



Full wwPDB EM Validation Report ⓘ

Nov 10, 2024 – 03:18 pm GMT

PDB ID : 7Z12
EMDB ID : EMD-14438
Title : VAR2 complex with PAM1.4
Authors : Raghavan, S.S.R.; Wang, K.T.
Deposited on : 2022-02-24
Resolution : 3.00 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.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

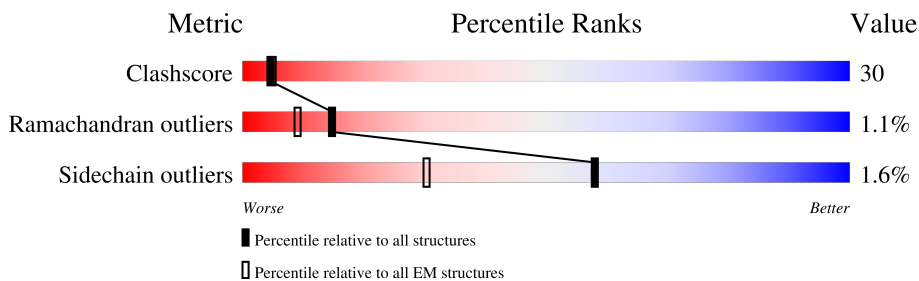
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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	B	472	
2	C	233	
3	A	2040	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18352 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 PAM1.4, Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	221	Total	C	N	O	S	0	0
			1650	1042	283	319	6		

- Molecule 2 is a protein called PAM1.4, light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	212	Total	C	N	O	S	0	0
			1631	1021	279	326	5		

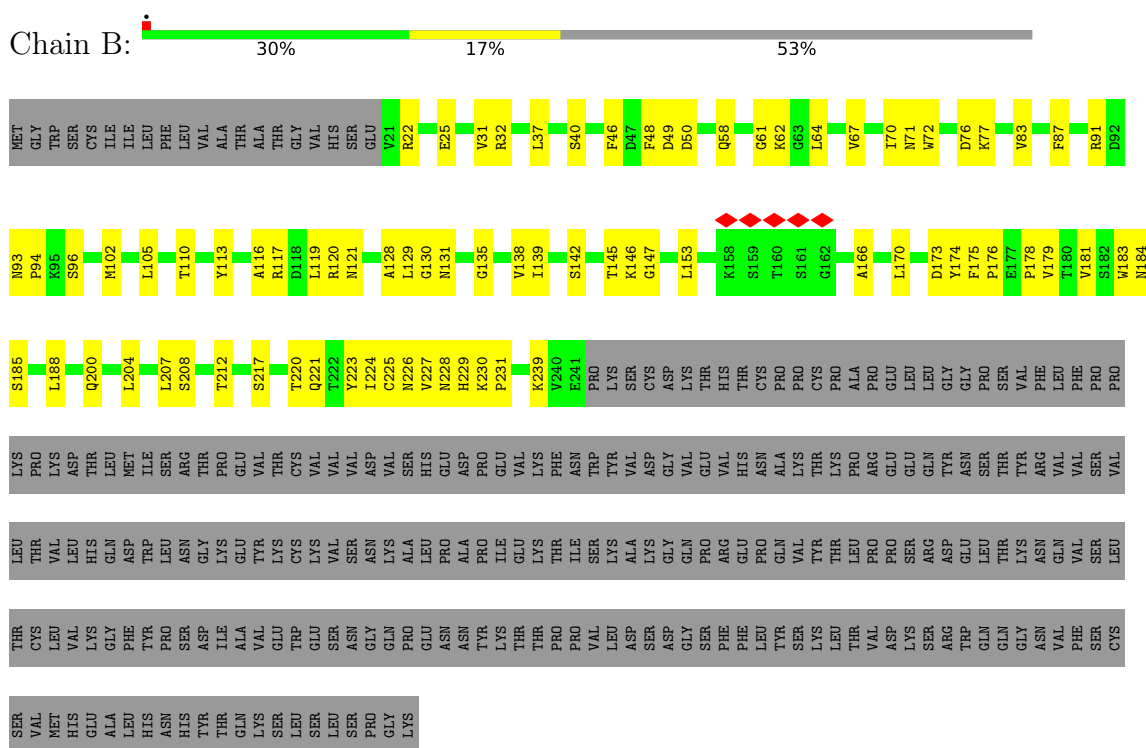
- Molecule 3 is a protein called VAR2CSA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	1853	Total	C	N	O	S	0	0
			15071	9402	2597	2973	99		

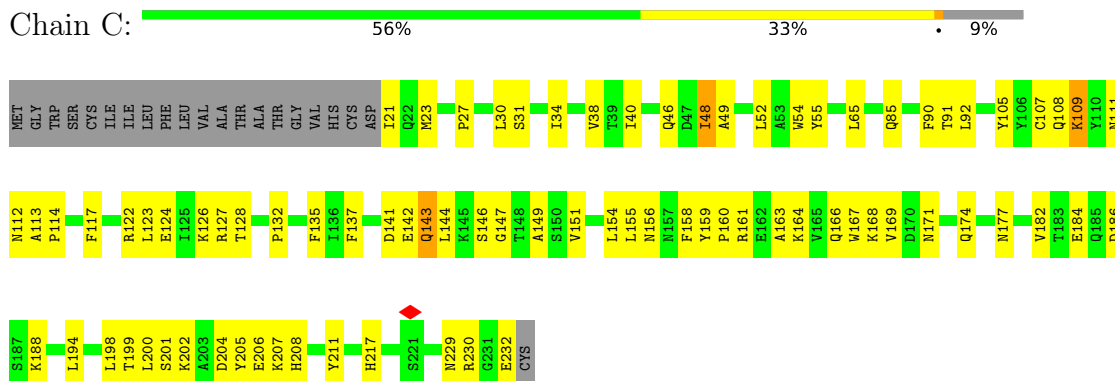
3 Residue-property plots

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.

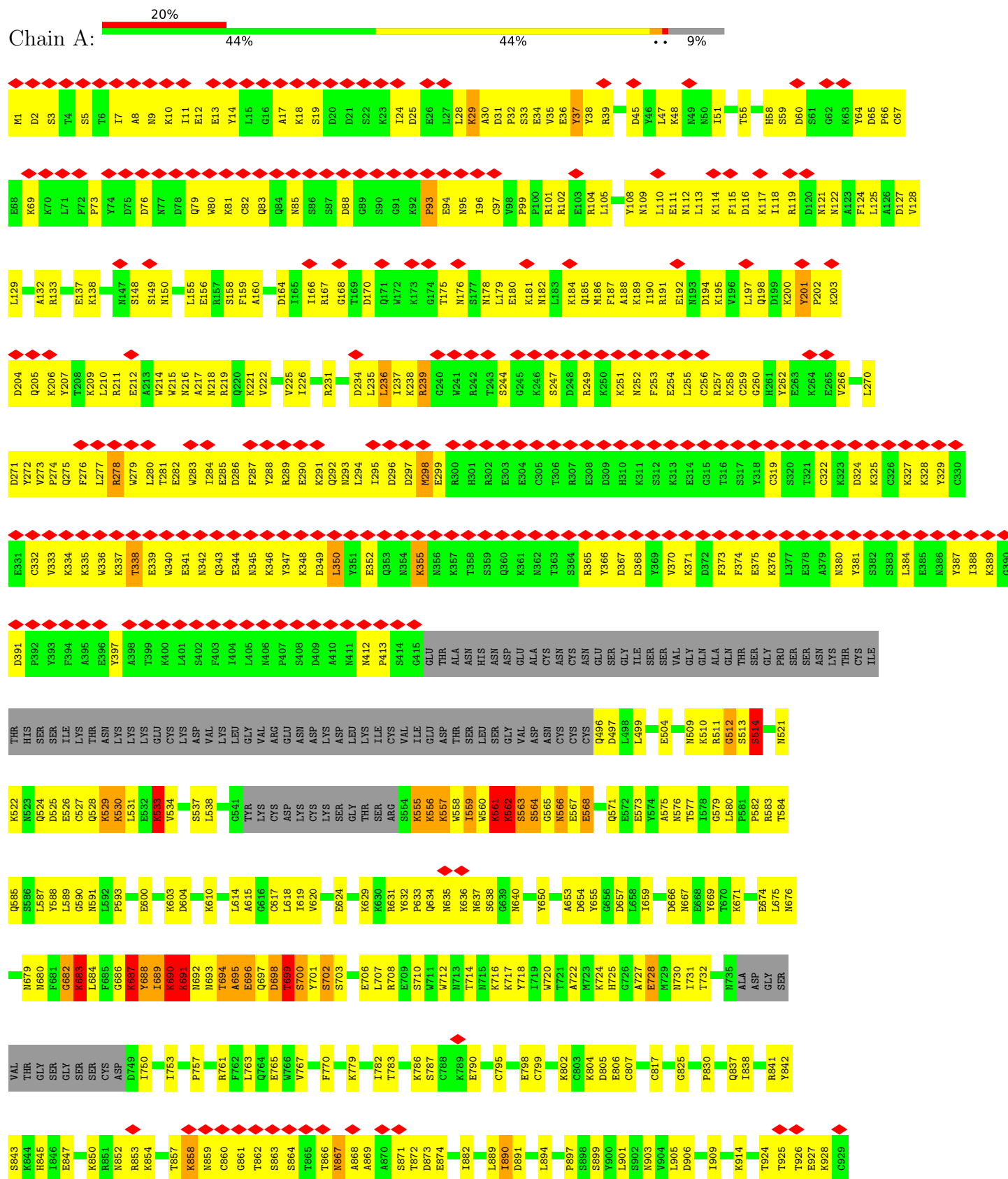
• Molecule 1: PAM1.4, Heavy Chain



• Molecule 2: PAM1.4, light Chain



● Molecule 3: VAR2CSA



N930	R995	SER	A1129	E1206	N1271	G1332	V1394	R1465	N1556	R1664	Q1765	E1875
K931	G996	ASP	M1130	S1207	L1272	K1333	G1395	L1466	Y1561	E1665	R1769	D1879
E932	Y997	GLU	K1131	T1208	C1273	M1334	S1396	R1467	Y1561	A1666	Y1770	Y1880
R933	N999	THR	G1132	D1209	G1274	D1335	S1397	Y1468	Y1564	Y1667	P1780	L1883
D934	D1000	PRO	S1133	E1210	E1275	P1336	T1398	L1470	Y1564	L1669	L1781	M1884
K935	M1001	LYS	Q1134	N1211	G1276	L1339	E1399	R1471	D1569	K1471	L1788	V1888
S936	Y1002	VAL	K1136	I1212	L1277	P1340	N1400	I1472	Y1561	Y1472	C1762	M1888
S938	E1003	ARG	K1137	I1213	D1278	K1341	A1401	A1473	Y1573	A1474	G1763	L1889
Q939	L1004	GLY	Y1138	N1213	K1280	G1342	A1402	A1475	I1573	C1476	I1764	M1893
Q939	C1005	THR	S1139	K1214	S1281	F1343	W1404	T1477	Q1578	T1477	I1790	A1791
S941	K1006	GLU	S1140	S1215	G1283	A1344	W1405	I1478	Y1581	I1478	Q1794	Q1794
S940	K1007	TJR	S1141	E1216	G1284	C1345	K1406	K1479	Y1582	K1479	R1797	G1798
V946	Y1007	ASN	N1142	I1217	R1285	G1346	K1406	K1480	K1583	K1480	L1798	L1799
V947	M1008	ASN	S1143	S1218	R1286	Q1348	K1406	K1481	Y1584	N1482	R1799	G1800
V948	Y1009	THR	F1145	C1219	G1287	Q1349	K1406	K1481	Y1584	N1482	R1799	E1801
V949	C1005	THR	F1147	D1220	N1287	Q1349	K1406	K1481	Y1584	N1482	R1799	E1801
P950	K1006	THR	S1148	I1222	I1288	F1351	A1411	E1483	E1588	K1483	Y1696	G1913
P951	Y1017	THR	W1150	N1222	K1289	D1352	E1411	K1484	K1589	K1484	D1697	A1914
S951	T1015	GLN	I1154	A1223	N1290	Y1354	D1414	K1485	K1590	K1485	L1698	S1919
P952	T1016	GLY	Q1155	T1224	D1291	K1355	A1415	S1489	L1594	S1489	F1814	G1920
P952	R1018	THR	K1156	N1225	E1294	M1357	A1415	K1490	C1596	K1490	K1818	T1921
L953	S1019	C1093	K1156	Y1226	L1295	I1358	A1418	Q1493	K1599	Q1493	C1821	V1922
T956	N1020	E1095	M1159	I1227	L1296	L1359	A1418	K1496	K1599	K1496	D1822	N1923
P957	S1021	K1096	G1160	R1228	K1297	G1360	A1419	I1497	K1612	K1497	P1823	K1924
Y958	G1026	C1097	D1161	G1229	E1298	T1361	I1420	I1497	K1612	I1497	P1824	K1925
R959	Y1029	K1098	W1162	C1230	K1299	S1362	K1422	I1498	N1615	I1498	R1825	K1926
Y960	Y1101	C1099	S1163	Q1231	K1300	N1364	I1423	G1499	G1616	G1499	R1826	Q1927
C964	M1033	K1101	I1165	Y1235	K1301	I1365	K1425	C1501	R1617	C1501	A1827	K1928
C965	E1041	K1102	I1165	I1236	N1302	I1365	K1426	C1502	P1626	C1502	D1828	K1929
K967	I1042	W1103	M1167	G1237	I1304	I1369	K1426	R1503	R1627	R1503	I1720	E1930
I968	Q1045	K1106	I1168	F1240	K1306	I1369	N1427	K1504	K1628	K1504	I1723	T1931
P969	I1046	D1107	E1174	G1241	K1307	H1368	N1429	G1370	Q1629	K1507	S1726	C1932
T970	I1047	D1109	F1175	G1242	E1307	I1369	S1430	L1372	Q1630	Y1508	D1832	E1933
E972	Y1048	Q1110	L1176	K1243	T1308	Q1373	I1431	Q1373	L1633	Y1511	T1729	C1934
C975	M1050	W1111	I1177	K1243	L1310	E1374	F1432	E1374	Y1634	Y1511	T1738	E1935
R978	T1051	K1113	S1184	E1246	L1311	D1375	N1433	D1375	E1635	W1519	R1738	E1936
K979	N1052	Q1115	G1187	K1247	Y1312	I1376	E1436	I1376	L1636	D1520	W1741	K1938
R980	A1053	K1115	G1187	Q1248	E1313	K1377	E1436	K1377	F1637	K1521	T1746	P1939
Y981	M1054	D1116	I1190	C1251	H1315	K1378	C1437	K1378	I1639	Q1522	T1746	L1940
M982	I1055	N1117	E1193	K1252	D1316	I1379	P1442	I1379	I1640	K1525	R1752	M1847
N983	S1056	Y1118	K1194	D1253	G1318	E1381	T1443	E1381	T1641	Y1526	R1753	R1853
Q984	C1057	N1119	E1197	T1254	T1319	K1382	G1444	G1382	G1444	Y1530	K1754	L1854
W985	I1058	F1121	A1198	I1255	A1320	G1383	N1445	K1383	N1445	Y1530	T1755	E1855
S986	T1059	R1122	E1199	I1256	I1321	T1384	D1446	T1384	D1446	Y1538	T1757	M1859
C987	GLY	S1123	E1199	H1257	I1322	T1385	Q1386	Q1385	Q1449	L1538	Q1758	Y1946
G988	LYS	Q1124	K1200	G1258	K1324	Q1386	Q1386	Q1387	Q1449	M1542	Q1758	E1951
S989	GLU	Q1125	K1201	D1259	M1325	Q1387	F1454	Q1387	F1454	Y1543	W1761	K1952
A990	VAL	I1126	C1202	T1260	K1326	K1388	K1455	K1388	K1455	Y1543	D1762	K1953
R991	LEU	Y1127	K1203	N1261	K1327	D1389	E1456	D1389	E1456	C1546	T1764	Y1954
T992	ASP	D1128	E1204	G1262	K1328	K1390	W1457	W1457	W1457	W1457	M1764	E1961
M993	SER	VAL	M1205	Y1265	Q1330	I1391	Q1460	Q1460	Q1460	M1550	N1871	K1961
K994	VAL	VAL		P1266	K1331	G1392	E1464	E1464	E1464			

[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50000	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	2.352	Depositor
Minimum map value	-0.906	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.043	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	366.08002, 366.08002, 366.08002	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.832, 0.832, 0.832	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	B	0.39	0/1688	0.53	0/2297
2	C	0.36	0/1665	0.51	0/2263
3	A	0.38	0/15370	0.57	2/20668 (0.0%)
All	All	0.38	0/18723	0.56	2/25228 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1
3	A	0	31
All	All	0	32

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	562	LYS	CB-CA-C	-7.20	95.99	110.40
3	A	1203	LYS	N-CA-C	6.14	127.59	111.00

There are no chirality outliers.

