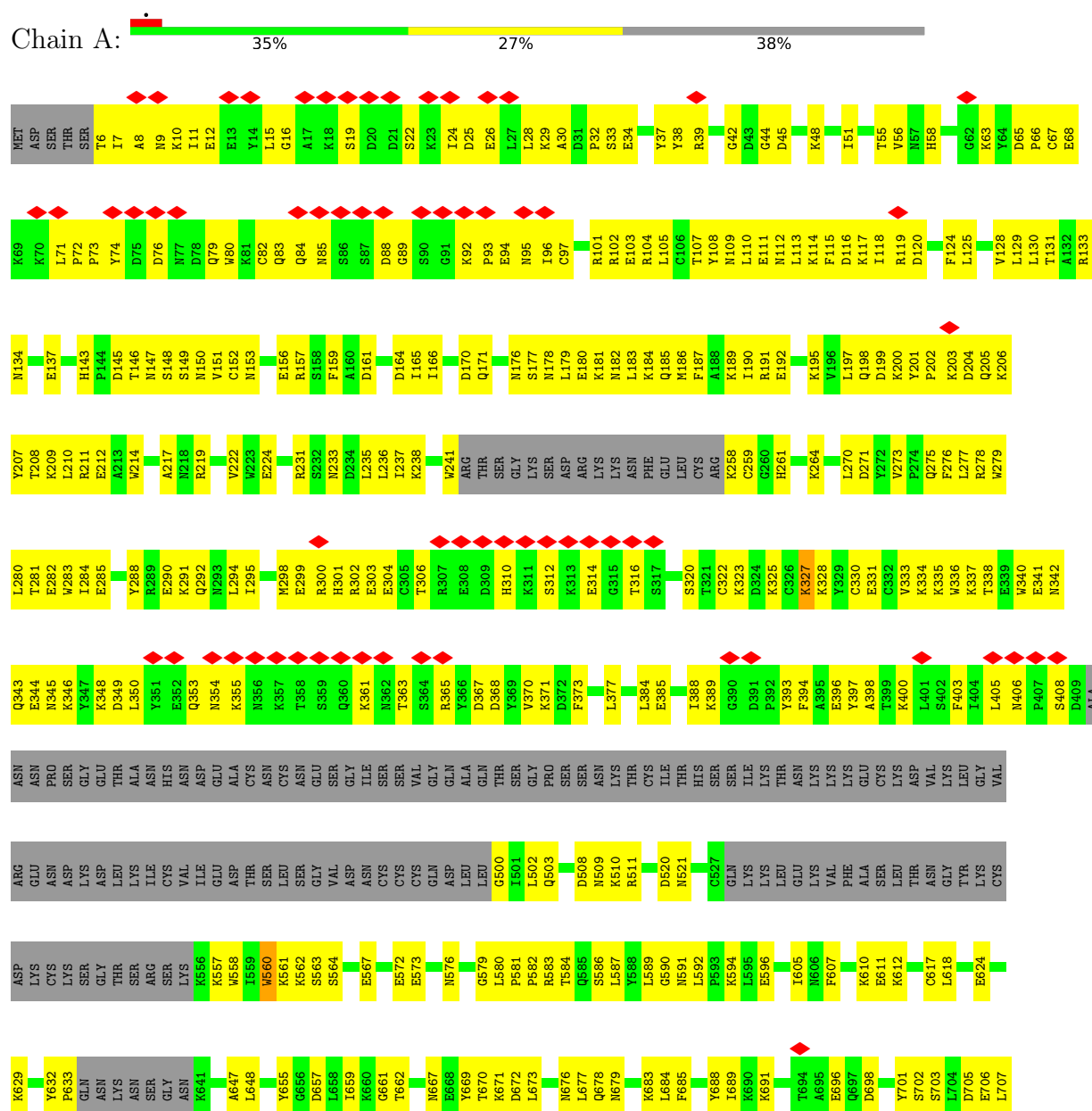
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1192	SER	ASN	conflict	UNP Q6UDW7
A	1728	ASN	ASP	conflict	UNP Q6UDW7
A	1876	ASP	GLY	conflict	UNP Q6UDW7
A	2241	GLN	ARG	conflict	UNP Q6UDW7

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: Erythrocyte membrane protein 1



I1788	A1791	Q1794	W1798	L1799	W1802	F1806	K1812	F1814	C1821	ASP	PRO	PRO	LYS	ARG	ALA	ASP	THR	M1730	D1731	T1734	Q1628	Q1630	I1631	C1632	I1636	M1850	P1851	K1852	R1853	M1859	I1866	Y1867	R1868	K1869	S1870	N1871	K1872	E1873	D1876	G1877	K1878	D1879	Y1880	M1884	T1887						
D1681	N1684	R1692	F1695	D1697	D1700	G1704	M1705	H1709	K1719	L1720	M1721	E1722	S1534	A1535	S1536	D1537	L1538	L1539	E1540	E1541	N1542	Y1543	P1544	E1545	C1546	I1547	F1551	D1552	F1553	I1554	F1555	N1556	D1557	E1560	Y1561	K1562	T1563	Y1564	Y1565	D1569	K1571	O1572	Y1573	C1574	S1575	K1583					
M1586	K1590	S1594	L1595	C1596	K1599	D1600	M1601	T1604	W1605	K1611	K1612	L1613	E1614	L1619	V1624	P1625	P1626	R1627	R1628	Q1629	Q1630	I1631	C1632	E1635	L1636	I1639	I1640	I1641	K1642	N1643	T1657	V1661	R1664	E1665	A1666	Y1667	W1670	K1671	O1672	Y1673	N1674	P1675	T1676	G1677	K1678						
GLY	GLN	Q1498	R1503	K1507	K1515	K1516	Q1517	E1518	W1519	Q1522	K1523	T1524	K1525	S1534	A1535	S1536	D1537	L1538	L1539	E1540	E1541	N1542	Y1543	P1544	E1545	C1546	I1547	F1551	D1552	F1553	I1554	F1555	N1556	D1557	E1560	Y1561	K1562	T1563	Y1564	Y1565	D1569	K1571	O1572	Y1573	C1574	S1575	K1583				
VAL	SER	THR	N1400	V1401	A1403	W1404	W1405	K1406	R1417	C1418	A1419	I1420	T1421	K1422	I1423	N1424	N1429	S1430	E1436	V1439	P1442	Q1449	W1453	F1454	W1457	C1462	E1469	Q1470	R1473	E1474	I1478	ASN	GLY	LYS	ASN	GLU	LYS	C1486	S1489	K1490	S1491										
K1306	Y1314	H1315	G1318	T1319	A1320	K1324	N1325	Q1330	K1331	G1332	L1339	P1340	F1343	R1349	I1352	D1353	Y1354	K1355	N1356	G1360	V1363	N1364	I1365	Y1366	E1367	H1368	I1369	G1370	K1371	L1372	Q1373	K1377	K1378	I1379	I1380	E1381	K1382	G1383	P1385	GLN	GLN	LYS	ASP	LYS	ILE	GLY					
G1229	C1230	Y1235	D1236	G1237	K1238	I1239	K1243	E1246	Q1247	Q1248	W1249	I1250	C1251	K1252	D1253	T1254	I1255	I1256	N1261	I1265	P1266	P1267	T1268	T1269	N1270	G1275	E1276	L1277	D1279	K1280	S1281	Y1282	G1283	G1284	N1287	I1288	D1291	T1292	K1293	E1298	K1299	I1300	K1301	H1305							
K1156	Y1157	F1158	N1159	GLY	ASP	T1163	K1164	I1165	N1167	I1168	E1174	I1177	C1180	G1181	N1183	H1186	G1187	E1188	K1194	L1195	K1196	K1200	K1201	C1202	K1203	GLU	ASN	GLU	SER	THR	THR	ASN	ILE	ASN	LYS	VAL	V1139	S1140	S1142	N1143	F1144	L1145	F1146	F1147	E1151	T1154	Q1155				
T1015	T1016	V1017	R1018	SER	ASN	SER	S1022	K1023	L1024	D1025	N1027	D1028	G954	N955	T956	F1031	Y958	K961	Y962	C964	C965	C966	T970	E973	Y981	Q984	Y985	S986	C987	G988	ALA	THR	ARG	THR	LEU	VAL	ASP	VAL	THR	GLY	THR	PRO	LYS	VAL	ARG	GLY	TYR	GLU	ASP		
SER	SER	THR	THR	ASN	ALA	ALA	SER	D873	C877	N878	Q879	D881	I882	K887	H888	L889	I890	L894	Q965	C966	E1047	T970	S987	S988	S989	Y900	L901	G923	S986	S987	D906	Y904	Y985	Y986	D913	K914	Y915	Y916	Y917	T918	T919	Y920	T921	T922	C928	C929	C1005	N1008	Y1013	P1014	
I762	T783	S710	C785	W711	K786	W713	T714	W715	K716	I719	W720	W723	K724	E798	C799	K800	T801	K802	D805	E806	K811	A820	G823	I824	T826	A827	G828	S829	P830	W831	R834	K840	R841	Y842	S843	K844	H845	I846	N852	R853	K854	A855	C856	THR	LYS	ASN	GLU	ARG	ASP	GLY	THR



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	102676	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.842	Depositor
Minimum map value	-0.736	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.065	Depositor
Recommended contour level	0.56	Depositor
Map size (Å)	365.19998, 365.19998, 365.19998	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	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	0.29	0/13462	0.49	0/18140

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1180	CYS	Peptide
1	A	1252	LYS	Peptide
1	A	1281	SER	Peptide
1	A	560	TRP	Peptide
1	A	879	GLN	Peptide
1	A	965	GLN	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	13186	0	12436	604	0
All	All	13186	0	12436	604	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 24.

All (604) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:691:LYS:HB2	1:A:702:SER:HB2	1.53	0.91
1:A:108:TYR:HA	1:A:111:GLU:HG2	1.55	0.87
1:A:1097:CYS:SG	1:A:1101:LYS:NZ	2.49	0.86
1:A:115:PHE:HE2	1:A:117:LYS:HG2	1.40	0.84
1:A:573:GLU:O	1:A:841:ARG:NH1	2.10	0.84
1:A:878:VAL:HG11	1:A:888:HIS:HB2	1.63	0.81
1:A:377:LEU:HD21	1:A:384:LEU:HB3	1.65	0.78
1:A:1145:LEU:HD12	1:A:1188:GLU:HB2	1.65	0.78
1:A:71:LEU:HD12	1:A:72:PRO:HD2	1.66	0.78
1:A:89:GLY:HA2	1:A:93:PRO:HA	1.67	0.77
1:A:1704:GLY:HA3	1:A:1738:ARG:HH12	1.49	0.76
1:A:688:TYR:O	1:A:702:SER:OG	2.03	0.75
1:A:114:LYS:HE3	1:A:182:ASN:HD21	1.52	0.75
1:A:1258:GLY:HA2	1:A:1364:ASN:H	1.50	0.75
1:A:1611:LYS:HB3	1:A:1709:HIS:HD2	1.51	0.75
1:A:895:THR:O	1:A:899:SER:OG	2.06	0.74
1:A:1942:LEU:HA	1:A:1945:GLU:HB3	1.69	0.74
1:A:164:ASP:OD2	1:A:278:ARG:NH1	2.21	0.73
1:A:343:GLN:HA	1:A:346:LYS:HD2	1.70	0.73
1:A:558:TRP:HB2	1:A:825:GLY:HA2	1.70	0.73
1:A:178:ASN:O	1:A:182:ASN:ND2	2.22	0.72
1:A:1674:ASN:ND2	1:A:1684:ASN:OD1	2.22	0.72
1:A:45:ASP:HA	1:A:48:LYS:HG2	1.71	0.72
1:A:288:TYR:O	1:A:292:GLN:NE2	2.23	0.72
1:A:691:LYS:NZ	1:A:696:GLU:O	2.18	0.72
1:A:130:LEU:O	1:A:134:ASN:ND2	2.23	0.72
1:A:829:SER:HB2	1:A:834:ARG:HE	1.54	0.71
1:A:842:TYR:OH	1:A:894:LEU:O	2.06	0.71
1:A:987:CYS:HA	1:A:1005:CYS:HA	1.72	0.71
1:A:25:ASP:O	1:A:29:LYS:N	2.22	0.71
1:A:1353:ASP:OD1	1:A:1449:GLN:NE2	2.24	0.70
1:A:111:GLU:O	1:A:114:LYS:NZ	2.21	0.70
1:A:206:LYS:HD3	1:A:210:LEU:HG	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:691:LYS:HE2	1:A:702:SER:H	1.55	0.70
1:A:852:ASN:O	1:A:887:LYS:NZ	2.22	0.70
1:A:1227:ILE:HG22	1:A:1229:GLY:H	1.55	0.70
1:A:25:ASP:HA	1:A:28:LEU:HB3	1.73	0.69
1:A:187:PHE:HB3	1:A:205:GLN:HE22	1.57	0.69
1:A:918:THR:HG22	1:A:919:THR:H	1.56	0.69
1:A:7:ILE:H	1:A:11:ILE:HD13	1.57	0.69
1:A:291:LYS:HZ1	1:A:397:TYR:H	1.41	0.69
1:A:1590:LYS:O	1:A:1664:ARG:NH2	2.18	0.69
1:A:956:THR:HB	1:A:961:LYS:HA	1.74	0.68
1:A:1151:GLU:HA	1:A:1154:ILE:HG22	1.74	0.68
1:A:97:CYS:SG	1:A:343:GLN:NE2	2.64	0.68
1:A:103:GLU:OE1	1:A:104:ARG:NH1	2.25	0.68
1:A:314:GLU:HG3	1:A:316:THR:HG22	1.75	0.68
1:A:186:MET:HA	1:A:189:LYS:HD2	1.75	0.67
1:A:1027:ASN:O	1:A:1030:THR:OG1	2.11	0.67
1:A:73:PRO:HA	1:A:104:ARG:HG2	1.75	0.67
1:A:153:ASN:HB3	1:A:157:ARG:HE	1.60	0.66
1:A:115:PHE:CE2	1:A:117:LYS:HG2	2.29	0.66
1:A:96:ILE:HD11	1:A:276:PHE:HA	1.78	0.66
1:A:235:LEU:HA	1:A:258:LYS:HB3	1.78	0.66
1:A:84:GLN:HA	1:A:89:GLY:HA3	1.78	0.65
1:A:1565:TYR:OH	1:A:1635:GLU:OE2	2.14	0.65
1:A:1599:LYS:NZ	1:A:1665:GLU:OE1	2.29	0.65
1:A:679:ASN:O	1:A:683:LYS:NZ	2.28	0.65
1:A:757:PRO:HB3	1:A:882:ILE:HG13	1.79	0.65
1:A:1291:ASP:OD1	1:A:1292:THR:N	2.29	0.65
1:A:96:ILE:HG13	1:A:279:TRP:HE3	1.61	0.65
1:A:1143:ASN:HD22	1:A:1973:LEU:HD21	1.61	0.65
1:A:164:ASP:OD2	1:A:275:GLN:NE2	2.30	0.65
1:A:187:PHE:HA	1:A:190:ILE:HD12	1.80	0.64
1:A:1101:LYS:HZ1	1:A:1202:CYS:HB2	1.61	0.64
1:A:1261:ASN:OD1	1:A:1525:LYS:NZ	2.30	0.64
1:A:367:ASP:HA	1:A:371:LYS:HE2	1.79	0.64
1:A:906:ASP:HB2	1:A:909:ILE:HG23	1.78	0.64
1:A:330:CYS:O	1:A:334:LYS:HG2	1.97	0.64
1:A:1557:ASP:O	1:A:1562:LYS:NZ	2.30	0.64
1:A:1600:ASP:OD1	1:A:1601:ASN:N	2.29	0.63
1:A:1473:ARG:NH2	1:A:1641:ILE:O	2.29	0.63
1:A:1420:ILE:O	1:A:1424:ASN:ND2	2.31	0.63
1:A:922:THR:HG22	1:A:949:VAL:HG12	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:VAL:HA	1:A:130:LEU:HD21	1.80	0.63
1:A:270:LEU:O	1:A:278:ARG:NH2	2.29	0.63
1:A:1100:TYR:HA	1:A:1103:TRP:CD1	2.34	0.63
1:A:65:ASP:O	1:A:109:ASN:ND2	2.32	0.63
1:A:846:ILE:HG13	1:A:895:THR:HG23	1.81	0.62
1:A:1692:ARG:NE	1:A:1903:ASN:OD1	2.32	0.62
1:A:66:PRO:HA	1:A:109:ASN:HD21	1.64	0.62
1:A:780:ASP:O	1:A:783:THR:OG1	2.17	0.62
1:A:306:THR:N	1:A:322:CYS:SG	2.72	0.62
1:A:191:ARG:NH2	1:A:200:LYS:O	2.33	0.62
1:A:915:ALA:HB2	1:A:958:TYR:HB2	1.82	0.62
1:A:1250:ILE:O	1:A:1265:ILE:N	2.27	0.62
1:A:7:ILE:HG23	1:A:9:ASN:H	1.65	0.62
1:A:846:ILE:HG23	1:A:890:ILE:HD11	1.81	0.62
1:A:124:PHE:HZ	1:A:166:ILE:HD11	1.66	0.61
1:A:207:TYR:O	1:A:211:ARG:HB2	1.99	0.61
1:A:1869:LYS:HB3	1:A:1873:GLU:HG2	1.83	0.61
1:A:1002:TYR:OH	1:A:1028:ASP:OD1	2.19	0.61
1:A:784:ASN:HB2	1:A:806:GLU:OE1	2.01	0.60
1:A:558:TRP:CD2	1:A:582:PRO:HD3	2.36	0.60
1:A:984:GLN:HG3	1:A:1008:ASN:HD21	1.67	0.60
1:A:657:ASP:OD1	1:A:662:THR:OG1	2.19	0.60
1:A:1174:GLU:N	1:A:1174:GLU:OE1	2.32	0.60
1:A:1356:ASN:ND2	1:A:1449:GLN:OE1	2.24	0.60
1:A:202:PRO:HD2	1:A:206:LYS:HB2	1.82	0.60
1:A:345:ASN:O	1:A:349:ASP:N	2.31	0.59
1:A:573:GLU:HG3	1:A:841:ARG:HH22	1.66	0.59
1:A:1259:ASP:H	1:A:1364:ASN:HB2	1.67	0.59
1:A:92:LYS:HB2	1:A:361:LYS:HE3	1.84	0.59
1:A:1041:GLU:OE2	1:A:1853:ARG:NH1	2.35	0.59
1:A:509:ASN:HB3	1:A:511:ARG:HH22	1.67	0.59
1:A:1002:TYR:HE2	1:A:1028:ASP:HA	1.67	0.59
1:A:1036:GLU:OE2	1:A:1850:ASN:ND2	2.36	0.59
1:A:1159:ASN:H	1:A:1163:SER:HA	1.66	0.59
1:A:1249:TRP:CH2	1:A:1457:TRP:HB2	2.38	0.58
1:A:1420:ILE:HG12	1:A:1436:GLU:HG3	1.83	0.58
1:A:1671:LYS:HD3	1:A:1675:PRO:HG3	1.85	0.58
1:A:113:LEU:HD11	1:A:182:ASN:HB3	1.85	0.58
1:A:765:GLU:O	1:A:766:TRP:HB3	2.03	0.58
1:A:1325:ASN:H	1:A:1330:GLN:HA	1.67	0.58
1:A:1627:ARG:NH1	1:A:1697:ASP:OD2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:ILE:O	1:A:258:LYS:NZ	2.37	0.58
1:A:920:TYR:HA	1:A:951:SER:HA	1.85	0.58
1:A:179:LEU:HA	1:A:182:ASN:HD22	1.69	0.58
1:A:587:LEU:HD13	1:A:655:TYR:HE1	1.68	0.58
1:A:1369:ILE:O	1:A:1372:LEU:N	2.35	0.58
1:A:34:GLU:HB2	1:A:37:TYR:HE1	1.68	0.58
1:A:1047:GLU:OE2	1:A:1194:LYS:NZ	2.27	0.58
1:A:1093:CYS:SG	1:A:1094:LYS:N	2.77	0.58
1:A:1163:SER:N	1:A:1166:LYS:HZ3	2.01	0.58
1:A:1256:ILE:O	1:A:1257:HIS:ND1	2.36	0.58
1:A:560:TRP:CE2	1:A:579:GLY:HA3	2.39	0.58
1:A:1158:PHE:HD1	1:A:1166:LYS:HE2	1.69	0.58
1:A:203:LYS:HE3	1:A:204:ASP:HA	1.86	0.57
1:A:231:ARG:CZ	1:A:233:ASN:HB3	2.34	0.57
1:A:775:GLN:HA	1:A:778:VAL:HG12	1.86	0.57
1:A:895:THR:HG22	1:A:896:THR:H	1.68	0.57
1:A:981:TYR:O	1:A:1049:TYR:OH	2.14	0.57
1:A:1266:PRO:O	1:A:1269:THR:OG1	2.19	0.57
1:A:842:TYR:CG	1:A:897:PRO:HG3	2.40	0.57
1:A:1417:ARG:NE	1:A:1439:VAL:O	2.37	0.57
1:A:1537:ASP:O	1:A:1540:LYS:N	2.37	0.57
1:A:1583:LYS:N	1:A:1586:ASN:OD1	2.38	0.57
1:A:224:GLU:OE2	1:A:261:HIS:NE2	2.30	0.57
1:A:842:TYR:HE2	1:A:895:THR:HA	1.70	0.57
1:A:39:ARG:NH2	1:A:1782:CYS:O	2.37	0.57
1:A:1293:LYS:HE3	1:A:1380:ILE:HA	1.86	0.57
1:A:882:ILE:H	1:A:882:ILE:HD12	1.69	0.57
1:A:826:THR:OG1	1:A:829:SER:O	2.22	0.57
1:A:905:LEU:HD13	1:A:909:ILE:HD11	1.86	0.57
1:A:1278:TRP:CZ2	1:A:1284:GLY:HA2	2.40	0.57
1:A:39:ARG:NH2	1:A:1780:PRO:O	2.38	0.56
1:A:67:CYS:HB2	1:A:108:TYR:HB2	1.86	0.56
1:A:984:GLN:OE1	1:A:984:GLN:N	2.31	0.56
1:A:1156:LYS:HE3	1:A:1157:TYR:CZ	2.41	0.56
1:A:1280:LYS:HB3	1:A:1283:GLY:HA2	1.86	0.56
1:A:1570:TYR:O	1:A:1574:CYS:HB3	2.06	0.56