All (32) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	1125	GLN	Peptide
3	A	1134	GLN	Peptide
3	A	1136	LYS	Peptide
3	A	1184	SER	Peptide
3	A	1201	LYS	Peptide
3	A	1202	CYS	Peptide

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Mol	Chain	Res	Type	Group
3	A	1299	LYS	Peptide
3	A	1308	THR	Peptide
3	A	1365	ILE	Peptide
3	A	1399	GLU	Peptide
3	A	1403	ALA	Peptide
3	A	1408	ILE	Peptide
3	A	1409	GLU	Peptide
3	A	1822	ASP	Peptide
3	A	201	TYR	Peptide
3	A	236	LEU	Peptide
3	A	239	ARG	Peptide
3	A	278	ARG	Peptide
3	A	298	MET	Peptide
3	A	338	THR	Peptide
3	A	349	ASP	Peptide
3	A	355	LYS	Peptide
3	A	37	TYR	Peptide
3	A	529	LYS	Peptide
3	A	533	LYS	Peptide
3	A	698	ASP	Peptide
3	A	728	GLU	Peptide
3	A	786	LYS	Peptide
3	A	952	PRO	Peptide
3	A	965	GLN	Peptide
3	A	966	CYS	Peptide
2	C	48	ILE	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	B	1650	0	1628	59	0
2	C	1631	0	1599	60	0
3	A	15071	0	14624	984	0
All	All	18352	0	17851	1093	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 30.