1:A:182:ASN:O	1:A:185:GLN:HG2	2.06	0.56
1:A:292:GLN:HA	1:A:295:ILE:HG22	1.86	0.56
1:A:63:LYS:NZ	1:A:114:LYS:O	2.39	0.56
1:A:37:TYR:HB2	1:A:42:GLY:HA3	1.88	0.56
1:A:96:ILE:HG13	1:A:279:TRP:CE3	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1352:ILE:HD11	1:A:1442:PRO:HB2	1.86	0.56
1:A:1605:TRP:CE2	1:A:1626:PRO:HD3	2.41	0.56
1:A:337:LYS:O	1:A:341:GLU:HG2	2.06	0.56
1:A:1626:PRO:O	1:A:1630:GLN:HG2	2.06	0.56
1:A:1887:THR:HG23	1:A:1890:ASP:H	1.70	0.56
1:A:129:LEU:HD11	1:A:222:VAL:HA	1.89	0.55
1:A:398:ALA:HB3	1:A:400:LYS:HE3	1.88	0.55
1:A:118:ILE:O	1:A:119:ARG:HG2	2.06	0.55
1:A:1378:LYS:O	1:A:1382:LYS:HG2	2.06	0.55
1:A:33:SER:HA	1:A:44:GLY:HA2	1.88	0.55
1:A:159:PHE:HE1	1:A:222:VAL:HG13	1.71	0.55
1:A:192:GLU:O	1:A:198:GLN:NE2	2.40	0.55
1:A:605:ILE:HG22	1:A:607:PHE:H	1.72	0.55
1:A:1611:LYS:HB3	1:A:1709:HIS:CD2	2.37	0.55
1:A:109:ASN:HB2	1:A:131:THR:HG22	1.88	0.55
1:A:29:LYS:HD2	1:A:217:ALA:HB1	1.89	0.55
1:A:706:GLU:O	1:A:710:SER:HB3	2.08	0.54
1:A:191:ARG:HA	1:A:197:LEU:HD23	1.88	0.54
1:A:560:TRP:CE3	1:A:834:ARG:HD2	2.42	0.54
1:A:689:ILE:HD13	1:A:707:LEU:HD12	1.89	0.54
1:A:827:ALA:O	1:A:834:ARG:NH1	2.40	0.54
1:A:629:LYS:NZ	1:A:728:GLU:HB2	2.23	0.54
1:A:1183:ASN:HB2	1:A:1186:HIS:ND1	2.23	0.54
1:A:1381:GLU:OE1	1:A:1400:ASN:ND2	2.34	0.54
1:A:152:CYS:SG	1:A:238:LYS:NZ	2.70	0.54
1:A:1276:GLU:O	1:A:1287:ASN:ND2	2.27	0.54
1:A:1626:PRO:HA	1:A:1629:GLN:HE21	1.73	0.54
1:A:178:ASN:HA	1:A:181:LYS:NZ	2.22	0.54
1:A:1046:ILE:O	1:A:1050:MET:HG2	2.08	0.54
1:A:12:GLU:O	1:A:16:GLY:N	2.32	0.54
1:A:919:THR:O	1:A:921:THR:HG23	2.08	0.54
1:A:1024:LEU:HD12	1:A:1963:GLU:HG2	1.90	0.54
1:A:1122:ARG:O	1:A:1126:ILE:N	2.41	0.54
1:A:1553:PHE:HE2	1:A:1569:ASP:HA	1.73	0.54
1:A:1945:GLU:HG3	1:A:1951:ASP:HB3	1.88	0.54
1:A:24:ILE:O	1:A:28:LEU:N	2.37	0.53
1:A:93:PRO:HG2	1:A:342:ASN:ND2	2.24	0.53
1:A:1002:TYR:CE2	1:A:1028:ASP:HA	2.43	0.53
1:A:898:SER:HB2	1:A:917:TRP:O	2.08	0.53
1:A:94:GLU:OE2	1:A:97:CYS:HA	2.09	0.53
1:A:273:VAL:O	1:A:278:ARG:NH2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1368:HIS:O	1:A:1371:LYS:HG2	2.08	0.53
1:A:350:LEU:HD21	1:A:363:THR:H	1.72	0.53
1:A:1419:ALA:O	1:A:1423:ILE:HG12	2.09	0.53
1:A:1965:TYR:O	1:A:1969:VAL:HG23	2.08	0.53
1:A:270:LEU:O	1:A:273:VAL:HG22	2.08	0.53
1:A:288:TYR:HE2	1:A:394:PHE:HA	1.73	0.53
1:A:590:GLY:O	1:A:669:TYR:HB2	2.09	0.53
1:A:760:LEU:HD12	1:A:900:TYR:CZ	2.42	0.53
1:A:1572:SER:O	1:A:1574:CYS:N	2.41	0.53
1:A:370:VAL:HG13	1:A:371:LYS:HD3	1.91	0.53
1:A:1100:TYR:CE2	1:A:1104:ILE:HD11	2.44	0.53
1:A:1250:ILE:HB	1:A:1265:ILE:HB	1.89	0.53
1:A:1561:TYR:HE1	1:A:1596:CYS:HA	1.74	0.53
1:A:1604:THR:O	1:A:1629:GLN:NE2	2.41	0.53
1:A:1026:GLY:O	1:A:1029:VAL:HG12	2.09	0.53
1:A:146:THR:N	1:A:147:ASN:HA	2.24	0.53
1:A:238:LYS:HA	1:A:241:TRP:HB3	1.91	0.53
1:A:561:LYS:HG3	1:A:562:LYS:N	2.23	0.53
1:A:1366:TYR:HB3	1:A:1369:ILE:HD11	1.89	0.53
1:A:1544:PRO:HA	1:A:1547:ILE:HD11	1.91	0.53
1:A:1305:HIS:ND1	1:A:1419:ALA:HB2	2.24	0.52
1:A:1454:PHE:CE2	1:A:1535:ALA:HB1	2.44	0.52
1:A:342:ASN:O	1:A:346:LYS:HG3	2.09	0.52
1:A:729:MET:HG3	1:A:733:THR:HG21	1.91	0.52
1:A:1227:ILE:HG21	1:A:1275:GLY:HA2	1.91	0.52
1:A:780:ASP:OD1	1:A:781:VAL:N	2.42	0.52
1:A:291:LYS:NZ	1:A:397:TYR:HB3	2.25	0.52
1:A:1470:GLN:NE2	1:A:1474:GLU:OE2	2.39	0.52
1:A:1320:ALA:O	1:A:1324:LYS:HG3	2.09	0.52
1:A:152:CYS:SG	1:A:153:ASN:N	2.83	0.52
1:A:161:ASP:O	1:A:165:ILE:HG12	2.10	0.52
1:A:618:LEU:HD23	1:A:719:ILE:HD13	1.92	0.52
1:A:1377:LYS:HD3	1:A:1381:GLU:HG3	1.92	0.52
1:A:157:ARG:HD3	1:A:282:GLU:OE1	2.10	0.52
1:A:1594:SER:OG	1:A:1664:ARG:NH1	2.42	0.52
1:A:93:PRO:HG2	1:A:342:ASN:HD21	1.75	0.51
1:A:703:SER:O	1:A:706:GLU:N	2.43	0.51
1:A:96:ILE:HG12	1:A:171:GLN:HB2	1.93	0.51
1:A:950:PRO:HB3	1:A:953:LEU:HG	1.92	0.51
1:A:176:ASN:O	1:A:180:GLU:N	2.41	0.51
1:A:560:TRP:NE1	1:A:579:GLY:HA3	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1277:LEU:HD11	1:A:1300:ILE:HA	1.91	0.51
1:A:1403:ALA:HA	1:A:1406:LYS:HD2	1.91	0.51
1:A:39:ARG:HH22	1:A:1784:GLY:N	2.09	0.51
1:A:629:LYS:O	1:A:633:PRO:HD2	2.10	0.51
1:A:281:THR:O	1:A:285:GLU:HG2	2.11	0.51
1:A:344:GLU:HG3	1:A:348:LYS:HD2	1.93	0.51
1:A:1628:ARG:O	1:A:1628:ARG:NH1	2.36	0.51
1:A:648:LEU:HD11	1:A:723:MET:HG2	1.93	0.51
1:A:720:TRP:NE1	1:A:724:LYS:HD2	2.26	0.51
1:A:973:GLU:OE1	1:A:973:GLU:N	2.33	0.51
1:A:116:ASP:HA	1:A:189:LYS:HZ3	1.76	0.51
1:A:288:TYR:CE2	1:A:394:PHE:HA	2.46	0.51
1:A:233:ASN:OD1	1:A:678:GLN:NE2	2.44	0.51
1:A:503:GLN:HB2	1:A:714:THR:HG21	1.91	0.51
1:A:672:ASP:OD1	1:A:673:LEU:N	2.42	0.51
1:A:895:THR:O	1:A:896:THR:OG1	2.29	0.51
1:A:587:LEU:HD13	1:A:655:TYR:CE1	2.45	0.50
1:A:1349:ARG:NH2	1:A:1543:TYR:OH	2.41	0.50
1:A:1745:GLU:HA	1:A:1755:THR:HA	1.92	0.50
1:A:560:TRP:CD1	1:A:579:GLY:HA3	2.47	0.50
1:A:1013:LYS:H	1:A:1950:MET:CE	2.25	0.50
1:A:1120:LYS:HB3	1:A:1124:LYS:NZ	2.26	0.50
1:A:1469:GLU:HB2	1:A:1570:TYR:OH	2.11	0.50
1:A:1613:LEU:HD23	1:A:1614:GLU:HG2	1.94	0.50
1:A:1360:GLY:HA2	1:A:1373:GLN:HG2	1.92	0.50
1:A:1516:LYS:HA	1:A:1555:PHE:HD1	1.75	0.50
1:A:560:TRP:CZ3	1:A:834:ARG:HD2	2.45	0.50
1:A:1280:LYS:HG3	1:A:1284:GLY:H	1.77	0.50
1:A:1742:TRP:CE2	1:A:1757:ARG:HB3	2.46	0.50
1:A:303:GLU:HG2	1:A:304:GLU:HG2	1.92	0.50
1:A:1237:GLY:O	1:A:1314:TYR:OH	2.15	0.50
1:A:80:TRP:CZ3	1:A:283:TRP:HD1	2.30	0.50
1:A:557:LYS:H	1:A:582:PRO:HB3	1.76	0.50
1:A:191:ARG:HD3	1:A:205:GLN:HE21	1.77	0.50
1:A:350:LEU:HG	1:A:353:GLN:HE21	1.76	0.50
1:A:781:VAL:HA	1:A:806:GLU:OE1	2.12	0.50
1:A:1146:PHE:HE1	1:A:1181:GLY:HA3	1.76	0.50
1:A:63:LYS:HB3	1:A:112:ASN:O	2.12	0.49
1:A:393:TYR:CD1	1:A:396:GLU:HG3	2.48	0.49
1:A:1613:LEU:HD12	1:A:1619:LEU:HD22	1.94	0.49
1:A:180:GLU:O	1:A:183:LEU:HG	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:LYS:O	1:A:331:GLU:HG3	2.13	0.49
1:A:918:THR:O	1:A:919:THR:OG1	2.29	0.49
1:A:1624:VAL:HG11	1:A:1629:GLN:HB3	1.94	0.49
1:A:1339:LEU:HD23	1:A:1343:PHE:CE2	2.48	0.49
1:A:32:PRO:HG2	1:A:51:ILE:HD11	1.93	0.49
1:A:92:LYS:HZ3	1:A:346:LYS:HD3	1.77	0.49
1:A:405:LEU:HG	1:A:406:ASN:H	1.77	0.49
1:A:1740:ASP:HA	1:A:1743:GLU:HB2	1.95	0.49
1:A:918:THR:HG22	1:A:919:THR:N	2.26	0.49
1:A:37:TYR:H	1:A:42:GLY:HA3	1.78	0.49
1:A:182:ASN:HB3	1:A:186:MET:HE1	1.94	0.49
1:A:705:ASP:O	1:A:709:GLU:N	2.34	0.49
1:A:970:THR:N	1:A:973:GLU:OE2	2.40	0.49
1:A:589:LEU:HD12	1:A:592:LEU:HD12	1.95	0.49
1:A:801:THR:C	1:A:802:LYS:HD2	2.33	0.49
1:A:917:TRP:HA	1:A:952:PRO:HD3	1.95	0.49
1:A:114:LYS:CE	1:A:182:ASN:HD21	2.25	0.48
1:A:283:TRP:CZ3	1:A:340:TRP:HD1	2.30	0.48
1:A:393:TYR:HD1	1:A:396:GLU:HG3	1.78	0.48
1:A:1238:LYS:NZ	1:A:1243:LYS:O	2.34	0.48
1:A:510:LYS:HG2	1:A:888:HIS:CE1	2.48	0.48
1:A:587:LEU:HD12	1:A:589:LEU:H	1.78	0.48
1:A:896:THR:O	1:A:899:SER:N	2.45	0.48
1:A:1278:TRP:HE1	1:A:1371:LYS:HZ1	1.60	0.48
1:A:840:LYS:HE2	1:A:1884:MET:HB3	1.95	0.48
1:A:1280:LYS:O	1:A:1281:SER:OG	2.31	0.48
1:A:92:LYS:NZ	1:A:346:LYS:HD3	2.29	0.48
1:A:384:LEU:N	1:A:403:PHE:O	2.45	0.48
1:A:1235:TYR:HA	1:A:1247:LYS:HG3	1.96	0.48
1:A:561:LYS:HG3	1:A:562:LYS:H	1.79	0.48
1:A:102:ARG:HG2	1:A:279:TRP:CH2	2.48	0.48
1:A:896:THR:O	1:A:898:SER:N	2.47	0.48
1:A:1719:LYS:O	1:A:1722:GLU:HG2	2.13	0.48
1:A:55:THR:H	1:A:58:HIS:CE1	2.32	0.48
1:A:143:HIS:HE1	1:A:150:ASN:HB3	1.79	0.48
1:A:1516:LYS:HA	1:A:1555:PHE:CD1	2.48	0.48
1:A:350:LEU:HG	1:A:353:GLN:NE2	2.29	0.47
1:A:1002:TYR:O	1:A:1117:ASN:ND2	2.25	0.47
1:A:1731:ASP:O	1:A:1735:LYS:HG2	2.13	0.47
1:A:56:VAL:HG21	1:A:66:PRO:HD3	1.95	0.47
1:A:89:GLY:CA	1:A:93:PRO:HA	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:ARG:HA	1:A:222:VAL:HG12	1.95	0.47
1:A:310:HIS:NE2	1:A:323:LYS:HD3	2.29	0.47
1:A:841:ARG:O	1:A:844:LYS:HG3	2.13	0.47
1:A:1636:LEU:HD21	1:A:1661:VAL:HG11	1.97	0.47
1:A:1681:ASP:N	1:A:1681:ASP:OD2	2.47	0.47
1:A:855:ALA:O	1:A:879:GLN:NE2	2.36	0.47
1:A:1239:ILE:HA	1:A:1319:THR:HG21	1.95	0.47
1:A:1739:THR:O	1:A:1742:TRP:HB3	2.14	0.47
1:A:205:GLN:HB3	1:A:207:TYR:CE2	2.49	0.47
1:A:38:TYR:OH	1:A:118:ILE:HA	2.15	0.47
1:A:581:PRO:O	1:A:584:THR:OG1	2.32	0.47
1:A:720:TRP:CE2	1:A:751:PRO:HD3	2.50	0.47
1:A:1876:ASP:HB2	1:A:1878:LYS:HD3	1.97	0.47
1:A:610:LYS:HE2	1:A:685:PHE:CE1	2.50	0.47
1:A:1667:TYR:HD1	1:A:1771:ALA:HB2	1.80	0.47
1:A:771:CYS:HB3	1:A:910:CYS:HB3	1.26	0.47
1:A:1572:SER:O	1:A:1575:SER:N	2.45	0.47
1:A:1639:ILE:O	1:A:1643:ASN:N	2.43	0.47
1:A:811:LYS:HD3	1:A:955:ASN:HB2	1.95	0.47
1:A:895:THR:C	1:A:896:THR:HG1	2.18	0.47
1:A:1382:LYS:HA	1:A:1382:LYS:HD3	1.74	0.47
1:A:624:GLU:HG3	1:A:655:TYR:OH	2.14	0.47
1:A:629:LYS:HZ2	1:A:728:GLU:HB2	1.78	0.47
1:A:1670:TRP:CH2	1:A:1780:PRO:HG3	2.49	0.47
1:A:684:LEU:H	1:A:684:LEU:HD23	1.78	0.47
1:A:1258:GLY:H	1:A:1364:ASN:C	2.19	0.47
1:A:1625:PRO:HG3	1:A:1798:TRP:CD1	2.50	0.47
1:A:1734:THR:O	1:A:1738:ARG:HG2	2.15	0.47
1:A:191:ARG:HH22	1:A:201:TYR:HA	1.80	0.46
1:A:564:SER:HB2	1:A:567:GLU:O	2.15	0.46
1:A:677:LEU:HD23	1:A:708:ARG:HH11	1.80	0.46
1:A:152:CYS:HB2	1:A:236:LEU:HA	1.97	0.46
1:A:502:LEU:O	1:A:503:GLN:NE2	2.48	0.46
1:A:1519:TRP:CH2	1:A:1523:LYS:HD3	2.51	0.46
1:A:511:ARG:NH1	1:A:520:ASP:H	2.13	0.46
1:A:751:PRO:O	1:A:753:ILE:N	2.44	0.46
1:A:829:SER:HB2	1:A:834:ARG:NE	2.27	0.46
1:A:195:LYS:HA	1:A:198:GLN:OE1	2.16	0.46
1:A:563:SER:OG	1:A:572:GLU:HA	2.16	0.46
1:A:1154:ILE:HG12	1:A:1164:LYS:HD2	1.96	0.46
1:A:148:SER:OG	1:A:149:SER:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:LYS:HD2	1:A:207:TYR:CE2	2.50	0.46
1:A:300:ARG:HG3	1:A:301:HIS:H	1.81	0.46
1:A:696:GLU:O	1:A:698:ASP:N	2.49	0.46
1:A:769:ASN:O	1:A:772:GLU:HG3	2.16	0.46
1:A:1794:GLN:OE1	1:A:1794:GLN:N	2.43	0.46
1:A:1196:LYS:O	1:A:1200:LYS:HG2	2.15	0.46
1:A:1235:TYR:HB2	1:A:1267:PRO:HB2	1.96	0.46
1:A:1639:ILE:HD11	1:A:1657:THR:HG21	1.97	0.46
1:A:1799:LEU:HD13	1:A:1859:MET:HE2	1.98	0.46
1:A:701:TYR:O	1:A:707:LEU:HG	2.16	0.46
1:A:1632:CYS:HB3	1:A:1665:GLU:HG2	1.98	0.46
1:A:1870:SER:H	1:A:1873:GLU:CD	2.20	0.46
1:A:191:ARG:O	1:A:198:GLN:HG3	2.16	0.45
1:A:354:ASN:HA	1:A:355:LYS:HA	1.46	0.45
1:A:334:LYS:O	1:A:338:THR:HG23	2.16	0.45
1:A:509:ASN:HB2	1:A:521:ASN:O	2.16	0.45
1:A:1515:LYS:HA	1:A:1518:GLU:HB3	1.97	0.45
1:A:1896:CYS:HB2	1:A:1907:CYS:O	2.16	0.45
1:A:333:VAL:O	1:A:337:LYS:HG2	2.16	0.45
1:A:1560:GLU:HA	1:A:1563:THR:HG22	1.99	0.45
1:A:170:ASP:OD1	1:A:171:GLN:N	2.50	0.45
1:A:949:VAL:N	1:A:950:PRO:HD3	2.31	0.45
1:A:1355:LYS:HG3	1:A:1405:TRP:NE1	2.31	0.45
1:A:15:LEU:HD21	1:A:368:ASP:HB3	1.99	0.45
1:A:586:SER:HA	1:A:591:ASN:ND2	2.32	0.45
1:A:1032:PHE:O	1:A:1036:GLU:N	2.37	0.45
1:A:1042:ILE:O	1:A:1046:ILE:HG12	2.16	0.45
1:A:281:THR:HG21	1:A:388:ILE:HD12	1.97	0.45
1:A:632:TYR:HE2	1:A:647:ALA:HB3	1.82	0.45
1:A:1118:TYR:CD1	1:A:1141:LEU:HB2	2.52	0.45
1:A:166:ILE:HG12	1:A:214:TRP:CZ3	2.52	0.45
1:A:1100:TYR:HA	1:A:1103:TRP:NE1	2.31	0.45
1:A:1147:PHE:CZ	1:A:1969:VAL:HG22	2.52	0.45
1:A:117:LYS:HG3	1:A:117:LYS:O	2.17	0.45
1:A:180:GLU:O	1:A:184:LYS:HG2	2.17	0.45
1:A:1959:MET:O	1:A:1963:GLU:HG3	2.17	0.45
1:A:1980:ILE:O	1:A:1984:LYS:HG2	2.16	0.44
1:A:896:THR:HG23	1:A:1870:SER:HB3	1.98	0.44
1:A:1013:LYS:H	1:A:1950:MET:HE1	1.82	0.44
1:A:101:ARG:NH1	1:A:161:ASP:OD2	2.51	0.44
1:A:1158:PHE:HB3	1:A:1163:SER:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:ILE:H	1:A:11:ILE:HD12	1.82	0.44
1:A:145:ASP:HB3	1:A:150:ASN:HD22	1.82	0.44
1:A:895:THR:HB	1:A:1870:SER:HB2	2.00	0.44
1:A:7:ILE:HD11	1:A:385:GLU:HG3	1.99	0.44
1:A:22:SER:O	1:A:25:ASP:N	2.31	0.44
1:A:147:ASN:HB2	1:A:151:VAL:HG13	2.00	0.44
1:A:203:LYS:HA	1:A:205:GLN:H	1.81	0.44
1:A:772:GLU:O	1:A:775:GLN:HG3	2.18	0.44
1:A:1503:ARG:O	1:A:1507:LYS:HG3	2.17	0.44
1:A:1700:ASP:O	1:A:1704:GLY:N	2.50	0.44
1:A:105:LEU:O	1:A:107:THR:N	2.49	0.44
1:A:340:TRP:CE3	1:A:400:LYS:HB2	2.52	0.44
1:A:949:VAL:HG11	1:A:1867:TYR:OH	2.18	0.44
1:A:1288:ILE:O	1:A:1288:ILE:HG13	2.17	0.44
1:A:706:GLU:O	1:A:710:SER:CB	2.65	0.44
1:A:753:ILE:HG13	1:A:756:ILE:HD12	2.00	0.44
1:A:1225:ASN:OD1	1:A:1306:LYS:HD3	2.18	0.44
1:A:1315:HIS:HB3	1:A:1340:PRO:HB2	1.99	0.44
1:A:1866:ILE:HD11	1:A:1880:TYR:CE1	2.53	0.44
1:A:83:GLN:O	1:A:85:ASN:ND2	2.51	0.44
1:A:560:TRP:CD1	1:A:579:GLY:CA	3.01	0.44
1:A:610:LYS:HG3	1:A:611:GLU:OE2	2.18	0.44
1:A:689:ILE:HA	1:A:702:SER:HB3	1.99	0.44
1:A:1454:PHE:CD1	1:A:1522:GLN:HB3	2.53	0.44
1:A:786:LYS:HD2	1:A:786:LYS:HA	1.74	0.43
1:A:873:ASP:N	1:A:879:GLN:OE1	2.51	0.43
1:A:1457:TRP:CH2	1:A:1519:TRP:HB2	2.53	0.43
1:A:1696:TYR:CD1	1:A:1791:ALA:HB2	2.52	0.43
1:A:76:ASP:OD1	1:A:79:GLN:NE2	2.50	0.43
1:A:153:ASN:O	1:A:156:GLU:HG2	2.19	0.43
1:A:1421:THR:HA	1:A:1424:ASN:HD21	1.83	0.43
1:A:1537:ASP:O	1:A:1541:GLU:OE1	2.35	0.43
1:A:74:TYR:CE2	1:A:143:HIS:HA	2.53	0.43
1:A:110:LEU:HG	1:A:131:THR:HG21	2.00	0.43
1:A:199:ASP:HB2	1:A:200:LYS:NZ	2.33	0.43
1:A:273:VAL:HG23	1:A:278:ARG:HB2	2.01	0.43
1:A:288:TYR:HA	1:A:291:LYS:HG2	2.01	0.43
1:A:767:VAL:HG21	1:A:901:LEU:HD11	2.00	0.43
1:A:965:GLN:O	1:A:967:LYS:HG2	2.18	0.43
1:A:1049:TYR:HD2	1:A:1103:TRP:CZ2	2.36	0.43
1:A:1705:ASN:HA	1:A:1878:LYS:HE3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:576:ASN:N	1:A:576:ASN:OD1	2.52	0.43
1:A:691:LYS:CE	1:A:702:SER:H	2.27	0.43
1:A:1462:CYS:HB3	1:A:1546:CYS:HB3	1.35	0.43
1:A:1870:SER:O	1:A:1872:LYS:N	2.52	0.43
1:A:33:SER:OG	1:A:48:LYS:N	2.52	0.43
1:A:277:LEU:O	1:A:280:LEU:HG	2.19	0.43
1:A:312:SER:OG	1:A:320:SER:HB2	2.19	0.43
1:A:670:THR:HG22	1:A:671:LYS:H	1.84	0.43
1:A:696:GLU:C	1:A:698:ASP:H	2.22	0.43
1:A:1534:SER:OG	1:A:1537:ASP:OD2	2.36	0.43