All (1093) 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)
3:A:924:THR:HA	3:A:946:VAL:O	1.27	1.31
3:A:251:LYS:HB3	3:A:566:ASN:HB2	1.21	1.12
3:A:325:LYS:O	3:A:329:TYR:HB2	1.60	0.99
3:A:83:GLN:HB3	3:A:95:ASN:HD21	1.28	0.97
3:A:559:ILE:HG22	3:A:561:LYS:HG2	1.48	0.95
3:A:328:LYS:HG3	3:A:332:CYS:HB3	1.50	0.94
3:A:1413:TRP:HA	3:A:1416:VAL:HG12	1.50	0.94
3:A:340:TRP:O	3:A:344:GLU:HB3	1.68	0.93
3:A:1154:ILE:HG21	3:A:1164:LYS:HG3	1.51	0.93
3:A:691:LYS:HB3	3:A:694:THR:HA	1.50	0.92
3:A:1307:GLU:HA	3:A:1310:LEU:HB2	1.54	0.90
3:A:333:VAL:HA	3:A:337:LYS:HB2	1.52	0.89
3:A:1302:ASN:HA	3:A:1305:HIS:HB2	1.54	0.89
3:A:19:SER:HA	3:A:216:ASN:HB3	1.55	0.88
3:A:133:ARG:HH12	3:A:137:GLU:HB3	1.38	0.87
3:A:278:ARG:O	3:A:282:GLU:HB2	1.73	0.87
3:A:499:LEU:HD13	3:A:701:TYR:HE1	1.37	0.86
3:A:191:ARG:NH2	3:A:205:GLN:O	2.08	0.85
3:A:186:MET:SD	3:A:189:LYS:NZ	2.49	0.85
3:A:1356:ASN:HB3	3:A:1449:GLN:HE21	1.42	0.85
3:A:338:THR:HA	3:A:342:ASN:HB2	1.59	0.84
3:A:610:LYS:HA	3:A:684:LEU:HD21	1.60	0.84
3:A:1257:HIS:ND1	3:A:1364:ASN:O	2.09	0.83
3:A:1301:LYS:HD3	3:A:1422:LYS:HD2	1.60	0.83
3:A:365:ARG:HH12	3:A:374:PHE:HB2	1.43	0.83
3:A:1199:GLU:HB3	3:A:1203:LYS:HG3	1.60	0.83
3:A:717:LYS:HA	3:A:750:ILE:HD11	1.59	0.82
3:A:294:LEU:HA	3:A:298:MET:HB2	1.61	0.82
3:A:854:LYS:HA	3:A:869:ALA:HB3	1.60	0.82
3:A:725:HIS:HA	3:A:730:ASN:HD21	1.43	0.81
3:A:1352:ILE:HD11	3:A:1442:PRO:HG2	1.62	0.81
3:A:562:LYS:HB2	3:A:575:ALA:HB1	1.60	0.81
3:A:276:PHE:O	3:A:280:LEU:N	2.13	0.81
3:A:235:LEU:HA	3:A:258:LYS:HG2	1.60	0.81
3:A:1278:TRP:HB2	3:A:1372:LEU:HD11	1.63	0.81
3:A:345:ASN:HB3	3:A:352:GLU:H	1.47	0.80
3:A:795:CYS:HB3	3:A:967:LYS:HD2	1.64	0.80
3:A:942:ASP:HA	3:A:946:VAL:HA	1.61	0.80
3:A:96:ILE:HD11	3:A:346:LYS:HB3	1.63	0.80
3:A:1125:GLN:HG3	3:A:1128:ASP:HB3	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:LEU:HB3	2:C:137:PHE:HD1	1.47	0.79
3:A:1193:GLU:O	3:A:1197:ASN:N	2.15	0.79
1:B:117:ARG:NH1	1:B:131:ASN:OD1	2.14	0.79
3:A:281:THR:HG23	3:A:285:GLU:HB3	1.64	0.79
3:A:1013:LYS:HB2	3:A:1018:ARG:HH22	1.47	0.79
3:A:989:SER:O	3:A:1110:GLN:NE2	2.16	0.79
3:A:1396:SER:HA	3:A:1399:GLU:HG2	1.63	0.78
3:A:1497:ILE:HG22	3:A:1499:GLY:H	1.47	0.78
3:A:1376:ILE:HD13	3:A:1380:ILE:HG13	1.66	0.78
3:A:1375:ASP:O	3:A:1379:ILE:N	2.16	0.78
3:A:1125:GLN:HA	3:A:1128:ASP:H	1.49	0.78
3:A:997:TYR:H	3:A:1003:GLU:HG3	1.48	0.77
3:A:234:ASP:O	3:A:238:LYS:NZ	2.17	0.77
3:A:925:THR:H	3:A:946:VAL:HG12	1.49	0.77
3:A:251:LYS:HB3	3:A:566:ASN:CB	2.08	0.77
3:A:524:GLN:HG3	3:A:527:CYS:HB2	1.67	0.76
3:A:872:THR:OG1	3:A:874:GLU:O	2.02	0.76
3:A:530:LYS:HD2	3:A:531:LEU:HB2	1.67	0.76
3:A:164:ASP:OD1	3:A:167:ARG:NH1	2.19	0.75
3:A:188:ALA:HA	3:A:191:ARG:HG2	1.68	0.75
3:A:1424:ASN:ND2	3:A:1430:SER:O	2.15	0.75
3:A:1471:ASN:HB3	3:A:1504:LYS:HD2	1.68	0.75
3:A:1126:ILE:O	3:A:1130:ASN:ND2	2.19	0.75
3:A:927:GLU:HB2	3:A:943:THR:HA	1.69	0.75
3:A:1933:CYS:H	3:A:1934:GLU:HG3	1.51	0.75
3:A:987:CYS:SG	3:A:995:ARG:N	2.57	0.75
3:A:1356:ASN:O	3:A:1360:GLY:N	2.20	0.75
3:A:499:LEU:HD13	3:A:701:TYR:CE1	2.20	0.74
3:A:1826:ARG:HG3	3:A:1831:GLY:HA2	1.67	0.74
3:A:1422:LYS:HA	3:A:1425:LYS:HG2	1.68	0.74
3:A:102:ARG:HH22	3:A:282:GLU:HG3	1.53	0.74
3:A:1627:ARG:NH2	3:A:1801:GLU:OE2	2.15	0.73
3:A:121:ASN:HA	3:A:124:PHE:HB3	1.69	0.73
1:B:220:THR:OG1	1:B:221:GLN:OE1	2.07	0.73
3:A:38:TYR:O	3:A:39:ARG:NH1	2.19	0.73
3:A:188:ALA:O	3:A:192:GLU:N	2.22	0.73
3:A:1355:LYS:HE3	3:A:1406:LYS:HE3	1.71	0.73
3:A:113:LEU:H	3:A:182:ASN:HD21	1.35	0.72
3:A:25:ASP:HA	3:A:28:LEU:HB3	1.70	0.72
1:B:49:ASP:OD2	1:B:93:ASN:ND2	2.22	0.72
3:A:802:LYS:O	3:A:805:ASP:N	2.17	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1408:ILE:O	3:A:1412:MET:N	2.23	0.72
3:A:275:GLN:HG3	3:A:279:TRP:CZ3	2.25	0.72
3:A:563:SER:O	3:A:564:SER:C	2.28	0.72
3:A:830:PRO:HG3	3:A:928:LYS:HD3	1.70	0.72
3:A:939:GLN:H	3:A:943:THR:HG21	1.53	0.71
3:A:1268:ARG:NH2	3:A:1353:ASP:OD2	2.16	0.71
3:A:1380:ILE:O	3:A:1384:THR:OG1	2.08	0.71
3:A:195:LYS:HD3	3:A:201:TYR:HE1	1.54	0.71
3:A:277:LEU:HA	3:A:280:LEU:HB2	1.72	0.71
3:A:1356:ASN:HA	3:A:1359:LEU:HG	1.71	0.71
3:A:324:ASP:OD1	3:A:325:LYS:N	2.24	0.71
3:A:33:SER:HA	3:A:48:LYS:NZ	2.06	0.71
3:A:1042:ILE:HD11	3:A:1107:ILE:HD12	1.71	0.71
3:A:80:TRP:HA	3:A:97:CYS:HA	1.71	0.70
3:A:698:ASP:H	3:A:699:THR:HB	1.54	0.70
3:A:1893:ASN:ND2	3:A:1933:CYS:O	2.22	0.70
3:A:73:PRO:O	3:A:104:ARG:NH1	2.24	0.70
3:A:344:GLU:HA	3:A:347:TYR:HB2	1.73	0.70
3:A:972:GLU:HA	3:A:1102:LEU:HD21	1.74	0.70
3:A:1315:HIS:HD2	3:A:1342:GLY:HA3	1.56	0.70
3:A:1136:LYS:HE2	3:A:1140:SER:H	1.57	0.70
2:C:49:ALA:O	2:C:85:GLN:NE2	2.24	0.70
3:A:1485:LYS:HE2	3:A:1489:SER:HB2	1.74	0.69
3:A:1252:LYS:HG3	3:A:1521:LYS:HG3	1.75	0.69
2:C:149:ALA:HB3	2:C:200:LEU:H	1.58	0.68
3:A:1594:SER:O	3:A:1664:ARG:NH2	2.27	0.68
3:A:573:GLU:OE2	3:A:841:ARG:NH1	2.26	0.68
3:A:1310:LEU:O	3:A:1314:TYR:HB3	1.93	0.68
3:A:1359:LEU:O	3:A:1373:GLN:NE2	2.25	0.68
3:A:111:GLU:HA	3:A:179:LEU:HD13	1.74	0.68
3:A:529:LYS:NZ	3:A:531:LEU:O	2.27	0.68
3:A:576:ASN:O	3:A:837:GLN:NE2	2.27	0.68
3:A:206:LYS:HB3	3:A:209:LYS:HB3	1.76	0.68
3:A:273:VAL:HG13	3:A:277:LEU:HD23	1.74	0.68
3:A:850:LYS:HZ1	3:A:890:ILE:HD13	1.57	0.68
3:A:987:CYS:HB2	3:A:1005:CYS:HA	1.73	0.68
3:A:637:ASN:ND2	3:A:640:ASN:O	2.22	0.68
3:A:251:LYS:CB	3:A:566:ASN:HB2	2.14	0.68
3:A:271:ASP:O	3:A:278:ARG:NH2	2.26	0.68
3:A:583:ARG:NH2	3:A:765:GLU:OE1	2.27	0.67
3:A:1136:LYS:HE2	3:A:1139:VAL:HA	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1411:GLU:HA	3:A:1414:ASP:HB2	1.75	0.67
3:A:691:LYS:HB3	3:A:694:THR:CA	2.21	0.67
3:A:293:ASN:HA	3:A:296:ASP:HB2	1.76	0.67
3:A:1823:PRO:HB3	3:A:1828:ASP:HB2	1.76	0.67
3:A:1325:ASN:O	3:A:1467:ARG:NH2	2.27	0.67
3:A:236:LEU:HD13	3:A:259:CYS:HA	1.76	0.67
3:A:1933:CYS:HB2	3:A:1934:GLU:HA	1.75	0.67
1:B:174:TYR:HE2	1:B:178:PRO:HA	1.60	0.67
3:A:864:SER:HA	3:A:1790:ILE:HG21	1.75	0.66
3:A:1246:GLU:O	3:A:1248:GLN:NE2	2.28	0.66
3:A:701:TYR:HB3	3:A:706:GLU:OE1	1.95	0.66
1:B:184:ASN:HD22	1:B:188:LEU:HD13	1.60	0.66
3:A:504:GLU:HG3	3:A:521:ASN:HD21	1.60	0.66
1:B:173:ASP:HA	1:B:204:LEU:HB3	1.76	0.66
3:A:984:GLN:HB3	3:A:1007:TYR:CE2	2.30	0.66
3:A:1154:ILE:HG22	3:A:1161:ASP:HA	1.78	0.66
3:A:1125:GLN:HG2	3:A:1137:LYS:O	1.96	0.65
3:A:1988:LEU:HG	3:A:1989:ASP:H	1.60	0.65
3:A:1827:ALA:O	3:A:1830:CYS:N	2.27	0.65
3:A:689:ILE:HD12	3:A:701:TYR:HB2	1.79	0.65
3:A:1412:MET:HA	3:A:1415:ALA:HB3	1.77	0.65
3:A:1938:GLY:O	3:A:1940:LEU:N	2.29	0.65
3:A:1013:LYS:O	3:A:1018:ARG:NH1	2.21	0.65
3:A:181:LYS:HA	3:A:184:LYS:HE2	1.77	0.65
3:A:1594:SER:OG	3:A:1635:GLU:OE2	2.12	0.65
3:A:1692:ARG:NH2	3:A:1903:ASN:OD1	2.27	0.65
3:A:698:ASP:N	3:A:699:THR:HB	2.10	0.65
3:A:951:SER:O	3:A:953:LEU:N	2.26	0.65
3:A:1411:GLU:O	3:A:1415:ALA:N	2.29	0.65
2:C:229:ASN:HB3	2:C:232:GLU:HG3	1.77	0.65
3:A:244:SER:O	3:A:257:ARG:NH2	2.30	0.65
3:A:529:LYS:HG3	3:A:530:LYS:H	1.60	0.65
3:A:1321:ILE:HG21	3:A:1460:GLN:HG2	1.77	0.65
3:A:1252:LYS:NZ	3:A:1261:ASN:O	2.30	0.64
3:A:842:TYR:OH	3:A:889:LEU:HD21	1.97	0.64
1:B:110:THR:HG23	1:B:139:ILE:HA	1.78	0.64
3:A:256:CYS:HA	3:A:257:ARG:HG2	1.80	0.64
3:A:562:LYS:O	3:A:564:SER:N	2.31	0.64
3:A:1305:HIS:HE1	3:A:1423:ILE:HA	1.62	0.64
3:A:333:VAL:O	3:A:338:THR:OG1	2.15	0.64
3:A:560:TRP:HA	3:A:579:GLY:HA2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1096:LYS:HD2	3:A:1201:LYS:HG2	1.79	0.64
1:B:221:GLN:NE2	1:B:223:TYR:OH	2.31	0.64
3:A:1127:TYR:O	3:A:1131:LYS:NZ	2.24	0.63
3:A:1251:CYS:SG	3:A:1252:LYS:N	2.71	0.63
3:A:1496:LYS:NZ	3:A:1497:ILE:O	2.29	0.63
3:A:325:LYS:HA	3:A:328:LYS:HB3	1.80	0.63
3:A:600:GLU:O	3:A:603:LYS:NZ	2.27	0.63
3:A:583:ARG:NH1	3:A:654:ASP:OD2	2.31	0.63
3:A:587:LEU:HD13	3:A:655:TYR:HE1	1.62	0.63
3:A:32:PRO:O	3:A:48:LYS:NZ	2.23	0.63
3:A:274:PRO:O	3:A:278:ARG:N	2.25	0.63
3:A:924:THR:OG1	3:A:945:VAL:HG22	1.99	0.63
3:A:1202:CYS:N	3:A:1204:GLU:HA	2.13	0.63
3:A:1295:LEU:O	3:A:1299:LYS:N	2.25	0.63
3:A:1409:GLU:HA	3:A:1412:MET:HB3	1.81	0.63
3:A:1058:ILE:HG23	3:A:1201:LYS:HB2	1.81	0.63
1:B:70:ILE:HD13	1:B:91:ARG:HG3	1.81	0.62
3:A:1166:LYS:HD3	3:A:1168:ILE:HG12	1.81	0.62
3:A:1313:GLU:O	3:A:1317:THR:OG1	2.12	0.62
3:A:1260:THR:HA	3:A:1363:VAL:HG12	1.81	0.62
3:A:1307:GLU:O	3:A:1311:LEU:N	2.33	0.62
1:B:121:ASN:ND2	3:A:958:TYR:OH	2.22	0.62
3:A:1320:ALA:HB3	3:A:1323:SER:HB3	1.80	0.62
3:A:1391:ILE:O	3:A:1400:ASN:ND2	2.32	0.62
3:A:80:TRP:O	3:A:81:LYS:HD2	2.00	0.62
3:A:149:SER:HA	3:A:238:LYS:HD3	1.81	0.62
3:A:799:CYS:HB2	3:A:802:LYS:HA	1.82	0.62
3:A:1280:LYS:O	3:A:1285:ARG:NH1	2.32	0.62
3:A:1418:CYS:HA	3:A:1421:THR:HG22	1.81	0.62
3:A:583:ARG:NH2	3:A:650:TYR:HB3	2.14	0.62
3:A:1484:LYS:HE2	3:A:1573:ILE:HG13	1.82	0.62
3:A:587:LEU:HD12	3:A:590:GLY:H	1.64	0.62
3:A:857:THR:OG1	3:A:871:SER:O	2.18	0.62
3:A:83:GLN:N	3:A:95:ASN:OD1	2.32	0.62
3:A:332:CYS:SG	3:A:336:TRP:N	2.73	0.62
2:C:141:ASP:OD2	2:C:142:GLU:N	2.32	0.62
3:A:65:ASP:OD1	3:A:66:PRO:HD2	2.00	0.62
3:A:236:LEU:HB2	3:A:259:CYS:N	2.14	0.61
3:A:852:ASN:ND2	3:A:854:LYS:O	2.33	0.61
3:A:1304:ILE:HA	3:A:1307:GLU:HB3	1.81	0.61
1:B:229:HIS:CD2	1:B:231:PRO:HD2	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1843:ALA:O	3:A:1847:ASN:ND2	2.33	0.61
3:A:132:ALA:HB1	3:A:226:ILE:HB	1.83	0.61
3:A:1550:ASN:HD22	3:A:1711:GLU:HG2	1.65	0.61
3:A:1863:TYR:HA	3:A:1866:ILE:HG22	1.81	0.61
3:A:1274:VAL:HG12	3:A:1278:TRP:H	1.65	0.61
3:A:1187:GLY:O	3:A:1190:ILE:HG22	2.00	0.61
3:A:200:LYS:NZ	3:A:209:LYS:O	2.33	0.61
3:A:1314:TYR:HA	3:A:1319:THR:OG1	2.01	0.61
3:A:1469:GLU:OE2	3:A:1473:ARG:NE	2.25	0.61
3:A:1581:TYR:N	3:A:1656:GLU:OE1	2.27	0.61
3:A:568:GLU:HG3	3:A:667:ASN:HB3	1.83	0.61
3:A:1296:LEU:O	3:A:1300:ILE:N	2.34	0.61
3:A:1301:LYS:HG2	3:A:1419:ALA:HA	1.82	0.61
3:A:278:ARG:HA	3:A:281:THR:HB	1.83	0.61
1:B:184:ASN:HD21	1:B:223:TYR:HD1	1.47	0.61
3:A:38:TYR:HE1	3:A:118:ILE:HB	1.65	0.61
3:A:182:ASN:OD1	3:A:185:GLN:NE2	2.34	0.61
3:A:983:ASN:HA	3:A:991:ARG:HB3	1.83	0.61
3:A:555:LYS:HD2	3:A:585:GLN:HG3	1.82	0.60
3:A:1402:ASN:HB3	3:A:1406:LYS:HD3	1.83	0.60
2:C:54:TRP:CZ3	2:C:107:CYS:HB3	2.36	0.60
3:A:861:GLY:N	3:A:891:ASP:OD1	2.33	0.60
3:A:1237:GLY:H	3:A:1246:GLU:HA	1.67	0.60
3:A:925:THR:N	3:A:946:VAL:H	1.98	0.60
3:A:176:ASN:O	3:A:180:GLU:N	2.27	0.60
3:A:176:ASN:HA	3:A:179:LEU:HB3	1.82	0.60
3:A:873:ASP:OD1	3:A:874:GLU:N	2.33	0.60
3:A:990:ALA:C	3:A:991:ARG:HE	2.05	0.60
3:A:1212:ILE:O	3:A:1417:ARG:NH1	2.34	0.60
3:A:13:GLU:HA	3:A:17:ALA:HB2	1.83	0.60
3:A:81:LYS:N	3:A:96:ILE:O	2.25	0.60
3:A:287:PHE:CD1	3:A:291:LYS:HE2	2.37	0.60
3:A:850:LYS:CE	3:A:890:ILE:HG21	2.32	0.60
3:A:1053:ALA:O	3:A:1059:ASP:HB2	2.00	0.60
3:A:1272:LEU:HB2	3:A:1354:TYR:HE1	1.67	0.60
3:A:277:LEU:HD12	3:A:280:LEU:HB2	1.84	0.60
3:A:1125:GLN:HB3	3:A:1129:ALA:CB	2.31	0.60
3:A:1564:TYR:CD2	3:A:1594:SER:HA	2.36	0.60
3:A:288:TYR:O	3:A:292:GLN:HB2	2.01	0.59
2:C:113:ALA:HB3	2:C:114:PRO:HD3	1.83	0.59
3:A:155:LEU:HD11	3:A:226:ILE:HG12	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:182:ASN:HA	3:A:185:GLN:HG3	1.84	0.59
3:A:689:ILE:HD13	3:A:707:LEU:HB2	1.84	0.59
3:A:1348:GLN:NE2	3:A:1437:CYS:SG	2.62	0.59
3:A:30:ALA:HB3	3:A:125:LEU:HD22	1.84	0.59
3:A:231:ARG:N	3:A:234:ASP:OD2	2.32	0.59
3:A:236:LEU:HB2	3:A:259:CYS:H	1.67	0.59
3:A:805:ASP:OD1	3:A:806:GLU:N	2.35	0.59
3:A:45:ASP:OD2	3:A:1901:ASN:ND2	2.35	0.59
3:A:1454:PHE:CE1	3:A:1522:GLN:HB3	2.38	0.59
3:A:1497:ILE:HG21	3:A:1501:CYS:HB3	1.85	0.59
3:A:1590:LYS:O	3:A:1664:ARG:NH1	2.35	0.59
3:A:787:SER:N	3:A:790:GLU:O	2.36	0.59
3:A:1274:VAL:HG11	3:A:1278:TRP:HB3	1.85	0.59
3:A:88:ASP:HB2	3:A:93:PRO:HA	1.83	0.59
3:A:1361:THR:OG1	3:A:1449:GLN:OE1	2.11	0.59
3:A:1655:LEU:HD13	3:A:1756:ILE:HD12	1.84	0.59
2:C:38:VAL:HG11	2:C:123:LEU:HD21	1.83	0.59
3:A:125:LEU:HG	3:A:129:LEU:HD13	1.83	0.59
3:A:275:GLN:OE1	3:A:278:ARG:NH1	2.35	0.59
3:A:509:ASN:HD22	3:A:513:SER:HB3	1.68	0.59
3:A:850:LYS:NZ	3:A:890:ILE:HD13	2.17	0.59
3:A:1147:PHE:CE2	3:A:1969:VAL:HG22	2.38	0.59
2:C:164:LYS:NZ	2:C:166:GLN:OE1	2.34	0.58
3:A:99:PRO:HD2	3:A:282:GLU:OE2	2.03	0.58
3:A:191:ARG:NH1	3:A:207:TYR:HA	2.18	0.58
3:A:1406:LYS:HA	3:A:1409:GLU:HB3	1.85	0.58
3:A:1412:MET:O	3:A:1416:VAL:N	2.34	0.58
2:C:204:ASP:HA	2:C:207:LYS:HB2	1.85	0.58
3:A:33:SER:HA	3:A:48:LYS:HZ1	1.68	0.58
3:A:281:THR:O	3:A:285:GLU:N	2.37	0.58
3:A:659:ILE:HD11	3:A:712:TRP:HE3	1.67	0.58
2:C:40:ILE:HD12	2:C:92:LEU:HD23	1.85	0.58
3:A:1050:MET:HE3	3:A:1198:ALA:HA	1.85	0.58
3:A:1304:ILE:HG22	3:A:1308:THR:HG23	1.84	0.58
3:A:1:MET:SD	3:A:2:ASP:N	2.77	0.58
3:A:1316:ASP:HB2	3:A:1340:PRO:HG3	1.86	0.58
3:A:1889:ILE:HD13	3:A:1941:ASP:HA	1.84	0.58
1:B:67:VAL:HG13	1:B:83:VAL:HG21	1.84	0.58
3:A:690:LYS:O	3:A:692:ASN:N	2.34	0.58
3:A:867:ASN:C	3:A:867:ASN:HD22	2.06	0.58
3:A:7:ILE:HG22	3:A:387:TYR:CE2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:924:THR:CA	3:A:946:VAL:O	2.24	0.58
3:A:254:GLU:O	3:A:258:LYS:N	2.37	0.58
3:A:985:TRP:H	3:A:991:ARG:HG3	1.69	0.58
3:A:339:GLU:HA	3:A:343:GLN:HB2	1.85	0.58
3:A:1901:ASN:OD1	3:A:1902:GLY:N	2.37	0.58
3:A:725:HIS:HA	3:A:730:ASN:ND2	2.17	0.57
3:A:1096:LYS:HA	3:A:1100:TYR:HB3	1.85	0.57
3:A:1202:CYS:N	3:A:1204:GLU:OE1	2.38	0.57
3:A:1883:ILE:O	3:A:1883:ILE:HG13	2.05	0.57
1:B:217:SER:HB2	1:B:221:GLN:HE22	1.69	0.57
3:A:336:TRP:HA	3:A:339:GLU:HB3	1.85	0.57
3:A:1929:LYS:HB3	3:A:1930:GLU:HG3	1.87	0.57
1:B:87:PHE:CZ	1:B:102:MET:HG2	2.39	0.57
3:A:1050:MET:CE	3:A:1198:ALA:HA	2.34	0.57
3:A:1201:LYS:HD3	3:A:1204:GLU:HB3	1.86	0.57
3:A:1715:TYR:OH	3:A:1719:LYS:NZ	2.23	0.57
3:A:293:ASN:OD1	3:A:297:ASP:HB2	2.03	0.57
3:A:562:LYS:C	3:A:564:SER:N	2.56	0.57
3:A:1818:LYS:HA	3:A:1957:HIS:HE1	1.69	0.57
3:A:689:ILE:CD1	3:A:707:LEU:HB2	2.34	0.57
3:A:1282:TYR:HB3	3:A:1285:ARG:HB2	1.85	0.57
1:B:94:PRO:HB2	3:A:1055:ILE:HG12	1.86	0.57
3:A:341:GLU:O	3:A:345:ASN:ND2	2.38	0.57
3:A:659:ILE:HD11	3:A:712:TRP:CE3	2.40	0.57
3:A:863:SER:HB3	3:A:1879:ASP:OD1	2.05	0.57
3:A:118:ILE:HD11	3:A:124:PHE:HB2	1.86	0.57
3:A:562:LYS:HB2	3:A:575:ALA:CB	2.34	0.57
3:A:575:ALA:O	3:A:577:THR:OG1	2.19	0.57
3:A:1235:TYR:HD1	3:A:1271:ASN:HD21	1.53	0.57
3:A:11:ILE:HA	3:A:14:TYR:HD2	1.70	0.56
3:A:178:ASN:O	3:A:182:ASN:HB2	2.06	0.56
3:A:689:ILE:HD11	3:A:703:SER:O	2.06	0.56
3:A:9:ASN:H	3:A:387:TYR:HE1	1.53	0.56
3:A:10:LYS:H	3:A:387:TYR:HE1	1.54	0.56
3:A:990:ALA:HA	3:A:1107:ILE:HD11	1.86	0.56
1:B:128:ALA:HB1	2:C:65:LEU:HD11	1.87	0.56
3:A:342:ASN:O	3:A:346:LYS:NZ	2.24	0.56
3:A:757:PRO:HB3	3:A:882:ILE:HD12	1.88	0.56
3:A:1120:LYS:O	3:A:1124:LYS:HG2	2.04	0.56
3:A:1320:ALA:O	3:A:1323:SER:OG	2.22	0.56
3:A:1386:GLN:HE21	3:A:1390:LYS:HA	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:184:LYS:HG3	3:A:207:TYR:CZ	2.40	0.56
3:A:591:ASN:HA	3:A:669:TYR:HD2	1.70	0.56
3:A:862:THR:HG22	3:A:1871:ASN:ND2	2.21	0.56
3:A:1339:LEU:HD22	3:A:1343:PHE:HD2	1.71	0.56
3:A:384:LEU:HB2	3:A:388:ILE:HG13	1.86	0.56
3:A:858:LYS:HD3	3:A:860:CYS:SG	2.46	0.56
3:A:1405:TRP:O	3:A:1409:GLU:HB2	2.06	0.56
3:A:862:THR:HG22	3:A:1871:ASN:HD21	1.71	0.56
3:A:1143:ASN:HB3	3:A:1973:LEU:HD21	1.88	0.55
3:A:1543:TYR:HB2	3:A:1546:CYS:SG	2.46	0.55
3:A:949:VAL:HG11	3:A:1867:TYR:OH	2.06	0.55
3:A:1118:TYR:OH	3:A:1139:VAL:O	2.16	0.55
3:A:1339:LEU:HD22	3:A:1343:PHE:CD2	2.40	0.55
3:A:1402:ASN:HA	3:A:1405:TRP:HB3	1.88	0.55
3:A:1402:ASN:O	3:A:1406:LYS:HB2	2.05	0.55
3:A:1436:GLU:HG2	3:A:1437:CYS:H	1.69	0.55
3:A:85:ASN:HD21	3:A:94:GLU:HB2	1.70	0.55
3:A:1125:GLN:HA	3:A:1128:ASP:N	2.20	0.55
3:A:1345:HIS:HB3	3:A:1349:ARG:HG3	1.88	0.55
3:A:577:THR:CG2	3:A:841:ARG:HB2	2.36	0.55
2:C:166:GLN:HE21	2:C:167:TRP:H	1.54	0.55
3:A:80:TRP:O	3:A:94:GLU:HG2	2.06	0.55
3:A:328:LYS:O	3:A:332:CYS:N	2.36	0.55
1:B:71:ASN:O	1:B:91:ARG:NH1	2.40	0.55
3:A:82:CYS:H	3:A:95:ASN:H	1.55	0.55
3:A:113:LEU:H	3:A:182:ASN:ND2	2.03	0.55
3:A:279:TRP:CD1	3:A:282:GLU:HB3	2.41	0.55
3:A:286:ASP:O	3:A:290:GLU:HG3	2.07	0.55
3:A:1308:THR:HA	3:A:1311:LEU:CB	2.36	0.55
3:A:127:ASP:OD1	3:A:128:VAL:N	2.40	0.55
3:A:686:GLY:O	3:A:687:LYS:C	2.45	0.55
3:A:187:PHE:HA	3:A:190:ILE:HG12	1.89	0.55
3:A:557:LYS:O	3:A:558:TRP:C	2.45	0.55
3:A:1299:LYS:HA	3:A:1303:ALA:H	1.72	0.55
3:A:1333:LYS:HE2	3:A:1341:LYS:HE2	1.88	0.55
3:A:113:LEU:HB2	3:A:186:MET:HG3	1.89	0.54
3:A:1199:GLU:C	3:A:1201:LYS:H	2.11	0.54
3:A:1315:HIS:CD2	3:A:1342:GLY:HA3	2.41	0.54
3:A:1599:LYS:HB2	3:A:1672:GLN:HB2	1.89	0.54
3:A:279:TRP:HB3	3:A:283:TRP:NE1	2.22	0.54
3:A:1053:ALA:C	3:A:1055:ILE:H	2.11	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:275:GLN:O	3:A:279:TRP:N	2.41	0.54
3:A:841:ARG:HE	3:A:845:HIS:CD2	2.26	0.54
3:A:1316:ASP:C	3:A:1330:GLN:HG3	2.28	0.54
3:A:55:THR:H	3:A:58:HIS:CD2	2.26	0.54
3:A:180:GLU:HG2	3:A:184:LYS:HZ3	1.72	0.54
3:A:1310:LEU:O	3:A:1314:TYR:CB	2.55	0.54
3:A:1396:SER:O	3:A:1400:ASN:ND2	2.40	0.54
3:A:1465:ARG:NH1	3:A:1569:ASP:OD2	2.40	0.54
3:A:1719:LYS:O	3:A:1723:ILE:HG12	2.07	0.54
3:A:28:LEU:O	3:A:121:ASN:ND2	2.41	0.54
3:A:1821:CYS:SG	3:A:1838:CYS:HB2	2.47	0.54
2:C:52:LEU:HD13	2:C:90:PHE:CG	2.43	0.54
3:A:259:CYS:SG	3:A:262:TYR:HB2	2.48	0.54
3:A:691:LYS:CB	3:A:694:THR:HA	2.32	0.54
3:A:862:THR:HG21	3:A:891:ASP:H	1.72	0.54
2:C:186:ASP:OD2	2:C:188:LYS:HG2	2.08	0.54
3:A:80:TRP:O	3:A:94:GLU:HA	2.08	0.54
3:A:1029:VAL:HG21	3:A:1959:MET:HE2	1.89	0.54
3:A:1298:GLU:O	3:A:1302:ASN:N	2.22	0.54
3:A:1409:GLU:HG3	3:A:1412:MET:HB3	1.90	0.54
3:A:287:PHE:HD1	3:A:291:LYS:HB2	1.72	0.54
3:A:1305:HIS:CE1	3:A:1423:ILE:HA	2.43	0.54
3:A:1305:HIS:HA	3:A:1308:THR:OG1	2.08	0.54
3:A:1372:LEU:O	3:A:1376:ILE:HG12	2.07	0.54
3:A:31:ASP:O	3:A:33:SER:N	2.41	0.54
3:A:121:ASN:CB	3:A:214:TRP:HE1	2.21	0.54
3:A:288:TYR:HB3	3:A:397:TYR:OH	2.07	0.54
3:A:295:ILE:HA	3:A:299:GLU:HB2	1.90	0.54
3:A:691:LYS:HZ1	3:A:700:SER:HB3	1.73	0.54
3:A:939:GLN:N	3:A:943:THR:HG21	2.23	0.54
3:A:112:ASN:HB3	3:A:114:LYS:NZ	2.22	0.53
3:A:926:THR:HG22	3:A:944:LEU:HD12	1.89	0.53
3:A:1364:ASN:HB3	3:A:1369:ILE:HG22	1.91	0.53
3:A:1445:ASN:O	3:A:1530:TYR:OH	2.25	0.53
3:A:1483:GLU:OE2	3:A:1578:GLN:N	2.41	0.53
1:B:71:ASN:HB2	1:B:76:ASP:HB3	1.90	0.53
2:C:127:ARG:NE	2:C:128:THR:O	2.38	0.53
3:A:113:LEU:N	3:A:182:ASN:HD21	2.06	0.53
3:A:1396:SER:HB3	3:A:1400:ASN:ND2	2.22	0.53
3:A:1413:TRP:CH2	3:A:1442:PRO:HD3	2.43	0.53
3:A:1936:GLU:HB2	3:A:1939:PRO:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:256:CYS:SG	3:A:257:ARG:NH1	2.81	0.53
3:A:337:LYS:HB3	3:A:341:GLU:OE2	2.08	0.53
3:A:345:ASN:HA	3:A:350:LEU:HA	1.91	0.53
3:A:927:GLU:OE2	3:A:933:ARG:N	2.33	0.53
2:C:27:PRO:HG2	2:C:30:LEU:HB2	1.89	0.53
3:A:191:ARG:NH1	3:A:210:LEU:HB3	2.24	0.53
3:A:281:THR:O	3:A:286:ASP:N	2.33	0.53
3:A:984:GLN:H	3:A:991:ARG:HB3	1.73	0.53
3:A:1240:PHE:CD1	3:A:1241:PRO:HA	2.43	0.53
2:C:111:ASN:ND2	2:C:112:ASN:OD1	2.42	0.53
3:A:1219:CYS:HB3	3:A:1422:LYS:HE2	1.91	0.53
3:A:1417:ARG:HA	3:A:1420:ILE:HG22	1.90	0.53
1:B:153:LEU:HB3	2:C:137:PHE:CD1	2.36	0.53
3:A:59:SER:OG	3:A:60:ASP:N	2.41	0.53
3:A:129:LEU:HD23	3:A:225:VAL:HG21	1.90	0.53
3:A:262:TYR:CE2	3:A:573:GLU:HB2	2.42	0.53
3:A:1006:LYS:NZ	3:A:1011:ASP:HA	2.23	0.53
3:A:1385:PRO:HB3	3:A:1404:TRP:CE3	2.44	0.53
3:A:1615:ASN:ND2	3:A:1875:GLU:OE2	2.42	0.53
3:A:1984:LYS:HE3	3:A:1984:LYS:HA	1.89	0.53
3:A:1:MET:SD	3:A:3:SER:N	2.82	0.53
3:A:36:GLU:HG2	3:A:1781:LEU:HB3	1.91	0.53
2:C:168:LYS:HB3	2:C:171:ASN:HA	1.90	0.53
3:A:239:ARG:HH12	3:A:249:ARG:HH12	1.57	0.53
3:A:993:MET:HG2	3:A:1008:ASN:HD21	1.73	0.53
3:A:1368:HIS:ND1	3:A:1371:LYS:HB3	2.24	0.53
3:A:38:TYR:HA	3:A:117:LYS:HE3	1.90	0.53
3:A:215:TRP:HZ3	3:A:272:TYR:HE1	1.57	0.53
3:A:940:SER:O	3:A:943:THR:HG22	2.09	0.53
3:A:1121:PHE:O	3:A:1125:GLN:OE1	2.26	0.53
3:A:562:LYS:C	3:A:564:SER:H	2.11	0.53
3:A:964:CYS:O	3:A:965:GLN:HG3	2.08	0.53
3:A:1369:ILE:HD12	3:A:1372:LEU:HD12	1.90	0.53
3:A:235:LEU:HD21	3:A:675:LEU:HD13	1.90	0.52
3:A:1015:THR:O	3:A:1018:ARG:NH1	2.41	0.52
3:A:1596:CYS:SG	3:A:1664:ARG:HG2	2.48	0.52
3:A:88:ASP:C	3:A:93:PRO:HB3	2.29	0.52
3:A:289:ARG:O	3:A:293:ASN:HB2	2.09	0.52
3:A:524:GLN:O	3:A:526:GLU:N	2.42	0.52
3:A:528:GLN:NE2	3:A:718:TYR:OH	2.42	0.52
3:A:587:LEU:HD13	3:A:655:TYR:CE1	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1202:CYS:H	3:A:1204:GLU:HA	1.72	0.52
3:A:279:TRP:HB3	3:A:283:TRP:CD1	2.45	0.52
3:A:499:LEU:HD11	3:A:522:LYS:HB3	1.91	0.52
3:A:1215:SER:HB3	3:A:1216:GLU:HG3	1.91	0.52
2:C:109:LYS:NZ	2:C:114:PRO:HD2	2.25	0.52
3:A:164:ASP:OD2	3:A:278:ARG:NH1	2.41	0.52
3:A:270:LEU:O	3:A:273:VAL:HB	2.09	0.52
3:A:632:TYR:O	3:A:637:ASN:N	2.41	0.52
3:A:1092:ASN:HA	3:A:1097:CYS:HB3	1.90	0.52
3:A:1269:THR:O	3:A:1272:LEU:HD22	2.09	0.52
3:A:1752:ASP:OD1	3:A:1753:ARG:N	2.37	0.52
3:A:180:GLU:HG2	3:A:184:LYS:NZ	2.24	0.52
3:A:1298:GLU:HA	3:A:1301:LYS:HD2	1.90	0.52
3:A:102:ARG:HH12	3:A:282:GLU:CD	2.13	0.52
3:A:121:ASN:O	3:A:125:LEU:N	2.43	0.52
3:A:850:LYS:HD2	3:A:864:SER:HB2	1.92	0.52
3:A:1129:ALA:O	3:A:1133:SER:N	2.43	0.52
3:A:1314:TYR:CD2	3:A:1320:ALA:HB2	2.45	0.52
3:A:1474:GLU:HA	3:A:1478:ILE:HB	1.90	0.52
3:A:1741:TRP:HA	3:A:1746:THR:HG21	1.91	0.52
3:A:29:LYS:HB3	3:A:217:ALA:HB1	1.91	0.52
3:A:1314:TYR:HA	3:A:1319:THR:HG1	1.75	0.52
3:A:1345:HIS:NE2	3:A:1543:TYR:HE1	2.07	0.52
3:A:1636:LEU:O	3:A:1640:ILE:HG12	2.10	0.52
3:A:680:ASN:C	3:A:682:GLY:N	2.62	0.52
3:A:159:PHE:HE1	3:A:222:VAL:HG13	1.74	0.52
3:A:207:TYR:HB3	3:A:211:ARG:NH1	2.25	0.52
3:A:852:ASN:OD1	3:A:853:ARG:N	2.41	0.52
3:A:1277:LEU:O	3:A:1288:ILE:HG23	2.10	0.51
3:A:1420:ILE:HD12	3:A:1423:ILE:HB	1.92	0.51
3:A:1984:LYS:C	3:A:1986:TYR:H	2.14	0.51
3:A:1356:ASN:HD22	3:A:1359:LEU:HD11	1.74	0.51
3:A:82:CYS:HB2	3:A:96:ILE:HB	1.93	0.51
3:A:511:ARG:O	3:A:512:GLY:C	2.49	0.51
3:A:1666:ALA:HB2	3:A:1764:MET:SD	2.49	0.51
3:A:935:LYS:HG3	3:A:936:SER:N	2.25	0.51
3:A:1627:ARG:NH1	3:A:1697:ASP:OD2	2.32	0.51
3:A:510:LYS:HE2	3:A:510:LYS:HA	1.91	0.51
3:A:559:ILE:HG22	3:A:561:LYS:CG	2.31	0.51
3:A:562:LYS:HZ3	3:A:576:ASN:HB2	1.76	0.51
3:A:1821:CYS:HA	3:A:1838:CYS:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:631:ARG:O	3:A:635:ASN:HB3	2.09	0.51
3:A:804:LYS:NZ	3:A:966:CYS:SG	2.82	0.51
1:B:119:LEU:HD12	1:B:120:ARG:HG3	1.91	0.51
3:A:207:TYR:O	3:A:211:ARG:HG2	2.10	0.51
3:A:251:LYS:HE3	3:A:566:ASN:O	2.11	0.51
3:A:1125:GLN:CA	3:A:1129:ALA:H	2.24	0.51
3:A:1550:ASN:ND2	3:A:1711:GLU:O	2.43	0.51
3:A:1814:PHE:CE2	3:A:1953:LYS:HE2	2.45	0.51
3:A:529:LYS:HB3	3:A:614:LEU:HD23	1.92	0.51
3:A:942:ASP:OD1	3:A:947:VAL:N	2.43	0.51
3:A:1436:GLU:OE1	3:A:1436:GLU:N	2.38	0.51
2:C:21:ILE:HG21	2:C:46:GLN:HG2	1.93	0.51
3:A:688:TYR:O	3:A:689:ILE:C	2.50	0.51
1:B:46:PHE:HE1	1:B:117:ARG:HE	1.58	0.50
1:B:48:PHE:HD2	1:B:96:SER:HA	1.75	0.50
3:A:537:SER:O	3:A:538:LEU:HG	2.11	0.50
3:A:988:GLY:HA2	3:A:1110:GLN:HG3	1.93	0.50
3:A:1262:GLY:HA2	3:A:1525:LYS:HE3	1.93	0.50
1:B:117:ARG:HD3	1:B:131:ASN:HB2	1.93	0.50
3:A:787:SER:OG	3:A:798:GLU:OE2	2.14	0.50
3:A:1199:GLU:HA	3:A:1202:CYS:O	2.11	0.50
3:A:1204:GLU:N	3:A:1205:ASN:HA	2.25	0.50
2:C:177:ASN:ND2	2:C:198:LEU:HD11	2.26	0.50
3:A:191:ARG:NE	3:A:205:GLN:HB3	2.26	0.50
3:A:277:LEU:HD22	3:A:373:PHE:CZ	2.46	0.50
3:A:562:LYS:NZ	3:A:576:ASN:HB2	2.26	0.50
3:A:1237:GLY:N	3:A:1246:GLU:HG3	2.26	0.50
3:A:1356:ASN:HB3	3:A:1449:GLN:NE2	2.21	0.50
3:A:925:THR:O	3:A:946:VAL:HG12	2.10	0.50
3:A:231:ARG:HG2	3:A:234:ASP:CG	2.32	0.50
3:A:770:PHE:CZ	3:A:953:LEU:HD23	2.47	0.50
3:A:1305:HIS:CE1	3:A:1427:ASN:HB2	2.47	0.50
3:A:1839:LYS:HG3	3:A:1964:VAL:HG22	1.93	0.50
3:A:38:TYR:CE1	3:A:118:ILE:HB	2.44	0.50
3:A:80:TRP:CD1	3:A:94:GLU:HB3	2.46	0.50
3:A:291:LYS:HD2	3:A:339:GLU:OE2	2.12	0.50
3:A:694:THR:O	3:A:695:ALA:HB2	2.10	0.50
3:A:905:LEU:HD22	3:A:909:ILE:HD11	1.94	0.50
3:A:1056:SER:HB3	3:A:1057:CYS:HB2	1.93	0.50
3:A:1124:LYS:O	3:A:1127:TYR:HB3	2.12	0.50
3:A:1721:ASN:OD1	3:A:1738:ARG:NH1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1939:PRO:O	3:A:1941:ASP:N	2.45	0.50
3:A:1977:ASP:OD1	3:A:1978:ASN:N	2.44	0.50
1:B:31:VAL:HG21	1:B:105:LEU:HD12	1.93	0.50
2:C:23:MET:SD	2:C:109:LYS:HG2	2.52	0.50
3:A:504:GLU:HG3	3:A:521:ASN:ND2	2.27	0.50
3:A:894:LEU:HD11	3:A:903:ASN:HD22	1.75	0.50
3:A:1209:ASP:HB3	3:A:1210:THR:OG1	2.11	0.50
3:A:1285:ARG:HG2	3:A:1287:ASN:HA	1.94	0.50
1:B:119:LEU:HB3	1:B:130:GLY:HA3	1.93	0.50
3:A:51:ILE:HG12	3:A:221:LYS:HE3	1.94	0.50
3:A:219:ARG:HH21	3:A:266:VAL:HG21	1.76	0.50
3:A:1657:THR:HA	3:A:1660:ILE:HG22	1.94	0.50
3:A:235:LEU:HD12	3:A:258:LYS:HG2	1.94	0.49
3:A:968:ILE:HB	3:A:969:PRO:HD2	1.94	0.49
3:A:1142:SER:HB3	3:A:1187:GLY:H	1.77	0.49
3:A:1414:ASP:O	3:A:1417:ARG:HG2	2.12	0.49