1:A:500:GLY:HA2	1:A:610:LYS:HB2	2.01	0.43
1:A:1047:GLU:O	1:A:1050:MET:HB2	2.18	0.43
1:A:7:ILE:HG21	1:A:10:LYS:HE2	2.01	0.43
1:A:72:PRO:O	1:A:104:ARG:NH2	2.52	0.43
1:A:83:GLN:CD	1:A:83:GLN:H	2.22	0.43
1:A:201:TYR:N	1:A:202:PRO:HD3	2.33	0.43
1:A:233:ASN:ND2	1:A:661:GLY:HA3	2.32	0.43
1:A:691:LYS:HG2	1:A:696:GLU:HG3	2.00	0.43
1:A:1100:TYR:O	1:A:1104:ILE:HG13	2.19	0.43
1:A:1120:LYS:HB3	1:A:1124:LYS:HZ1	1.84	0.43
1:A:1672:GLN:HE21	1:A:1672:GLN:HB3	1.71	0.43
1:A:8:ALA:HA	1:A:12:GLU:HG3	2.01	0.43
1:A:133:ARG:O	1:A:137:GLU:HG2	2.18	0.43
1:A:181:LYS:HA	1:A:184:LYS:HG2	2.01	0.43
1:A:586:SER:OG	1:A:586:SER:O	2.37	0.43
1:A:1177:ILE:HG13	1:A:1181:GLY:C	2.39	0.43
1:A:1221:LEU:H	1:A:1221:LEU:HD23	1.84	0.43
1:A:233:ASN:HD21	1:A:708:ARG:HH22	1.67	0.43
1:A:659:ILE:HA	1:A:677:LEU:HD21	2.01	0.43
1:A:1884:MET:SD	1:A:1884:MET:N	2.91	0.43
1:A:22:SER:O	1:A:24:ILE:N	2.52	0.43
1:A:48:LYS:HB3	1:A:48:LYS:HE3	1.77	0.43
1:A:118:ILE:O	1:A:120:ASP:N	2.52	0.43
1:A:805:ASP:OD1	1:A:806:GLU:N	2.50	0.43
1:A:145:ASP:HB3	1:A:150:ASN:ND2	2.34	0.42
1:A:152:CYS:HA	1:A:236:LEU:HD13	2.00	0.42
1:A:187:PHE:CE2	1:A:210:LEU:HB3	2.54	0.42
1:A:337:LYS:HE3	1:A:400:LYS:HB3	2.01	0.42
1:A:558:TRP:NE1	1:A:766:TRP:HB2	2.34	0.42
1:A:583:ARG:HD3	1:A:647:ALA:HB1	2.01	0.42
1:A:586:SER:HA	1:A:591:ASN:HD21	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:853:ARG:C	1:A:854:LYS:HD2	2.39	0.42
1:A:1259:ASP:HB3	1:A:1364:ASN:OD1	2.19	0.42
1:A:1913:GLY:HA3	1:A:1942:LEU:HD13	2.00	0.42
1:A:1202:CYS:SG	1:A:1203:LYS:HD2	2.59	0.42
1:A:1814:PHE:CZ	1:A:1953:LYS:HG2	2.54	0.42
1:A:670:THR:C	1:A:672:ASP:H	2.23	0.42
1:A:1049:TYR:O	1:A:1052:ASN:HB3	2.19	0.42
1:A:1101:LYS:NZ	1:A:1202:CYS:HB2	2.33	0.42
1:A:1399:GLU:N	1:A:1402:ASN:OD1	2.52	0.42
1:A:1417:ARG:O	1:A:1421:THR:HG23	2.19	0.42
1:A:84:GLN:HA	1:A:88:ASP:O	2.19	0.42
1:A:84:GLN:CA	1:A:89:GLY:HA3	2.48	0.42
1:A:110:LEU:HA	1:A:113:LEU:HD23	2.00	0.42
1:A:208:THR:OG1	1:A:209:LYS:N	2.52	0.42
1:A:967:LYS:HG3	1:A:967:LYS:O	2.20	0.42
1:A:1024:LEU:HD22	1:A:1028:ASP:OD2	2.20	0.42
1:A:1027:ASN:OD1	1:A:1028:ASP:N	2.52	0.42
1:A:1339:LEU:HD23	1:A:1343:PHE:CD2	2.54	0.42
1:A:1489:SER:HA	1:A:1498:GLN:CD	2.39	0.42
1:A:191:ARG:CD	1:A:205:GLN:HE21	2.32	0.42
1:A:335:LYS:HG3	1:A:336:TRP:N	2.34	0.42
1:A:510:LYS:HG2	1:A:888:HIS:NE2	2.35	0.42
1:A:557:LYS:N	1:A:582:PRO:HB3	2.35	0.42
1:A:562:LYS:HD2	1:A:563:SER:O	2.20	0.42
1:A:288:TYR:O	1:A:291:LYS:HG2	2.19	0.42
1:A:1278:TRP:HZ2	1:A:1284:GLY:HA2	1.85	0.42
1:A:56:VAL:HG21	1:A:65:ASP:HA	2.02	0.42
1:A:198:GLN:HA	1:A:201:TYR:CE2	2.55	0.42
1:A:344:GLU:HA	1:A:403:PHE:CE1	2.54	0.42
1:A:632:TYR:HE2	1:A:647:ALA:CB	2.32	0.42
1:A:880:SER:OG	1:A:881:ASP:N	2.48	0.42
1:A:903:ASN:C	1:A:903:ASN:HD22	2.21	0.42
1:A:1318:GLY:O	1:A:1324:LYS:HG2	2.20	0.42
1:A:184:LYS:HD2	1:A:207:TYR:CD2	2.55	0.42
1:A:277:LEU:HD12	1:A:280:LEU:HD11	2.01	0.42
1:A:278:ARG:O	1:A:281:THR:OG1	2.33	0.42
1:A:299:GLU:HA	1:A:302:ARG:HB3	2.01	0.42
1:A:509:ASN:O	1:A:511:ARG:NH1	2.51	0.42
1:A:667:ASN:H	1:A:670:THR:HB	1.85	0.42
1:A:323:LYS:NZ	1:A:327:LYS:HB3	2.35	0.42
1:A:1237:GLY:CA	1:A:1246:GLU:HG3	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1268:ARG:NH1	1:A:1353:ASP:OD2	2.44	0.42
1:A:1536:SER:HB2	1:A:1551:PHE:HD2	1.85	0.42
1:A:1720:LEU:HD23	1:A:1720:LEU:HA	1.90	0.42
1:A:1806:PHE:HD1	1:A:1852:LYS:HG2	1.84	0.42
1:A:19:SER:HB3	1:A:29:LYS:HZ1	1.85	0.41
1:A:264:LYS:HE2	1:A:264:LYS:HB2	1.93	0.41
1:A:617:CYS:HB3	1:A:719:ILE:HD11	2.02	0.41
1:A:913:ASP:OD1	1:A:913:ASP:N	2.53	0.41
1:A:1469:GLU:OE1	1:A:1570:TYR:OH	2.20	0.41
1:A:1873:GLU:N	1:A:1873:GLU:OE1	2.53	0.41
1:A:177:SER:HA	1:A:180:GLU:HB3	2.01	0.41
1:A:277:LEU:HD13	1:A:373:PHE:HE1	1.84	0.41
1:A:580:LEU:HD12	1:A:581:PRO:HD2	2.02	0.41
1:A:823:GLY:HA3	1:A:831:TRP:HZ2	1.86	0.41
1:A:1695:PHE:HE2	1:A:1788:ILE:HD11	1.85	0.41
1:A:275:GLN:HA	1:A:278:ARG:NH1	2.35	0.41
1:A:963:ALA:O	1:A:966:CYS:HA	2.20	0.41
1:A:1700:ASP:O	1:A:1705:ASN:N	2.54	0.41
1:A:34:GLU:HB2	1:A:37:TYR:CE1	2.52	0.41
1:A:74:TYR:HE2	1:A:143:HIS:HA	1.84	0.41
1:A:1298:GLU:OE2	1:A:1301:LYS:NZ	2.39	0.41
1:A:80:TRP:O	1:A:82:CYS:N	2.52	0.41
1:A:594:LYS:HG3	1:A:676:ASN:CG	2.41	0.41
1:A:594:LYS:HG3	1:A:676:ASN:ND2	2.35	0.41
1:A:917:TRP:HA	1:A:952:PRO:HG3	2.02	0.41
1:A:1537:ASP:O	1:A:1538:LEU:C	2.59	0.41
1:A:6:THR:HA	1:A:11:ILE:HB	2.02	0.41
1:A:291:LYS:HZ2	1:A:397:TYR:HB3	1.84	0.41
1:A:7:ILE:HG21	1:A:10:LYS:HZ3	1.85	0.41
1:A:68:GLU:HG2	1:A:108:TYR:HD2	1.86	0.41
1:A:281:THR:O	1:A:284:ILE:HG22	2.20	0.41
1:A:1158:PHE:CD1	1:A:1166:LYS:HE2	2.53	0.41
1:A:1168:ILE:O	1:A:1168:ILE:HG22	2.20	0.41
1:A:1418:CYS:O	1:A:1421:THR:OG1	2.33	0.41
1:A:92:LYS:HE3	1:A:95:ASN:OD1	2.21	0.41
1:A:290:GLU:O	1:A:294:LEU:HD23	2.20	0.41
1:A:408:SER:O	1:A:408:SER:OG	2.39	0.41
1:A:1457:TRP:CZ2	1:A:1515:LYS:HD2	2.56	0.41
1:A:25:ASP:OD2	1:A:26:GLU:N	2.53	0.41
1:A:200:LYS:HB3	1:A:210:LEU:HD11	2.03	0.41
1:A:385:GLU:C	1:A:389:LYS:HE3	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:ASN:HA	1:A:877:CYS:HB2	2.03	0.41
1:A:562:LYS:HD2	1:A:563:SER:N	2.36	0.41
1:A:712:TRP:O	1:A:716:LYS:HB3	2.21	0.41
1:A:799:CYS:HB3	1:A:966:CYS:HB3	1.52	0.41
1:A:985:TRP:NE1	1:A:1041:GLU:OE1	2.26	0.41
1:A:1227:ILE:HG21	1:A:1230:CYS:HB3	2.03	0.41
1:A:1523:LYS:HG3	1:A:1524:THR:N	2.35	0.41
1:A:1806:PHE:CD1	1:A:1852:LYS:HG2	2.56	0.41
1:A:7:ILE:CD1	1:A:385:GLU:HG3	2.51	0.41
1:A:30:ALA:HB3	1:A:125:LEU:HD22	2.03	0.41
1:A:703:SER:HB2	1:A:706:GLU:CD	2.41	0.41
1:A:1742:TRP:CZ2	1:A:1757:ARG:HB3	2.56	0.41
1:A:1266:PRO:HG2	1:A:1453:TRP:CD1	2.57	0.40
1:A:1278:TRP:CZ3	1:A:1366:TYR:HE2	2.39	0.40
1:A:101:ARG:HH21	1:A:282:GLU:HG2	1.85	0.40
1:A:508:ASP:HB3	1:A:878:VAL:O	2.21	0.40
1:A:1227:ILE:HD12	1:A:1276:GLU:H	1.86	0.40
1:A:1605:TRP:CH2	1:A:1802:TRP:HB2	2.55	0.40
1:A:231:ARG:NH2	1:A:233:ASN:HB3	2.37	0.40
1:A:298:MET:HA	1:A:325:LYS:NZ	2.37	0.40
1:A:561:LYS:HE2	1:A:567:GLU:OE2	2.22	0.40
1:A:596:GLU:OE1	1:A:605:ILE:HG12	2.21	0.40
1:A:1742:TRP:HE1	1:A:1757:ARG:HD2	1.87	0.40
1:A:1812:LYS:HE3	1:A:1813:TYR:CE1	2.56	0.40
1:A:206:LYS:HE2	1:A:209:LYS:HB2	2.02	0.40
1:A:208:THR:O	1:A:212:GLU:HG2	2.21	0.40
1:A:219:ARG:HH21	1:A:271:ASP:CG	2.25	0.40
1:A:236:LEU:HD23	1:A:259:CYS:HA	2.02	0.40
1:A:1177:ILE:HA	1:A:1181:GLY:H	1.87	0.40
1:A:1772:VAL:O	1:A:1776:ASN:N	2.54	0.40
1:A:10:LYS:HE2	1:A:10:LYS:HB2	1.86	0.40
1:A:128:VAL:O	1:A:131:THR:OG1	2.30	0.40
1:A:612:LYS:HA	1:A:612:LYS:HD3	1.82	0.40
1:A:841:ARG:HD2	1:A:845:HIS:CE1	2.56	0.40
1:A:1103:TRP:CZ3	1:A:1107:ILE:HG13	2.56	0.40
1:A:1719:LYS:HA	1:A:1722:GLU:HG2	2.04	0.40
1:A:1730:ASN:O	1:A:1734:THR:HG23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1599/2649 (60%)	1334 (83%)	262 (16%)	3 (0%)	44	74