3:A:1489:SER:HA	3:A:1498:GLN:HG2	1.94	0.49
3:A:1538:LEU:O	3:A:1542:ASN:ND2	2.44	0.49
3:A:290:GLU:OE2	3:A:291:LYS:HG3	2.12	0.49
3:A:1215:SER:HB3	3:A:1216:GLU:CG	2.42	0.49
3:A:1359:LEU:HD12	3:A:1360:GLY:N	2.28	0.49
3:A:1376:ILE:HA	3:A:1380:ILE:HB	1.92	0.49
3:A:95:ASN:ND2	3:A:346:LYS:HE3	2.27	0.49
3:A:256:CYS:HA	3:A:257:ARG:CG	2.41	0.49
3:A:287:PHE:HD1	3:A:291:LYS:HE2	1.77	0.49
3:A:560:TRP:O	3:A:576:ASN:HA	2.11	0.49
3:A:562:LYS:CB	3:A:575:ALA:HB1	2.36	0.49
3:A:563:SER:O	3:A:565:GLY:N	2.45	0.49
3:A:697:GLN:N	3:A:699:THR:HB	2.27	0.49
3:A:1398:THR:O	3:A:1402:ASN:HB2	2.12	0.49
3:A:1308:THR:HB	3:A:1429:ASN:HD21	1.77	0.49
3:A:1310:LEU:HD22	3:A:1314:TYR:HB2	1.93	0.49
3:A:1325:ASN:HD21	3:A:1328:LYS:CG	2.25	0.49
3:A:558:TRP:HB2	3:A:825:GLY:O	2.13	0.49
3:A:690:LYS:C	3:A:692:ASN:H	2.15	0.49
2:C:206:GLU:HG3	2:C:230:ARG:NH1	2.28	0.49
3:A:1307:GLU:C	3:A:1311:LEU:H	2.16	0.49
3:A:1485:LYS:HB2	3:A:1489:SER:HB2	1.94	0.49
3:A:1933:CYS:SG	3:A:1936:GLU:HB3	2.51	0.49
3:A:674:GLU:OE2	3:A:708:ARG:NH1	2.27	0.49
3:A:1500:ALA:O	3:A:1503:ARG:NH1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:GLU:HA	1:B:40:SER:O	2.13	0.49
1:B:181:VAL:HG22	1:B:227:VAL:HG12	1.93	0.49
3:A:216:ASN:O	3:A:219:ARG:HG2	2.13	0.49
3:A:699:THR:HG23	3:A:700:SER:O	2.13	0.49
3:A:1373:GLN:O	3:A:1377:LYS:HG2	2.12	0.49
3:A:1377:LYS:O	3:A:1381:GLU:HB2	2.13	0.49
3:A:1582:TYR:CD2	3:A:1589:LYS:HB2	2.47	0.49
3:A:817:CYS:SG	3:A:930:ASN:HB2	2.52	0.49
3:A:982:MET:H	3:A:991:ARG:NH1	2.11	0.49
2:C:31:SER:OG	2:C:124:GLU:OE2	2.28	0.48
3:A:76:ASP:HB2	3:A:104:ARG:HH22	1.77	0.48
3:A:289:ARG:O	3:A:293:ASN:CB	2.61	0.48
3:A:633:PRO:HA	3:A:634:GLN:HA	1.60	0.48
3:A:1626:PRO:O	3:A:1630:GLN:HG2	2.13	0.48
3:A:160:ALA:HB1	3:A:278:ARG:CZ	2.43	0.48
3:A:255:LEU:O	3:A:257:ARG:NH1	2.38	0.48
3:A:1822:ASP:CG	3:A:1823:PRO:HD3	2.33	0.48
2:C:135:PHE:HB2	2:C:154:LEU:HB3	1.95	0.48
3:A:559:ILE:HD11	3:A:585:GLN:OE1	2.13	0.48
3:A:559:ILE:C	3:A:561:LYS:H	2.16	0.48
3:A:1049:TYR:C	3:A:1053:ALA:HA	2.34	0.48
3:A:1118:TYR:HA	3:A:1121:PHE:HB3	1.94	0.48
3:A:1406:LYS:HA	3:A:1409:GLU:CB	2.42	0.48
2:C:206:GLU:HA	2:C:230:ARG:CZ	2.43	0.48
3:A:116:ASP:HB3	3:A:119:ARG:HH22	1.78	0.48
3:A:524:GLN:HB2	3:A:701:TYR:OH	2.13	0.48
3:A:1133:SER:HB2	3:A:1134:GLN:HG2	1.95	0.48
3:A:1311:LEU:HD21	3:A:1339:LEU:HB2	1.95	0.48
3:A:1688:CYS:SG	3:A:1783:MET:HG2	2.54	0.48
2:C:108:GLN:HG3	2:C:117:PHE:CE1	2.49	0.48
3:A:524:GLN:OE1	3:A:701:TYR:CZ	2.67	0.48
3:A:559:ILE:CG2	3:A:561:LYS:HG2	2.30	0.48
3:A:1443:THR:OG1	3:A:1446:ASP:OD2	2.23	0.48
3:A:1457:TRP:CH2	3:A:1519:TRP:HB2	2.49	0.48
3:A:513:SER:O	3:A:514:SER:C	2.52	0.48
3:A:767:VAL:HG11	3:A:901:LEU:HD21	1.94	0.48
3:A:1106:LYS:HB3	3:A:1110:GLN:NE2	2.28	0.48
3:A:1202:CYS:H	3:A:1204:GLU:CD	2.16	0.48
1:B:58:GLN:HB2	1:B:64:LEU:HD23	1.95	0.48
3:A:125:LEU:HG	3:A:129:LEU:CD1	2.43	0.48
3:A:1005:CYS:HB2	3:A:1114:GLN:NE2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1497:ILE:HB	3:A:1502:LYS:HE2	1.95	0.48
3:A:375:GLU:HA	3:A:380:ASN:HB3	1.95	0.48
3:A:1057:CYS:SG	3:A:1058:ILE:HB	2.53	0.48
3:A:1149:CYS:SG	3:A:1150:TRP:N	2.87	0.48
3:A:1408:ILE:HB	3:A:1411:GLU:HB3	1.94	0.48
3:A:60:ASP:O	3:A:64:TYR:HB3	2.13	0.48
3:A:1420:ILE:HG12	3:A:1436:GLU:HA	1.95	0.48
2:C:55:TYR:HE1	2:C:108:GLN:HB3	1.79	0.48
2:C:163:ALA:HB2	2:C:217:HIS:HD2	1.79	0.48
3:A:591:ASN:HA	3:A:669:TYR:CD2	2.48	0.48
3:A:1726:SER:N	3:A:1729:THR:OG1	2.46	0.48
3:A:102:ARG:NH2	3:A:282:GLU:HG3	2.27	0.47
3:A:560:TRP:HH2	3:A:838:ILE:CG1	2.27	0.47
3:A:1308:THR:HA	3:A:1311:LEU:HB2	1.96	0.47
3:A:5:SER:HB3	3:A:384:LEU:HD21	1.96	0.47
3:A:168:GLY:HA3	3:A:211:ARG:HH21	1.78	0.47
3:A:580:LEU:O	3:A:585:GLN:NE2	2.46	0.47
3:A:691:LYS:HB3	3:A:694:THR:HG23	1.95	0.47
3:A:1339:LEU:HD22	3:A:1343:PHE:HB3	1.95	0.47
1:B:228:ASN:HB3	1:B:230:LYS:NZ	2.29	0.47
3:A:689:ILE:HD11	3:A:703:SER:C	2.34	0.47
3:A:1404:TRP:O	3:A:1408:ILE:HG12	2.14	0.47
3:A:1757:ARG:NH2	3:A:1788:ILE:O	2.47	0.47
3:A:166:ILE:O	3:A:211:ARG:HD2	2.14	0.47
3:A:277:LEU:HD22	3:A:373:PHE:CE1	2.49	0.47
3:A:1408:ILE:C	3:A:1412:MET:H	2.16	0.47
3:A:1824:PRO:HG2	3:A:1832:ASP:H	1.79	0.47
3:A:275:GLN:O	3:A:275:GLN:NE2	2.44	0.47
3:A:687:LYS:O	3:A:688:TYR:C	2.53	0.47
3:A:1799:LEU:HD21	3:A:1888:VAL:HG23	1.95	0.47
1:B:224:ILE:HG22	1:B:239:LYS:HA	1.96	0.47
3:A:79:GLN:OE1	3:A:81:LYS:NZ	2.43	0.47
3:A:235:LEU:HD23	3:A:238:LYS:HE3	1.97	0.47
3:A:255:LEU:O	3:A:257:ARG:HD3	2.14	0.47
3:A:632:TYR:HB2	3:A:633:PRO:HD2	1.97	0.47
3:A:1250:ILE:HG12	3:A:1265:ILE:HB	1.95	0.47
3:A:1418:CYS:O	3:A:1422:LYS:HG2	2.14	0.47
3:A:1476:CYS:HA	3:A:1480:GLY:HA3	1.97	0.47
1:B:146:LYS:HD2	1:B:147:GLY:O	2.14	0.47
3:A:111:GLU:OE1	3:A:175:THR:OG1	2.33	0.47
3:A:187:PHE:HE2	3:A:191:ARG:HH11	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1316:ASP:O	3:A:1330:GLN:HG3	2.14	0.47
3:A:1324:LYS:HB3	3:A:1467:ARG:NH2	2.29	0.47
3:A:1454:PHE:HE1	3:A:1522:GLN:HB3	1.79	0.47
2:C:109:LYS:HZ2	2:C:114:PRO:HD2	1.80	0.47
3:A:202:PRO:HB2	3:A:206:LYS:HG2	1.97	0.47
3:A:258:LYS:HZ3	3:A:671:LYS:HA	1.79	0.47
3:A:691:LYS:O	3:A:694:THR:N	2.48	0.47
3:A:1111:TRP:O	3:A:1115:LYS:N	2.29	0.47
3:A:1274:VAL:CG1	3:A:1278:TRP:H	2.28	0.47
3:A:1278:TRP:HA	3:A:1287:ASN:HB3	1.95	0.47
3:A:1633:LEU:HD11	3:A:1712:TYR:HB3	1.96	0.47
3:A:33:SER:HA	3:A:48:LYS:HZ2	1.79	0.47
3:A:102:ARG:HA	3:A:105:LEU:CD1	2.45	0.47
3:A:254:GLU:HB3	3:A:258:LYS:O	2.15	0.47
3:A:365:ARG:NH2	3:A:370:VAL:O	2.48	0.47
3:A:562:LYS:HE2	3:A:576:ASN:ND2	2.30	0.47
3:A:617:CYS:HA	3:A:620:VAL:HG12	1.97	0.47
3:A:1499:GLY:HA2	3:A:1502:LYS:HB2	1.97	0.47
3:A:80:TRP:HB3	3:A:97:CYS:SG	2.55	0.47
3:A:164:ASP:O	3:A:168:GLY:N	2.48	0.47
3:A:236:LEU:HD22	3:A:260:GLY:N	2.30	0.47
3:A:1550:ASN:ND2	3:A:1711:GLU:HG2	2.30	0.47
3:A:1754:LYS:NZ	3:A:1762:ASP:OD2	2.38	0.47
3:A:18:LYS:HB3	3:A:216:ASN:ND2	2.30	0.46
3:A:167:ARG:C	3:A:211:ARG:HE	2.19	0.46
3:A:925:THR:O	3:A:946:VAL:HB	2.14	0.46
3:A:1397:SER:O	3:A:1401:VAL:HG22	2.15	0.46
2:C:151:VAL:HB	2:C:198:LEU:HB3	1.97	0.46
3:A:1114:GLN:NE2	3:A:1117:ASN:HD22	2.13	0.46
3:A:1305:HIS:CE1	3:A:1423:ILE:HG12	2.50	0.46
3:A:1312:TYR:O	3:A:1316:ASP:HB3	2.15	0.46
3:A:1419:ALA:O	3:A:1423:ILE:HG13	2.15	0.46
3:A:99:PRO:HB2	3:A:101:ARG:HB3	1.97	0.46
3:A:666:ASP:OD2	3:A:671:LYS:HE2	2.15	0.46
3:A:967:LYS:NZ	3:A:968:ILE:HG12	2.30	0.46
3:A:1348:GLN:O	3:A:1352:ILE:HB	2.16	0.46
1:B:175:PHE:HB3	1:B:204:LEU:HD13	1.97	0.46
3:A:12:GLU:OE1	3:A:12:GLU:N	2.44	0.46
3:A:252:ASN:OD1	3:A:253:PHE:N	2.43	0.46
3:A:290:GLU:OE2	3:A:291:LYS:NZ	2.45	0.46
3:A:632:TYR:HA	3:A:636:LYS:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:689:ILE:HG13	3:A:702:SER:O	2.14	0.46
3:A:798:GLU:HG3	3:A:966:CYS:HB3	1.97	0.46
3:A:999:ASN:ND2	3:A:1001:ASN:O	2.49	0.46
2:C:143:GLN:O	2:C:146:SER:OG	2.15	0.46
3:A:365:ARG:HH12	3:A:374:PHE:CB	2.21	0.46
3:A:1092:ASN:HB3	3:A:1094:LYS:O	2.14	0.46
3:A:1133:SER:HA	3:A:1134:GLN:HA	1.68	0.46
3:A:1203:LYS:HB3	3:A:1205:ASN:OD1	2.16	0.46
1:B:93:ASN:ND2	3:A:1615:ASN:OD1	2.49	0.46
3:A:85:ASN:ND2	3:A:94:GLU:HB2	2.30	0.46
3:A:112:ASN:HB3	3:A:114:LYS:HZ3	1.81	0.46
3:A:1096:LYS:HD2	3:A:1201:LYS:CG	2.45	0.46
3:A:1106:LYS:HE3	3:A:1110:GLN:HE22	1.80	0.46
3:A:1257:HIS:CD2	3:A:1265:ILE:HG13	2.51	0.46
1:B:145:THR:HA	1:B:176:PRO:HD3	1.97	0.46
1:B:212:THR:HG21	2:C:156:ASN:ND2	2.30	0.46
3:A:95:ASN:CG	3:A:346:LYS:HE3	2.36	0.46
3:A:200:LYS:HE3	3:A:210:LEU:HD13	1.98	0.46
3:A:291:LYS:O	3:A:294:LEU:HB2	2.15	0.46
3:A:388:ILE:HG22	3:A:389:LYS:HG2	1.98	0.46
3:A:614:LEU:O	3:A:618:LEU:HD23	2.16	0.46
3:A:615:ALA:O	3:A:619:ILE:HG12	2.15	0.46
3:A:1794:GLN:HG3	3:A:1797:ARG:NH2	2.31	0.46
3:A:1954:TYR:OH	3:A:1961:CYS:SG	2.59	0.46
2:C:184:GLU:HA	2:C:184:GLU:OE2	2.16	0.46
3:A:83:GLN:HB3	3:A:95:ASN:ND2	2.12	0.46
3:A:170:ASP:HA	3:A:279:TRP:HH2	1.81	0.46
3:A:203:LYS:HA	3:A:204:ASP:C	2.36	0.46
3:A:258:LYS:HE2	3:A:674:GLU:HG2	1.98	0.46
3:A:682:GLY:O	3:A:683:LYS:C	2.54	0.46
3:A:864:SER:HA	3:A:1790:ILE:CG2	2.44	0.46
3:A:978:ARG:HG3	3:A:980:GLU:OE2	2.16	0.46
3:A:24:ILE:HG22	3:A:24:ILE:O	2.16	0.46
3:A:148:SER:O	3:A:150:ASN:N	2.42	0.46
3:A:653:ALA:HB2	3:A:753:ILE:HG23	1.98	0.46
3:A:767:VAL:HG21	3:A:901:LEU:HD21	1.98	0.46
3:A:1094:LYS:HD2	3:A:1096:LYS:HE2	1.98	0.46
3:A:1670:TRP:CH2	3:A:1780:PRO:HG3	2.49	0.46
3:A:1822:ASP:HB3	3:A:1957:HIS:CE1	2.50	0.46
2:C:158:PHE:HD2	2:C:217:HIS:HE2	1.64	0.46
3:A:1123:SER:C	3:A:1126:ILE:H	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1125:GLN:HA	3:A:1129:ALA:H	1.81	0.46
3:A:1424:ASN:HA	3:A:1430:SER:O	2.16	0.46
3:A:1824:PRO:HD2	3:A:1828:ASP:HA	1.98	0.46
3:A:273:VAL:HG13	3:A:277:LEU:CD2	2.45	0.45
3:A:690:LYS:HE3	3:A:690:LYS:HB3	1.37	0.45
3:A:1667:TYR:OH	3:A:1671:LYS:NZ	2.42	0.45
3:A:319:CYS:HA	3:A:322:CYS:SG	2.57	0.45
3:A:779:LYS:O	3:A:783:THR:HG23	2.16	0.45
3:A:939:GLN:H	3:A:943:THR:CG2	2.25	0.45
3:A:1214:LYS:HG3	3:A:1414:ASP:OD2	2.16	0.45
3:A:38:TYR:CD2	3:A:59:SER:HA	2.52	0.45
3:A:185:GLN:NE2	3:A:186:MET:HG2	2.30	0.45
3:A:350:LEU:CB	3:A:355:LYS:H	2.30	0.45
3:A:894:LEU:HA	3:A:899:SER:OG	2.16	0.45
3:A:1136:LYS:HE2	3:A:1139:VAL:CA	2.46	0.45
3:A:1252:LYS:HG3	3:A:1521:LYS:HE2	1.97	0.45
2:C:40:ILE:O	2:C:91:THR:HA	2.16	0.45
3:A:367:ASP:HB3	3:A:371:LYS:HB2	1.98	0.45
3:A:998:LYS:HD2	3:A:998:LYS:HA	1.78	0.45
3:A:1311:LEU:HG	3:A:1340:PRO:HG2	1.99	0.45
3:A:32:PRO:HB2	3:A:47:LEU:HD23	1.98	0.45
3:A:1814:PHE:CZ	3:A:1953:LYS:HB3	2.51	0.45
3:A:1965:TYR:O	3:A:1969:VAL:HG23	2.17	0.45
2:C:144:LEU:HD11	2:C:205:TYR:CE2	2.52	0.45
3:A:562:LYS:HE2	3:A:576:ASN:HD22	1.82	0.45
3:A:582:PRO:HA	3:A:585:GLN:HG2	1.99	0.45
3:A:859:ASN:N	3:A:891:ASP:OD2	2.46	0.45
3:A:971:ASN:HB3	3:A:1098:LYS:HG2	1.97	0.45
3:A:993:MET:HG3	3:A:994:LYS:N	2.30	0.45
3:A:1224:THR:OG1	3:A:1225:ASN:N	2.49	0.45
3:A:1325:ASN:HD21	3:A:1328:LYS:HG2	1.82	0.45
3:A:1409:GLU:HA	3:A:1412:MET:CB	2.46	0.45
1:B:166:ALA:HB3	2:C:137:PHE:HZ	1.82	0.45
3:A:111:GLU:HG2	3:A:179:LEU:HB2	1.98	0.45
3:A:1103:TRP:HA	3:A:1106:LYS:HB2	1.97	0.45
3:A:1855:GLU:O	3:A:1859:MET:HG3	2.17	0.45
3:A:1960:LYS:HA	3:A:1963:GLU:HG2	1.98	0.45
3:A:989:SER:H	3:A:1110:GLN:CD	2.21	0.45
3:A:1299:LYS:HB3	3:A:1303:ALA:HB2	1.98	0.45
1:B:200:GLN:HG2	1:B:204:LEU:O	2.17	0.45
2:C:208:HIS:O	2:C:230:ARG:NE	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:327:LYS:HA	3:A:327:LYS:HD2	1.76	0.45
3:A:690:LYS:O	3:A:690:LYS:HG2	2.16	0.45
3:A:935:LYS:HE2	3:A:938:SER:O	2.16	0.45
3:A:247:SER:OG	3:A:391:ASP:OD1	2.30	0.45
3:A:293:ASN:O	3:A:297:ASP:N	2.48	0.45
3:A:680:ASN:C	3:A:682:GLY:H	2.19	0.45
3:A:345:ASN:HD22	3:A:352:GLU:HG3	1.82	0.44
3:A:679:ASN:O	3:A:683:LYS:HG2	2.17	0.44
3:A:984:GLN:H	3:A:991:ARG:CB	2.30	0.44
3:A:1007:TYR:HB3	3:A:1010:VAL:HG12	1.99	0.44
2:C:161:ARG:HH12	2:C:182:VAL:HG11	1.81	0.44
3:A:509:ASN:HD22	3:A:513:SER:CB	2.31	0.44
3:A:1455:LYS:HB3	3:A:1543:TYR:OH	2.17	0.44
3:A:710:SER:O	3:A:714:THR:HG22	2.17	0.44
3:A:712:TRP:O	3:A:716:LYS:HB3	2.17	0.44
3:A:997:TYR:N	3:A:1003:GLU:HG3	2.24	0.44
3:A:1033:ASN:OD1	3:A:1958:LYS:HD2	2.17	0.44
3:A:1520:ASP:OD2	3:A:1521:LYS:N	2.50	0.44
3:A:1706:ASP:OD1	3:A:1794:GLN:NE2	2.29	0.44
3:A:1972:GLN:O	3:A:1976:ILE:HG13	2.18	0.44
1:B:116:ALA:HB1	1:B:129:LEU:HB3	1.98	0.44
3:A:64:TYR:CE1	3:A:109:ASN:HB2	2.52	0.44
3:A:691:LYS:O	3:A:692:ASN:C	2.55	0.44
3:A:843:SER:O	3:A:847:GLU:HG2	2.17	0.44
3:A:956:THR:O	3:A:958:TYR:N	2.47	0.44
3:A:975:CYS:SG	3:A:1099:CYS:HA	2.57	0.44
3:A:1109:ASP:OD2	3:A:1113:LYS:NZ	2.47	0.44
3:A:1201:LYS:NZ	3:A:1207:SER:OG	2.50	0.44
3:A:1946:VAL:HA	3:A:1951:ASP:OD1	2.17	0.44
1:B:230:LYS:HA	1:B:230:LYS:HD3	1.72	0.44
2:C:48:ILE:HA	3:A:510:LYS:HD2	1.99	0.44
3:A:201:TYR:N	3:A:202:PRO:HD3	2.32	0.44
3:A:657:ASP:OD2	3:A:761:ARG:NH2	2.43	0.44
3:A:867:ASN:C	3:A:867:ASN:ND2	2.71	0.44
3:A:1000:ASP:HA	3:A:1120:LYS:HD3	2.00	0.44
3:A:1347:VAL:O	3:A:1351:PHE:HB3	2.17	0.44
3:A:589:LEU:HD13	3:A:620:VAL:HG21	1.99	0.44
3:A:1058:ILE:HG21	3:A:1200:LYS:HD3	1.98	0.44
3:A:1100:TYR:C	3:A:1102:LEU:H	2.20	0.44
3:A:1130:ASN:OD1	3:A:1131:LYS:N	2.51	0.44
1:B:25:GLU:N	1:B:25:GLU:OE1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:34:GLU:HG2	3:A:37:TYR:HE1	1.83	0.44
3:A:150:ASN:N	3:A:238:LYS:HD3	2.33	0.44
3:A:184:LYS:HG3	3:A:207:TYR:CE2	2.53	0.44
3:A:940:SER:H	3:A:943:THR:CG2	2.31	0.44
1:B:170:LEU:HA	1:B:208:SER:HA	2.00	0.44
2:C:54:TRP:CE3	2:C:107:CYS:HB3	2.52	0.44
3:A:30:ALA:HB1	3:A:122:ASN:HA	2.00	0.44
3:A:285:GLU:HA	3:A:288:TYR:HB2	1.98	0.44
3:A:366:TYR:CE1	3:A:368:ASP:HB2	2.52	0.44
3:A:993:MET:HG3	3:A:994:LYS:H	1.83	0.44
3:A:1143:ASN:HB3	3:A:1973:LEU:CD2	2.48	0.44
3:A:7:ILE:HG22	3:A:387:TYR:CZ	2.52	0.44
3:A:561:LYS:HB2	3:A:561:LYS:HE3	1.75	0.44
3:A:1635:GLU:O	3:A:1638:PRO:HD2	2.18	0.44
3:A:1755:THR:HG23	3:A:1758:GLN:H	1.83	0.44
2:C:55:TYR:O	2:C:105:TYR:HA	2.18	0.43
3:A:1277:LEU:O	3:A:1287:ASN:HB3	2.18	0.43
3:A:1476:CYS:HB3	3:A:1484:LYS:HG3	2.00	0.43
1:B:32:ARG:HH21	1:B:142:SER:HA	1.83	0.43
2:C:159:TYR:CG	2:C:160:PRO:HA	2.53	0.43
3:A:561:LYS:CG	3:A:562:LYS:N	2.80	0.43
3:A:659:ILE:O	3:A:708:ARG:NH2	2.45	0.43
3:A:782:ILE:HD13	3:A:960:TYR:CE2	2.53	0.43
3:A:799:CYS:HB2	3:A:802:LYS:CA	2.45	0.43
3:A:945:VAL:O	3:A:945:VAL:HG13	2.18	0.43
3:A:1006:LYS:HZ1	3:A:1011:ASP:HA	1.82	0.43
3:A:1125:GLN:HB3	3:A:1129:ALA:HB3	1.98	0.43
3:A:1939:PRO:O	3:A:1942:LEU:N	2.33	0.43
1:B:175:PHE:CZ	1:B:176:PRO:HB3	2.53	0.43
3:A:25:ASP:N	3:A:25:ASP:OD1	2.50	0.43
3:A:80:TRP:C	3:A:81:LYS:HD2	2.38	0.43
3:A:235:LEU:O	3:A:238:LYS:HG3	2.17	0.43
3:A:251:LYS:HE2	3:A:566:ASN:OD1	2.17	0.43
3:A:288:TYR:OH	3:A:348:LYS:HD3	2.17	0.43
3:A:807:CYS:HB2	3:A:964:CYS:SG	2.59	0.43
3:A:1428:ASN:HB3	3:A:1431:ILE:HD11	2.01	0.43
3:A:1761:TRP:HE1	3:A:1765:GLN:HE21	1.65	0.43
2:C:149:ALA:HB3	2:C:200:LEU:N	2.30	0.43
3:A:97:CYS:HB2	3:A:291:LYS:HD3	1.99	0.43
3:A:181:LYS:HA	3:A:184:LYS:HB2	2.00	0.43
3:A:235:LEU:HA	3:A:258:LYS:CG	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:629:LYS:HD3	3:A:728:GLU:HG3	2.01	0.43
3:A:1335:ASP:HB2	3:A:1336:PRO:HD2	2.00	0.43
1:B:183:TRP:CH2	1:B:225:CYS:HB3	2.54	0.43
2:C:126:LYS:HA	2:C:159:TYR:OH	2.18	0.43
3:A:231:ARG:HG2	3:A:234:ASP:OD2	2.18	0.43
3:A:1268:ARG:NH1	3:A:1350:SER:HA	2.33	0.43
3:A:1305:HIS:CE1	3:A:1427:ASN:HD22	2.36	0.43
3:A:1355:LYS:HA	3:A:1358:ILE:HD12	2.00	0.43
3:A:1526:TYR:CE1	3:A:1538:LEU:HD22	2.54	0.43
3:A:1823:PRO:CB	3:A:1828:ASP:HB2	2.47	0.43
3:A:167:ARG:HG3	3:A:212:GLU:HA	2.01	0.43
3:A:897:PRO:O	3:A:901:LEU:HB2	2.18	0.43
3:A:1136:LYS:HE2	3:A:1140:SER:N	2.30	0.43
3:A:1227:ILE:HG13	3:A:1299:LYS:HE3	2.00	0.43
3:A:1866:ILE:HD11	3:A:1880:TYR:CE1	2.54	0.43
3:A:38:TYR:HD2	3:A:59:SER:HA	1.84	0.43
3:A:763:LEU:HD13	3:A:838:ILE:HG21	2.01	0.43
3:A:850:LYS:HE3	3:A:890:ILE:HG21	1.99	0.43
3:A:934:ASP:O	3:A:935:LYS:HB2	2.18	0.43
3:A:1422:LYS:HB3	3:A:1422:LYS:HE3	1.81	0.43
1:B:113:TYR:O	1:B:135:GLY:HA2	2.18	0.43
3:A:8:ALA:N	3:A:387:TYR:OH	2.46	0.43
3:A:102:ARG:HA	3:A:105:LEU:HD12	2.01	0.43
3:A:588:TYR:CD2	3:A:620:VAL:HG23	2.54	0.43
3:A:1146:PHE:CD2	3:A:1184:SER:HB3	2.53	0.43
3:A:1164:LYS:HD3	3:A:1972:GLN:CD	2.39	0.43
3:A:1297:LYS:HE2	3:A:1297:LYS:HB3	1.87	0.43
3:A:1297:LYS:HG2	3:A:1301:LYS:HE2	2.01	0.43
2:C:147:GLY:HA2	2:C:202:LYS:NZ	2.34	0.43
3:A:35:VAL:HB	3:A:36:GLU:OE1	2.19	0.43
3:A:624:GLU:HB2	3:A:655:TYR:OH	2.19	0.43
3:A:905:LEU:HD23	3:A:905:LEU:HA	1.85	0.43
3:A:982:MET:SD	3:A:982:MET:N	2.92	0.43
3:A:1209:ASP:HA	3:A:1210:THR:HA	1.80	0.43
3:A:1346:ALA:O	3:A:1351:PHE:N	2.37	0.43
2:C:166:GLN:NE2	2:C:167:TRP:H	2.17	0.42
3:A:338:THR:HG22	3:A:338:THR:O	2.19	0.42
3:A:567:GLU:CD	3:A:567:GLU:H	2.21	0.42
3:A:1047:GLU:OE2	3:A:1194:LYS:HE3	2.19	0.42
3:A:1507:LYS:HG3	3:A:1508:TYR:N	2.33	0.42
3:A:1933:CYS:CB	3:A:1934:GLU:HA	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:PHE:CD2	1:B:96:SER:HA	2.54	0.42
2:C:122:ARG:HH22	2:C:161:ARG:HE	1.67	0.42
2:C:199:THR:O	2:C:200:LEU:HD23	2.19	0.42
3:A:69:LYS:HE2	3:A:69:LYS:HB3	1.86	0.42
3:A:604:ASP:OD1	3:A:604:ASP:N	2.52	0.42
3:A:618:LEU:HD13	3:A:722:ALA:HB2	2.00	0.42
3:A:637:ASN:OD1	3:A:638:SER:N	2.52	0.42
3:A:680:ASN:O	3:A:682:GLY:N	2.52	0.42
3:A:862:THR:HG21	3:A:890:ILE:HG13	2.00	0.42
3:A:1164:LYS:HD3	3:A:1972:GLN:NE2	2.34	0.42
3:A:1409:GLU:HA	3:A:1412:MET:H	1.83	0.42
3:A:1584:TYR:CE2	3:A:1769:ARG:HD2	2.54	0.42
3:A:1929:LYS:HA	3:A:1930:GLU:HA	1.62	0.42
1:B:61:GLY:O	1:B:62:LYS:HD2	2.19	0.42
2:C:132:PRO:HB3	2:C:158:PHE:HB3	2.01	0.42
3:A:29:LYS:HA	3:A:218:ASN:ND2	2.34	0.42
3:A:683:LYS:HE3	3:A:683:LYS:HB3	1.68	0.42
3:A:727:ALA:O	3:A:728:GLU:HG3	2.19	0.42
3:A:853:ARG:O	3:A:868:ALA:N	2.52	0.42
3:A:980:GLU:HB2	3:A:981:TYR:CE2	2.54	0.42
3:A:1266:PRO:O	3:A:1270:GLN:HG3	2.19	0.42
3:A:1556:ASN:HB2	3:A:1561:TYR:CD2	2.55	0.42
1:B:120:ARG:HG2	3:A:914:LYS:HB3	2.01	0.42
2:C:174:GLN:HB3	2:C:177:ASN:HD21	1.83	0.42
3:A:101:ARG:HD2	3:A:158:SER:OG	2.19	0.42
3:A:325:LYS:O	3:A:329:TYR:CB	2.48	0.42
3:A:344:GLU:HA	3:A:347:TYR:CD2	2.55	0.42
3:A:802:LYS:O	3:A:804:LYS:N	2.52	0.42
3:A:1216:GLU:HB3	3:A:1218:SER:H	1.83	0.42
3:A:1261:ASN:O	3:A:1525:LYS:HG3	2.19	0.42
3:A:1394:VAL:HA	3:A:1397:SER:HB3	2.01	0.42
1:B:37:LEU:HD23	1:B:138:VAL:HG13	2.00	0.42
3:A:81:LYS:HA	3:A:94:GLU:HA	2.01	0.42
3:A:346:LYS:HD3	3:A:346:LYS:N	2.34	0.42
3:A:376:LYS:HA	3:A:381:TYR:O	2.19	0.42
3:A:593:PRO:O	3:A:676:ASN:ND2	2.52	0.42
3:A:689:ILE:HA	3:A:701:TYR:O	2.20	0.42
3:A:731:ILE:HG23	3:A:732:THR:N	2.33	0.42
3:A:850:LYS:NZ	3:A:890:ILE:HG21	2.34	0.42
3:A:857:THR:OG1	3:A:872:THR:HB	2.19	0.42
3:A:1174:GLU:HG2	3:A:1175:PHE:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1464:GLU:HG3	3:A:1511:TYR:OH	2.19	0.42
3:A:104:ARG:HA	3:A:108:TYR:OH	2.20	0.42
3:A:342:ASN:O	3:A:345:ASN:HB2	2.20	0.42
3:A:497:ASP:HB2	3:A:526:GLU:OE2	2.20	0.42
3:A:610:LYS:N	3:A:684:LEU:HD11	2.35	0.42
3:A:1288:ILE:O	3:A:1288:ILE:HG13	2.20	0.42
3:A:1318:GLY:HA2	3:A:1323:SER:OG	2.20	0.42
3:A:1635:GLU:HB2	3:A:1661:VAL:CG2	2.50	0.42
3:A:1225:ASN:HB2	3:A:1295:LEU:HD21	2.01	0.42
3:A:1307:GLU:O	3:A:1307:GLU:HG3	2.19	0.42
3:A:1914:ALA:O	3:A:1953:LYS:HG3	2.20	0.42
3:A:194:ASP:HB2	3:A:197:LEU:HD11	2.02	0.42
3:A:332:CYS:SG	3:A:335:LYS:HB3	2.59	0.42
3:A:344:GLU:OE2	3:A:348:LYS:HE2	2.20	0.42
3:A:380:ASN:OD1	3:A:381:TYR:N	2.52	0.42
3:A:529:LYS:HG3	3:A:530:LYS:N	2.30	0.42
3:A:690:LYS:C	3:A:692:ASN:N	2.73	0.42
3:A:798:GLU:HB2	3:A:966:CYS:SG	2.60	0.42
3:A:853:ARG:O	3:A:869:ALA:N	2.43	0.42
3:A:949:VAL:O	3:A:949:VAL:HG13	2.20	0.42
3:A:1273:CYS:SG	3:A:1306:LYS:NZ	2.69	0.42
3:A:1397:SER:OG	3:A:1398:THR:N	2.53	0.42
3:A:1409:GLU:O	3:A:1413:TRP:HB2	2.20	0.42
3:A:1981:LYS:HE2	3:A:1988:LEU:HD23	2.01	0.42
2:C:155:LEU:HB2	2:C:194:LEU:HB3	2.02	0.42
3:A:7:ILE:HG12	3:A:7:ILE:O	2.19	0.42
3:A:8:ALA:H	3:A:387:TYR:HH	1.67	0.42
3:A:279:TRP:HA	3:A:282:GLU:HB3	2.02	0.42
3:A:1125:GLN:HB3	3:A:1129:ALA:HB2	2.01	0.42
3:A:1125:GLN:CA	3:A:1128:ASP:H	2.27	0.42
3:A:1300:ILE:HD13	3:A:1351:PHE:CE1	2.54	0.42
3:A:1484:LYS:HG2	3:A:1573:ILE:O	2.19	0.42
1:B:50:ASP:HA	1:B:72:TRP:HB2	2.02	0.42
3:A:39:ARG:HG2	3:A:115:PHE:CE2	2.55	0.42
3:A:928:LYS:HG3	3:A:931:LYS:O	2.20	0.42
3:A:1106:LYS:HB3	3:A:1106:LYS:HE3	1.75	0.42
3:A:1129:ALA:HA	3:A:1132:GLY:H	1.85	0.42
3:A:1308:THR:HA	3:A:1311:LEU:H	1.85	0.42
3:A:1315:HIS:HA	3:A:1323:SER:HB3	2.02	0.42
3:A:1833:ASN:CB	3:A:1838:CYS:HB3	2.50	0.42
3:A:1839:LYS:HD3	3:A:1968:HIS:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:274:PRO:HG2	3:A:373:PHE:CE2	2.55	0.41
3:A:1059:ASP:CG	3:A:1096:LYS:HD3	2.40	0.41
3:A:1919:SER:HA	3:A:1920:GLY:HA2	1.49	0.41
3:A:1982:ASP:HA	3:A:1990:ARG:C	2.40	0.41
3:A:365:ARG:NH1	3:A:374:PHE:HB2	2.23	0.41
3:A:688:TYR:O	3:A:700:SER:HB2	2.20	0.41
3:A:932:GLU:OE2	3:A:936:SER:OG	2.29	0.41
3:A:995:ARG:NH1	3:A:997:TYR:OH	2.53	0.41
3:A:1124:LYS:O	3:A:1128:ASP:N	2.53	0.41
3:A:1696:TYR:CD1	3:A:1791:ALA:HB2	2.54	0.41
3:A:1988:LEU:CG	3:A:1989:ASP:H	2.30	0.41
3:A:67:CYS:HA	3:A:108:TYR:HD2	1.85	0.41
3:A:236:LEU:HD22	3:A:260:GLY:H	1.85	0.41
3:A:287:PHE:HA	3:A:291:LYS:HZ3	1.85	0.41
3:A:342:ASN:HA	3:A:345:ASN:ND2	2.36	0.41
3:A:986:SER:HA	3:A:993:MET:HB3	2.02	0.41
3:A:1311:LEU:O	3:A:1316:ASP:N	2.53	0.41
3:A:1365:ILE:O	3:A:1365:ILE:HG23	2.20	0.41
1:B:179:VAL:HG12	1:B:229:HIS:HA	2.03	0.41
3:A:975:CYS:SG	3:A:1102:LEU:HD23	2.60	0.41
3:A:1617:ARG:HD3	3:A:1617:ARG:HA	1.72	0.41
3:A:1922:VAL:HG23	3:A:1922:VAL:O	2.20	0.41
3:A:339:GLU:HA	3:A:343:GLN:CB	2.50	0.41
3:A:1469:GLU:O	3:A:1473:ARG:HG2	2.20	0.41
3:A:1741:TRP:O	3:A:1746:THR:OG1	2.35	0.41
3:A:65:ASP:O	3:A:109:ASN:HB3	2.21	0.41
3:A:1041:GLU:OE1	3:A:1853:ARG:NH2	2.52	0.41
3:A:1097:CYS:HA	3:A:1101:LYS:HE3	2.03	0.41
3:A:1201:LYS:HD3	3:A:1201:LYS:HA	1.76	0.41
3:A:1626:PRO:HA	3:A:1629:GLN:HG2	2.02	0.41
3:A:7:ILE:HG13	3:A:376:LYS:HB2	2.02	0.41
3:A:97:CYS:HB2	3:A:291:LYS:CE	2.51	0.41
3:A:344:GLU:HA	3:A:347:TYR:CB	2.45	0.41
3:A:365:ARG:HH21	3:A:370:VAL:HG22	1.85	0.41
3:A:380:ASN:CG	3:A:381:TYR:H	2.23	0.41
3:A:687:LYS:HD2	3:A:688:TYR:CD2	2.55	0.41
3:A:1092:ASN:C	3:A:1094:LYS:H	2.23	0.41
3:A:1420:ILE:HA	3:A:1423:ILE:HD12	2.02	0.41
3:A:1572:SER:O	3:A:1642:LYS:HD2	2.20	0.41
3:A:1698:LEU:HD12	3:A:1698:LEU:HA	1.84	0.41
3:A:1978:ASN:HA	3:A:1981:LYS:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:TYR:OH	1:B:207:LEU:HD23	2.21	0.41
1:B:185:SER:H	1:B:226:ASN:ND2	2.19	0.41
3:A:284:ILE:O	3:A:287:PHE:HB3	2.21	0.41
3:A:1136:LYS:CE	3:A:1140:SER:H	2.31	0.41
3:A:1227:ILE:HD13	3:A:1276:GLU:OE2	2.20	0.41
3:A:1236:ASP:O	3:A:1243:LYS:NZ	2.31	0.41
3:A:1276:GLU:O	3:A:1287:ASN:ND2	2.53	0.41
3:A:1317:THR:HA	3:A:1330:GLN:NE2	2.35	0.41
1:B:175:PHE:CE2	1:B:176:PRO:HB3	2.56	0.41
2:C:108:GLN:HG3	2:C:117:PHE:CZ	2.55	0.41
2:C:169:VAL:HG13	2:C:211:TYR:HE1	1.86	0.41
3:A:25:ASP:O	3:A:29:LYS:HG3	2.21	0.41
3:A:109:ASN:OD1	3:A:110:LEU:N	2.52	0.41
3:A:111:GLU:HG2	3:A:179:LEU:HD22	2.03	0.41
3:A:236:LEU:CB	3:A:260:GLY:H	2.34	0.41
3:A:412:ASN:HB3	3:A:413:PRO:HD2	2.02	0.41
3:A:533:LYS:HB3	3:A:534:VAL:H	1.65	0.41
3:A:559:ILE:C	3:A:561:LYS:N	2.74	0.41
3:A:696:GLU:C	3:A:699:THR:HB	2.41	0.41
3:A:698:ASP:N	3:A:699:THR:CB	2.81	0.41
3:A:720:TRP:NE1	3:A:724:LYS:HE2	2.35	0.41
3:A:925:THR:N	3:A:946:VAL:N	2.66	0.41
3:A:1019:SER:OG	3:A:1026:GLY:HA2	2.21	0.41
3:A:1049:TYR:O	3:A:1053:ALA:HA	2.19	0.41
3:A:1058:ILE:HA	3:A:1059:ASP:HA	1.67	0.41
3:A:1174:GLU:O	3:A:1177:ILE:HG13	2.21	0.41
3:A:1221:LEU:HB3	3:A:1224:THR:HA	2.02	0.41
3:A:1379:ILE:O	3:A:1382:LYS:HG2	2.21	0.41
1:B:46:PHE:CE1	1:B:117:ARG:NE	2.88	0.41
2:C:55:TYR:CE1	2:C:108:GLN:HB3	2.56	0.41
2:C:201:SER:O	2:C:205:TYR:HB2	2.21	0.41
3:A:1029:VAL:HG21	3:A:1959:MET:CE	2.50	0.41
3:A:1355:LYS:O	3:A:1358:ILE:HB	2.21	0.41
3:A:1588:GLU:HG2	3:A:1770:TYR:OH	2.21	0.41
3:A:1933:CYS:HB2	3:A:1935:GLU:HA	2.03	0.41
2:C:34:ILE:HD12	2:C:34:ILE:H	1.85	0.40
3:A:34:GLU:OE1	3:A:34:GLU:N	2.55	0.40
3:A:334:LYS:HA	3:A:338:THR:OG1	2.21	0.40
3:A:562:LYS:O	3:A:563:SER:C	2.60	0.40
3:A:935:LYS:HG2	3:A:938:SER:C	2.42	0.40
3:A:1247:LYS:HD2	3:A:1271:ASN:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:ILE:HG13	1:B:77:LYS:HG2	2.03	0.40
3:A:156:GLU:OE1	3:A:270:LEU:HD22	2.21	0.40
3:A:529:LYS:HE3	3:A:718:TYR:CZ	2.56	0.40
3:A:1322:ILE:H	3:A:1322:ILE:HD12	1.86	0.40
3:A:1663:GLU:HB2	3:A:1763:ALA:HB1	2.04	0.40
3:A:1884:MET:O	3:A:1884:MET:HG2	2.20	0.40
3:A:1912:ILE:HG12	3:A:1913:GLY:N	2.37	0.40
3:A:344:GLU:C	3:A:347:TYR:H	2.25	0.40
3:A:853:ARG:HH22	3:A:866:THR:HG22	1.86	0.40
3:A:1294:GLU:O	3:A:1297:LYS:HB3	2.22	0.40
3:A:1313:GLU:HA	3:A:1317:THR:HG23	2.03	0.40
3:A:1612:LYS:HB2	3:A:1612:LYS:HE2	1.68	0.40
3:A:1943:MET:HA	3:A:1946:VAL:HG12	2.03	0.40
1:B:102:MET:HE3	1:B:105:LEU:HD21	2.04	0.40
3:A:277:LEU:HD13	3:A:373:PHE:CE1	2.56	0.40
3:A:560:TRP:HH2	3:A:838:ILE:HG13	1.87	0.40
3:A:584:THR:O	3:A:587:LEU:HG	2.22	0.40
3:A:731:ILE:HG23	3:A:732:THR:H	1.85	0.40
3:A:1045:GLN:NE2	3:A:1049:TYR:CD2	2.90	0.40
3:A:1109:ASP:O	3:A:1113:LYS:HG2	2.22	0.40
3:A:1424:ASN:O	3:A:1431:ILE:HG12	2.21	0.40
3:A:1596:CYS:HB2	3:A:1668:TYR:CD2	2.56	0.40
3:A:1697:ASP:O	3:A:1701:ILE:HG13	2.22	0.40
3:A:496:GLN:HB3	3:A:497:ASP:H	1.74	0.40
3:A:925:THR:O	3:A:946:VAL:CG1	2.70	0.40
3:A:1296:LEU:O	3:A:1300:ILE:HG13	2.22	0.40
3:A:1688:CYS:O	3:A:1692:ARG:HG2	2.22	0.40
3:A:1966:LEU:HD13	3:A:1966:LEU:HA	1.79	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	B	219/472 (46%)	205 (94%)	14 (6%)	0	100	100
2	C	210/233 (90%)	189 (90%)	21 (10%)	0	100	100
3	A	1843/2040 (90%)	1512 (82%)	305 (16%)	26 (1%)	9	37
All	All	2272/2745 (83%)	1906 (84%)	340 (15%)	26 (1%)	15	44