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1573	ILE
1	A	952	PRO
1	A	1572	SER

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1415/2404 (59%)	1407 (99%)	8 (1%)	84	88

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	327	LYS
1	A	365	ARG
1	A	844	LYS
1	A	903	ASN
1	A	1271	ASN
1	A	1601	ASN
1	A	1628	ARG
1	A	1672	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	GLN
1	A	83	GLN
1	A	85	ASN
1	A	109	ASN
1	A	134	ASN
1	A	182	ASN
1	A	205	GLN
1	A	275	GLN
1	A	353	GLN
1	A	1498	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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.

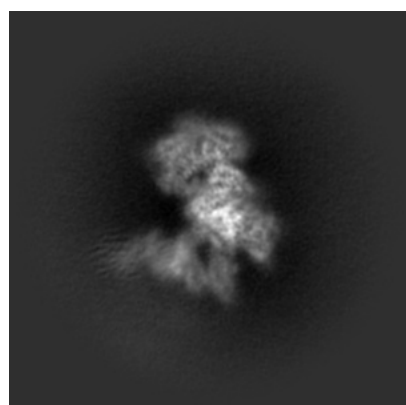
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12017. These allow visual inspection of the internal detail of the map and identification of artifacts.

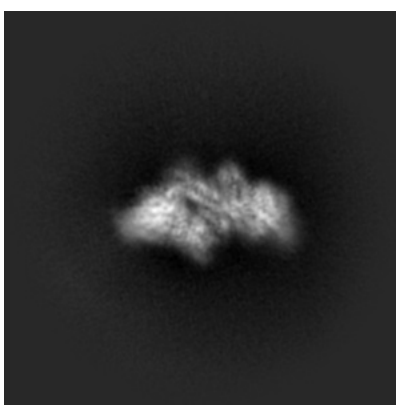
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

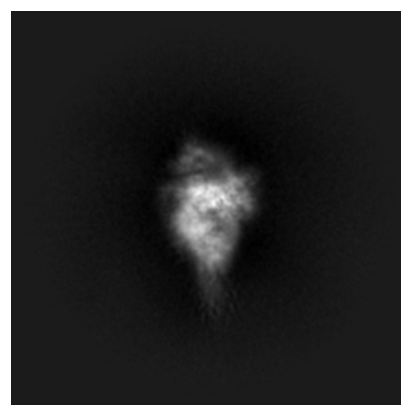
6.1.1 Primary map



X



Y

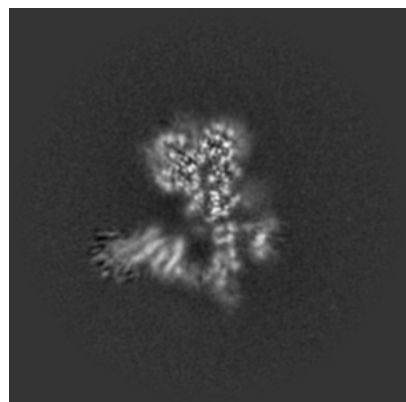


Z

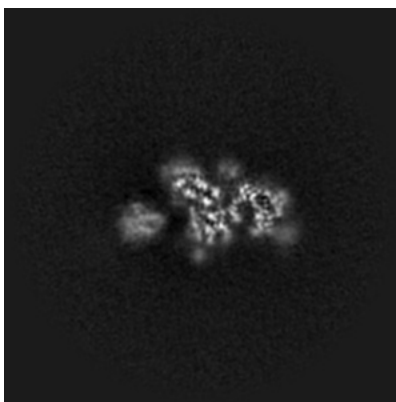
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

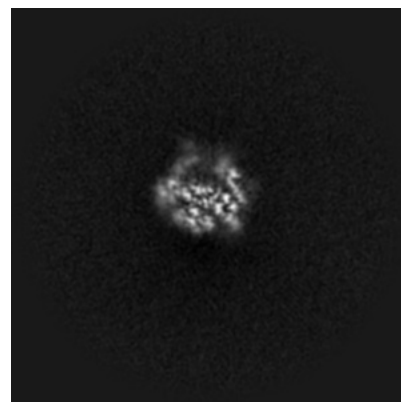
6.2.1 Primary map



X Index: 220



Y Index: 220

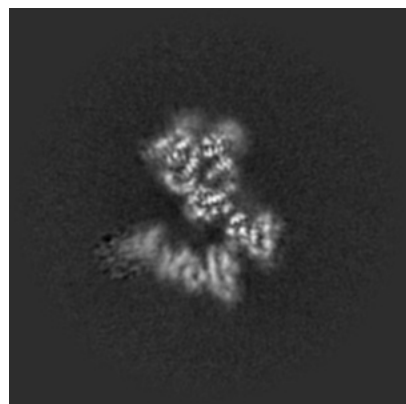


Z Index: 220

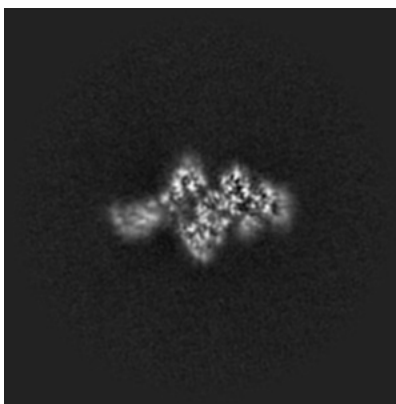
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

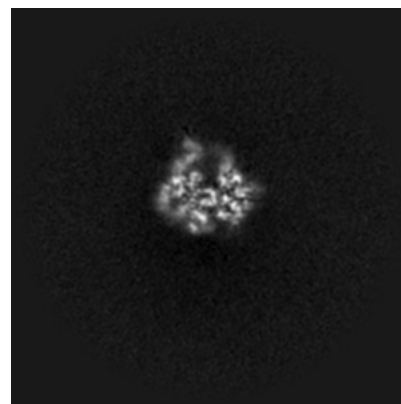
6.3.1 Primary map



X Index: 209



Y Index: 238

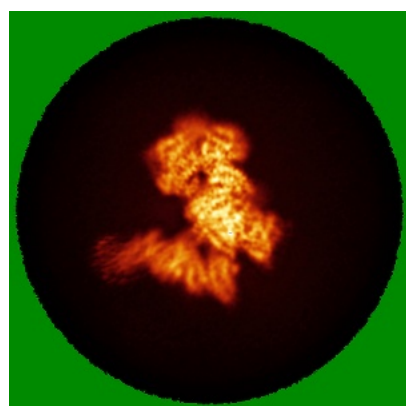


Z Index: 214

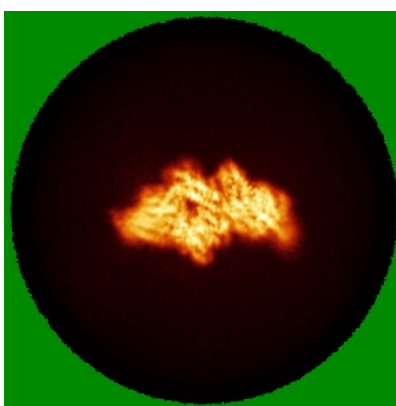
The images above show the largest variance slices of the map in three orthogonal directions.

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

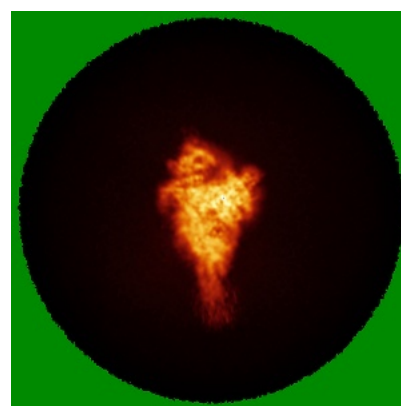
6.4.1 Primary map



X



Y

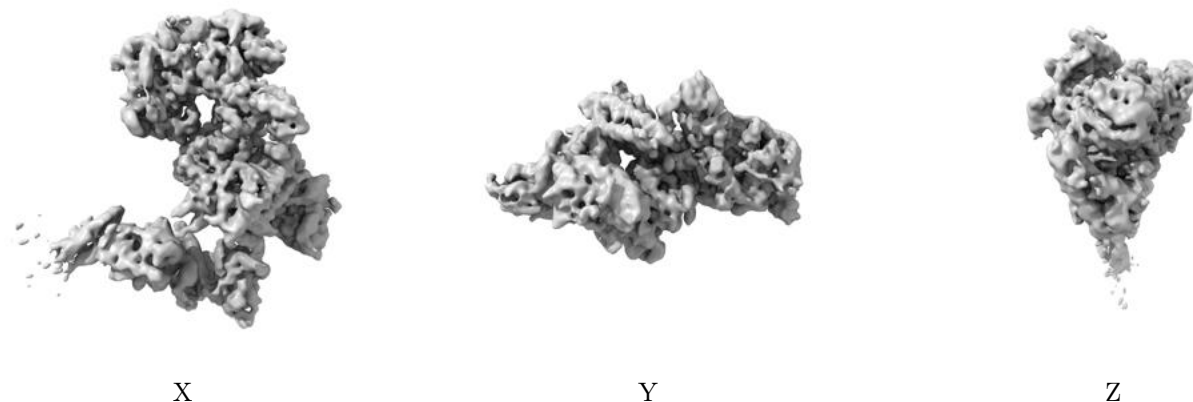


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.56. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