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	563	SER
3	A	566	ASN
3	A	683	LYS
3	A	690	LYS
3	A	699	THR
3	A	966	CYS
3	A	967	LYS
3	A	533	LYS
3	A	561	LYS
3	A	564	SER
3	A	695	ALA
3	A	512	GLY
3	A	525	ASP
3	A	556	LYS
3	A	571	GLN
3	A	687	LYS
3	A	688	TYR
3	A	691	LYS
3	A	702	SER
3	A	93	PRO
3	A	350	LEU
3	A	514	SER
3	A	965	GLN
3	A	906	ASP
3	A	237	ILE
3	A	682	GLY

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	181/411 (44%)	180 (99%)	1 (1%)	84	93
2	C	184/201 (92%)	182 (99%)	2 (1%)	70	87
3	A	1674/1839 (91%)	1644 (98%)	30 (2%)	54	80
All	All	2039/2451 (83%)	2006 (98%)	33 (2%)	58	82

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	22	ARG
2	C	109	LYS
2	C	143	GLN
3	A	29	LYS
3	A	138	LYS
3	A	198	GLN
3	A	514	SER
3	A	530	LYS
3	A	555	LYS
3	A	556	LYS
3	A	557	LYS
3	A	559	ILE
3	A	561	LYS
3	A	562	LYS
3	A	568	GLU
3	A	683	LYS
3	A	687	LYS
3	A	689	ILE
3	A	690	LYS
3	A	691	LYS
3	A	693	ASN
3	A	694	THR
3	A	696	GLU
3	A	699	THR
3	A	700	SER
3	A	858	LYS
3	A	867	ASN
3	A	890	ILE
3	A	1156	LYS
3	A	1490	LYS
3	A	1503	ARG
3	A	1628	ARG