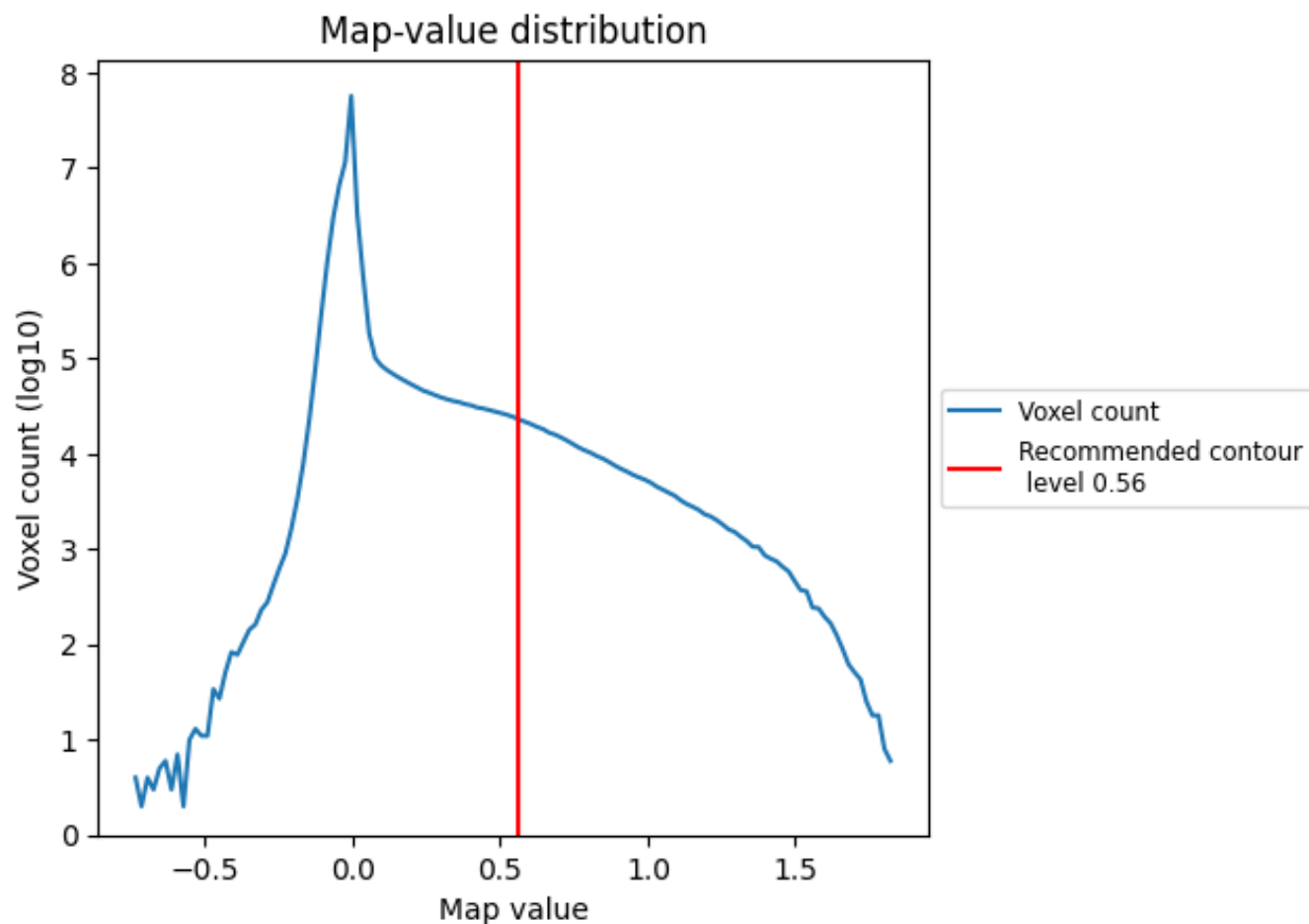
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

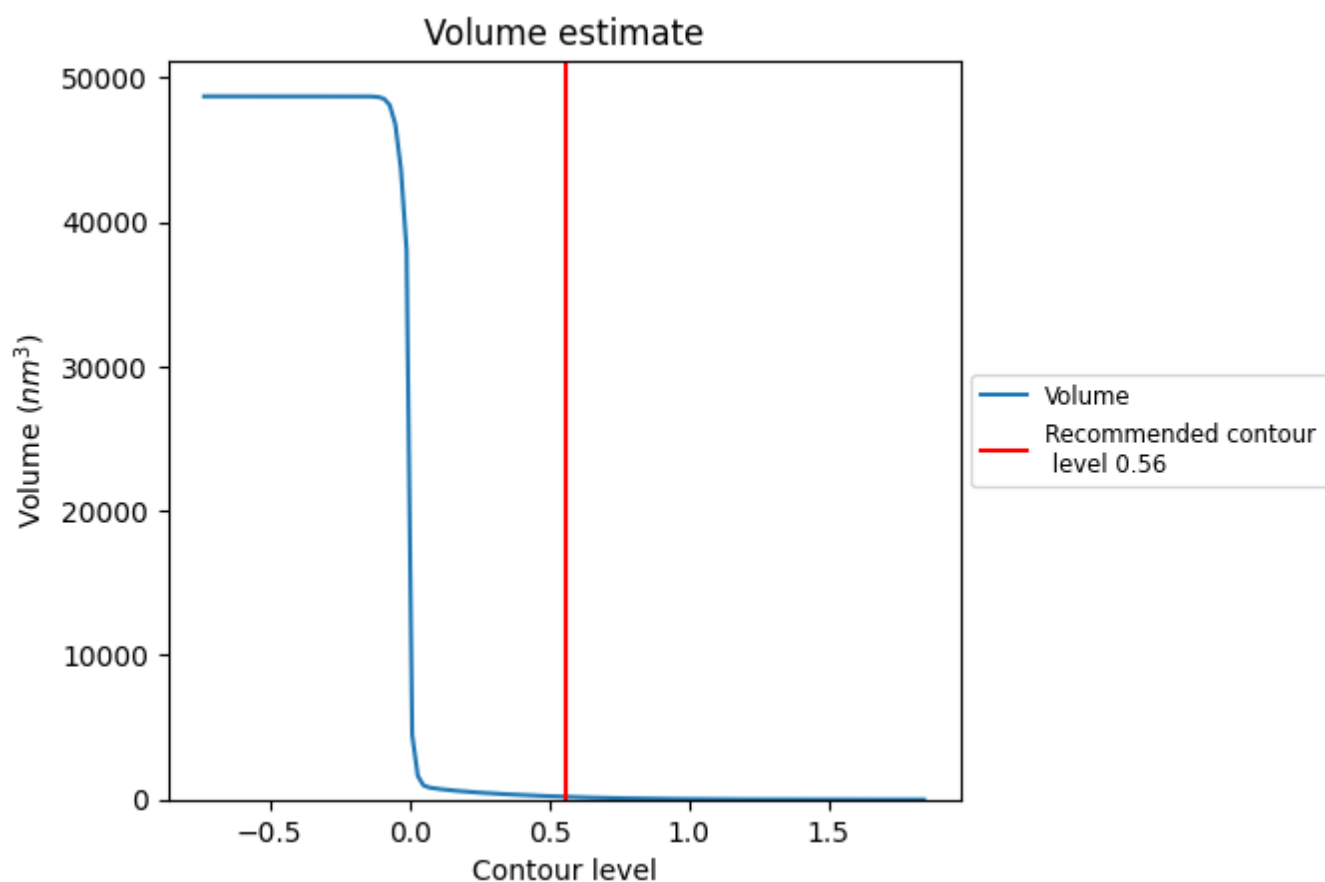
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

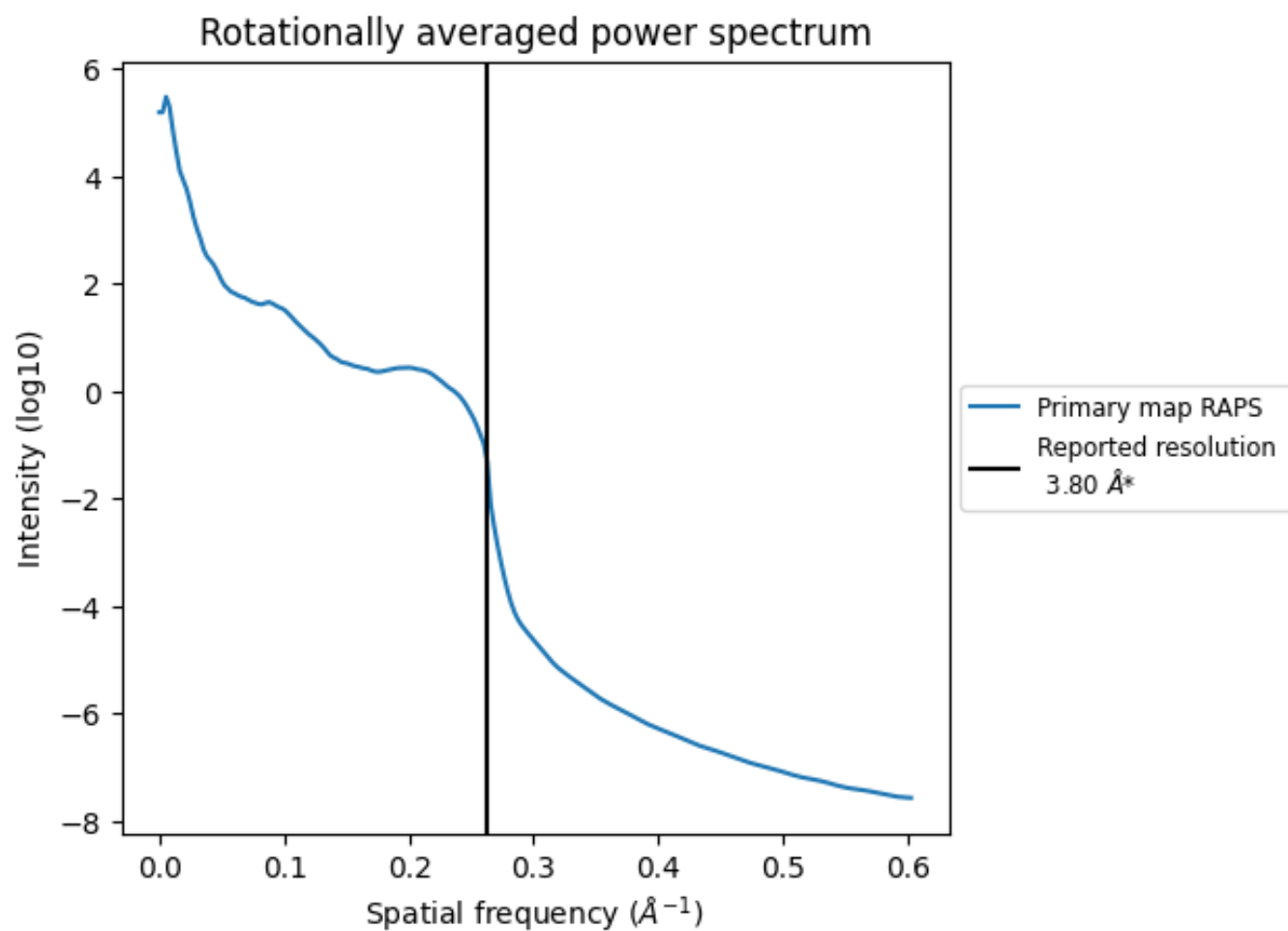
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 191 nm³; this corresponds to an approximate mass of 172 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 ⓘ

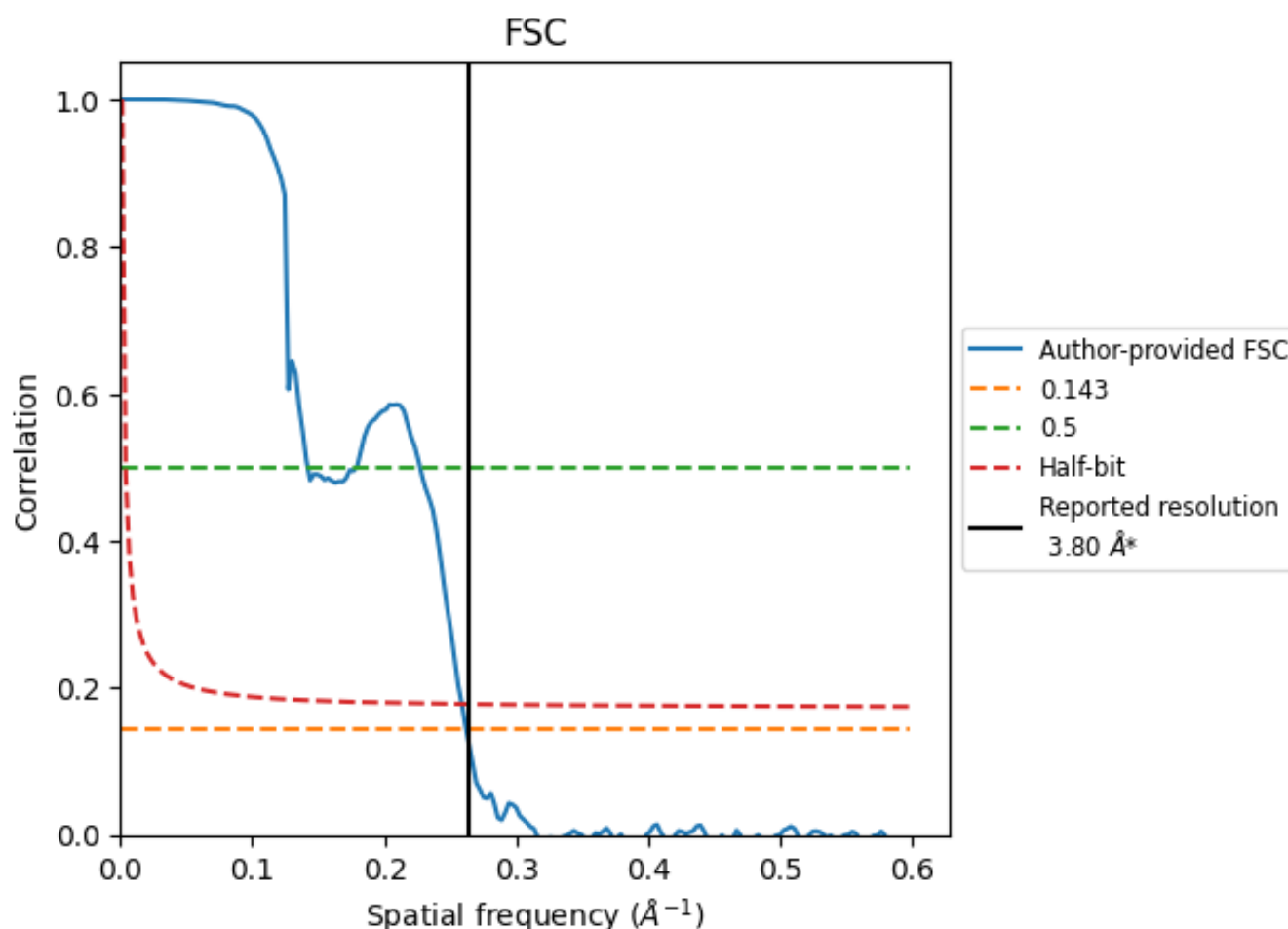


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

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 0.263 Å⁻¹

8.2 Resolution estimates [i](#)

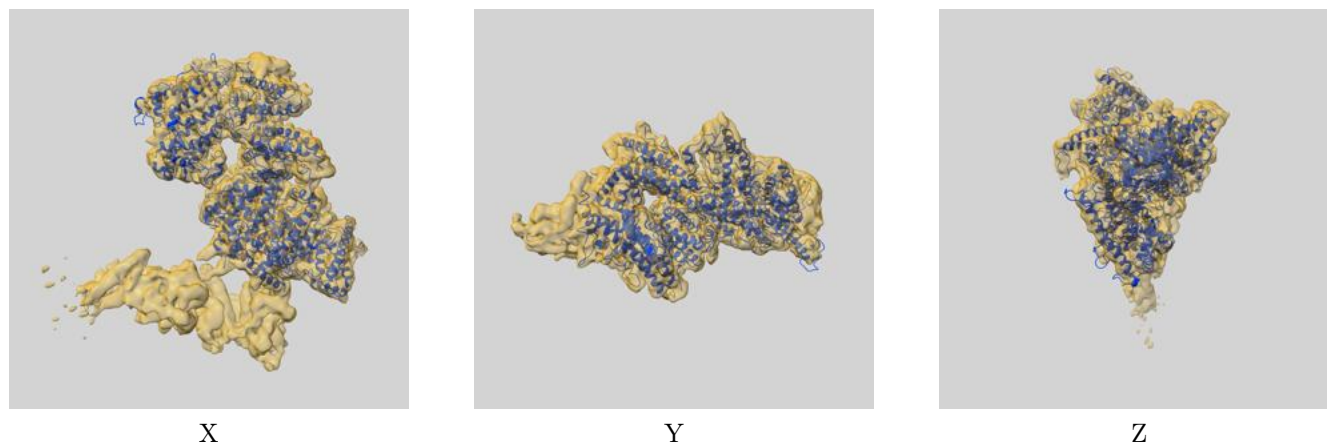
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.82	7.04	3.87
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

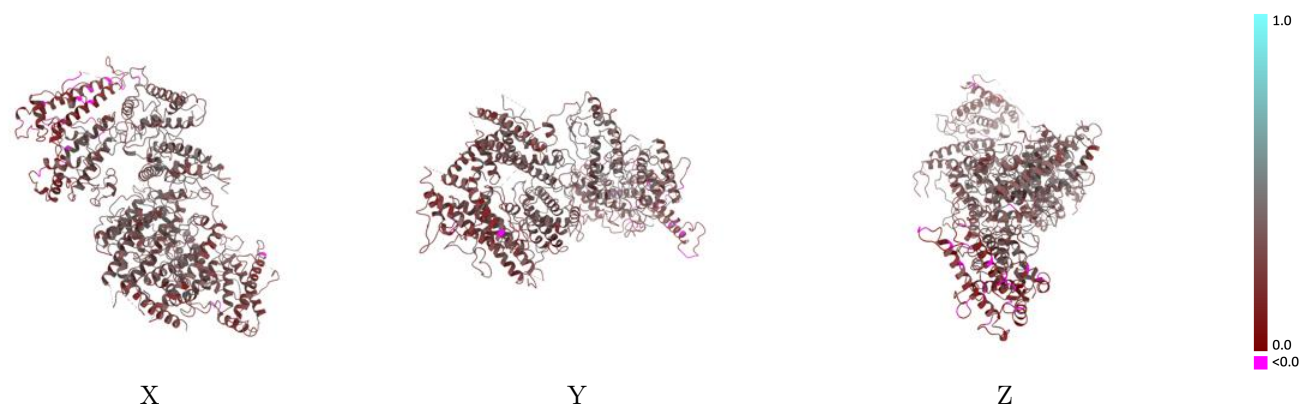
This section contains information regarding the fit between EMDB map EMD-12017 and PDB model 7B52. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



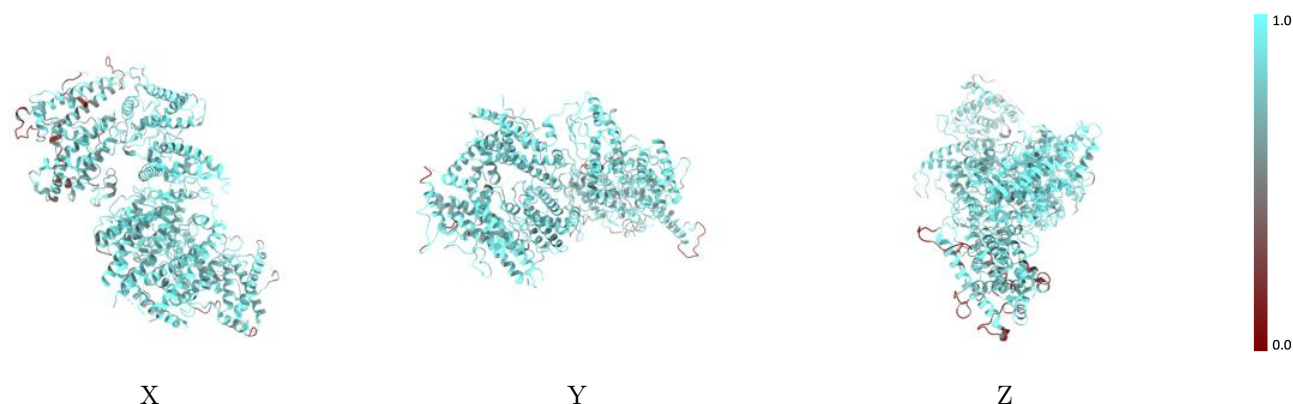
The images above show the 3D surface view of the map at the recommended contour level 0.56 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



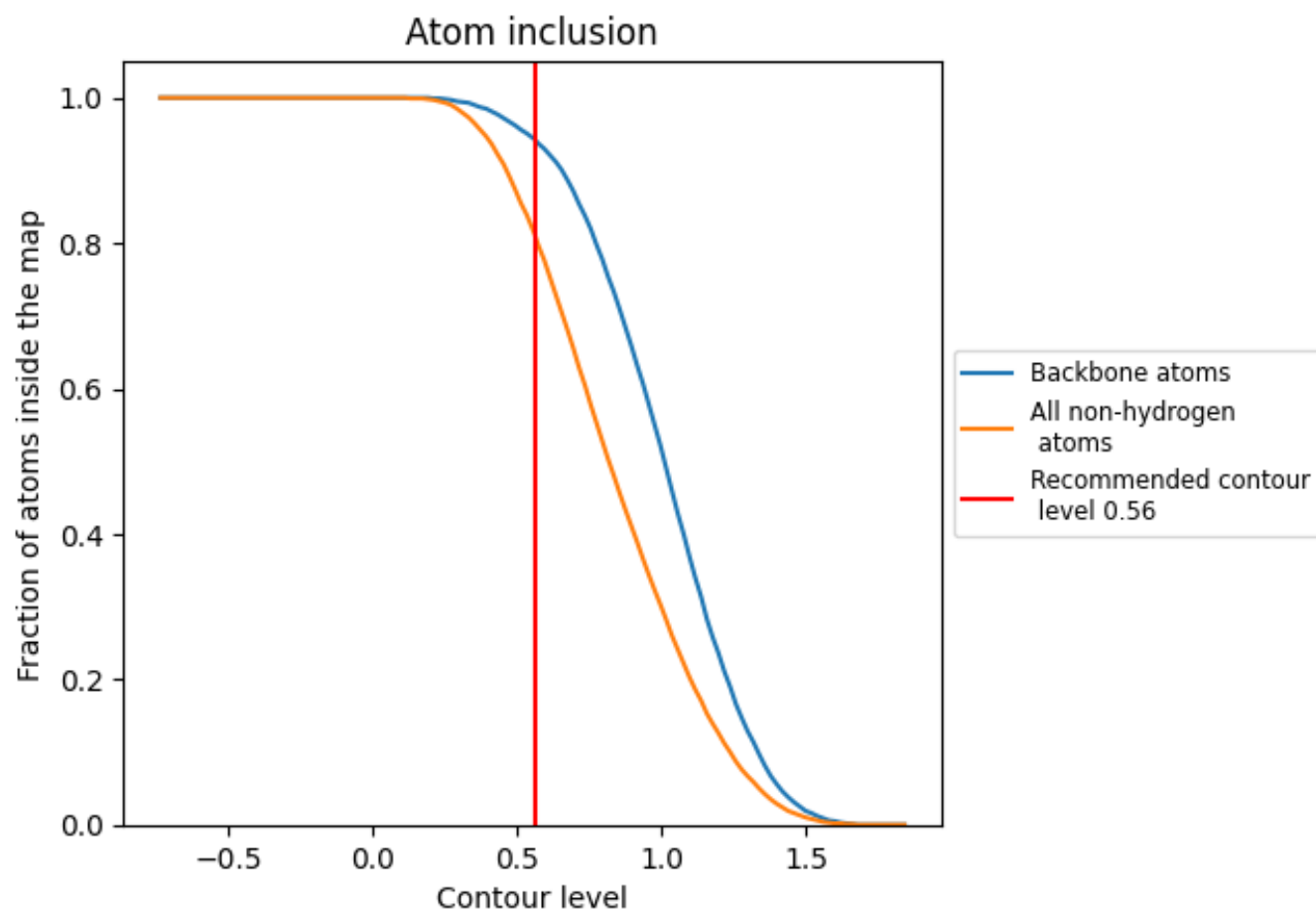
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.56).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 81% 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 (0.56) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8130	<div><div></div></div> 0.3060
A	<div><div></div></div> 0.8120	<div><div></div></div> 0.3060