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Mol	Chain	Res	Type
3	A	1980	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	198	GLN
3	A	353	GLN
3	A	509	ASN
3	A	1114	GLN
3	A	1305	HIS
3	A	1315	HIS
3	A	1348	GLN
3	A	1400	ASN
3	A	1427	ASN
3	A	1957	HIS
3	A	1972	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 ⓘ

There are no chain breaks in this entry.

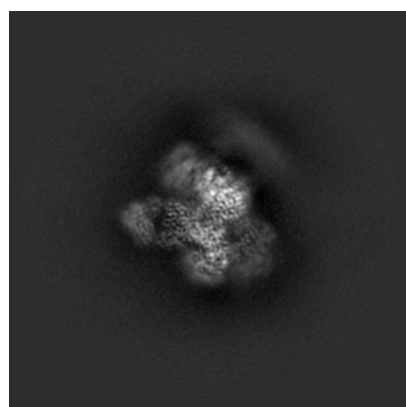
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14438. These allow visual inspection of the internal detail of the map and identification of artifacts.

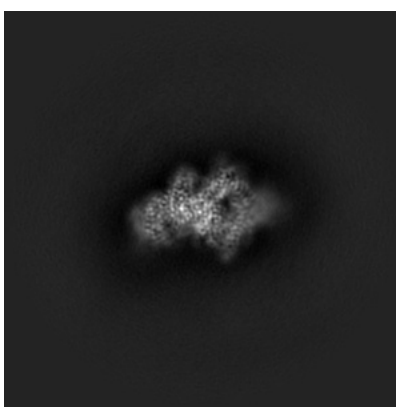
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

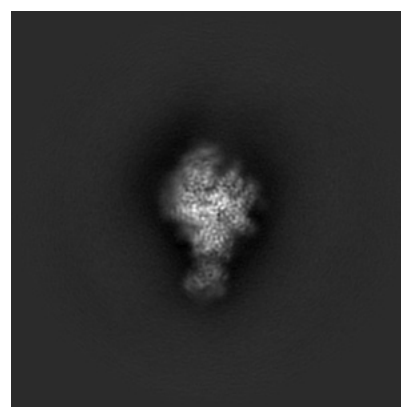
6.1.1 Primary map



X



Y

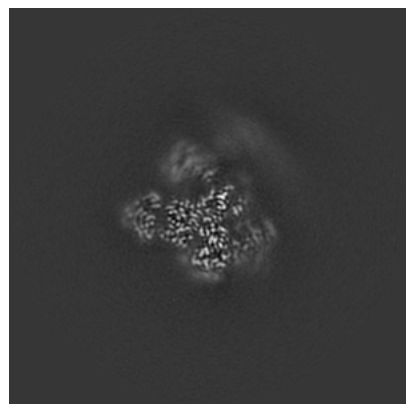


Z

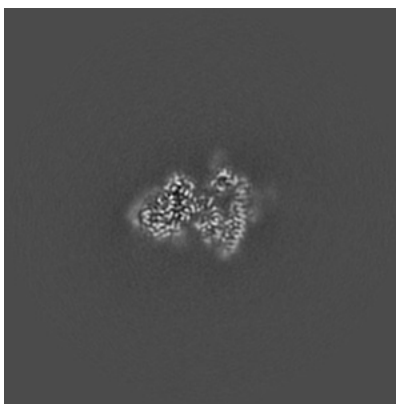
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

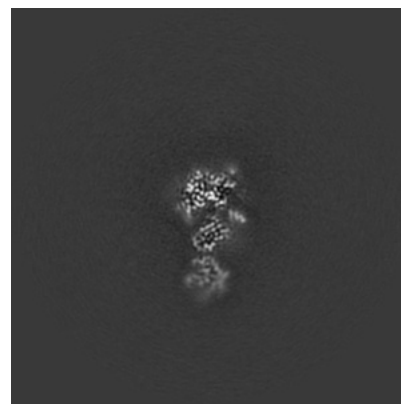
6.2.1 Primary map



X Index: 220



Y Index: 220

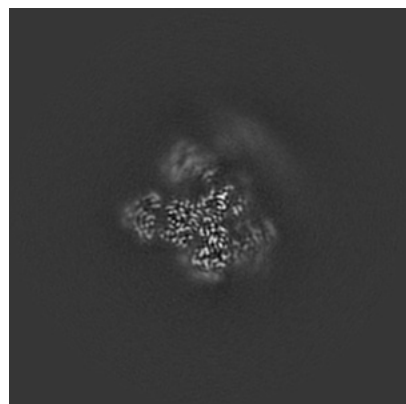


Z Index: 220

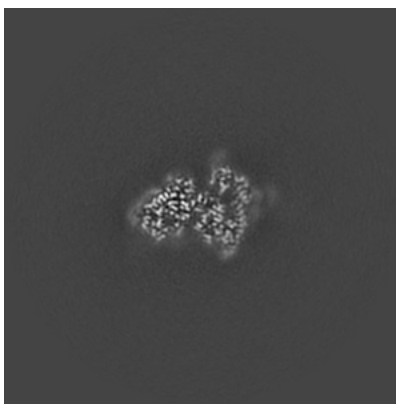
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

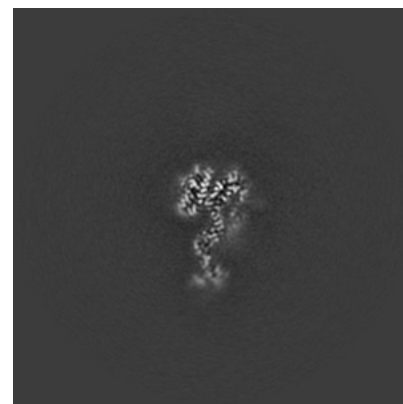
6.3.1 Primary map



X Index: 220



Y Index: 223

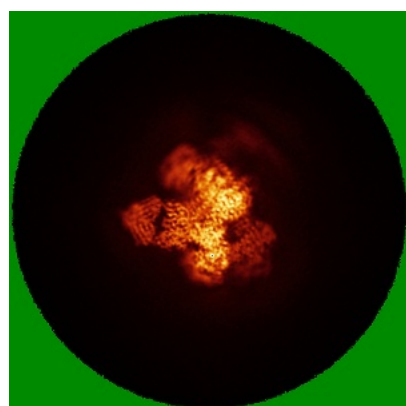


Z Index: 225

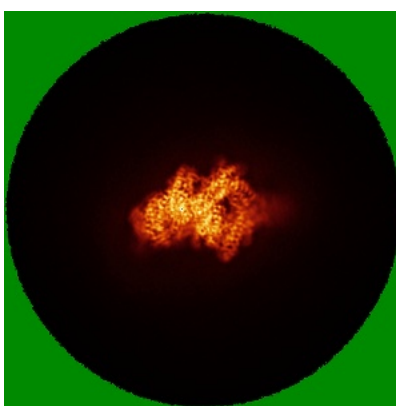
The images above show the largest variance slices of the map in three orthogonal directions.

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

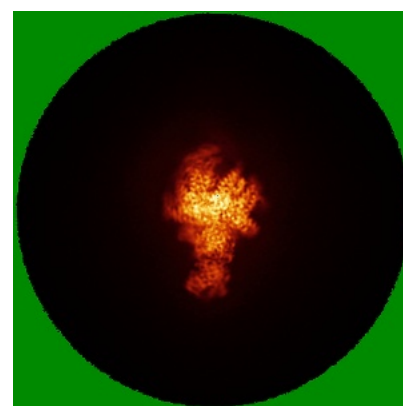
6.4.1 Primary map



X



Y

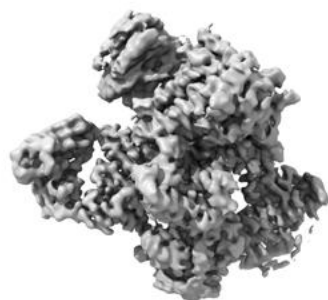


Z

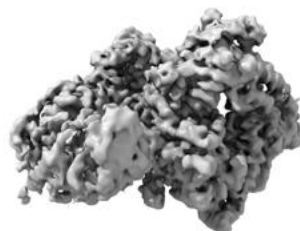
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

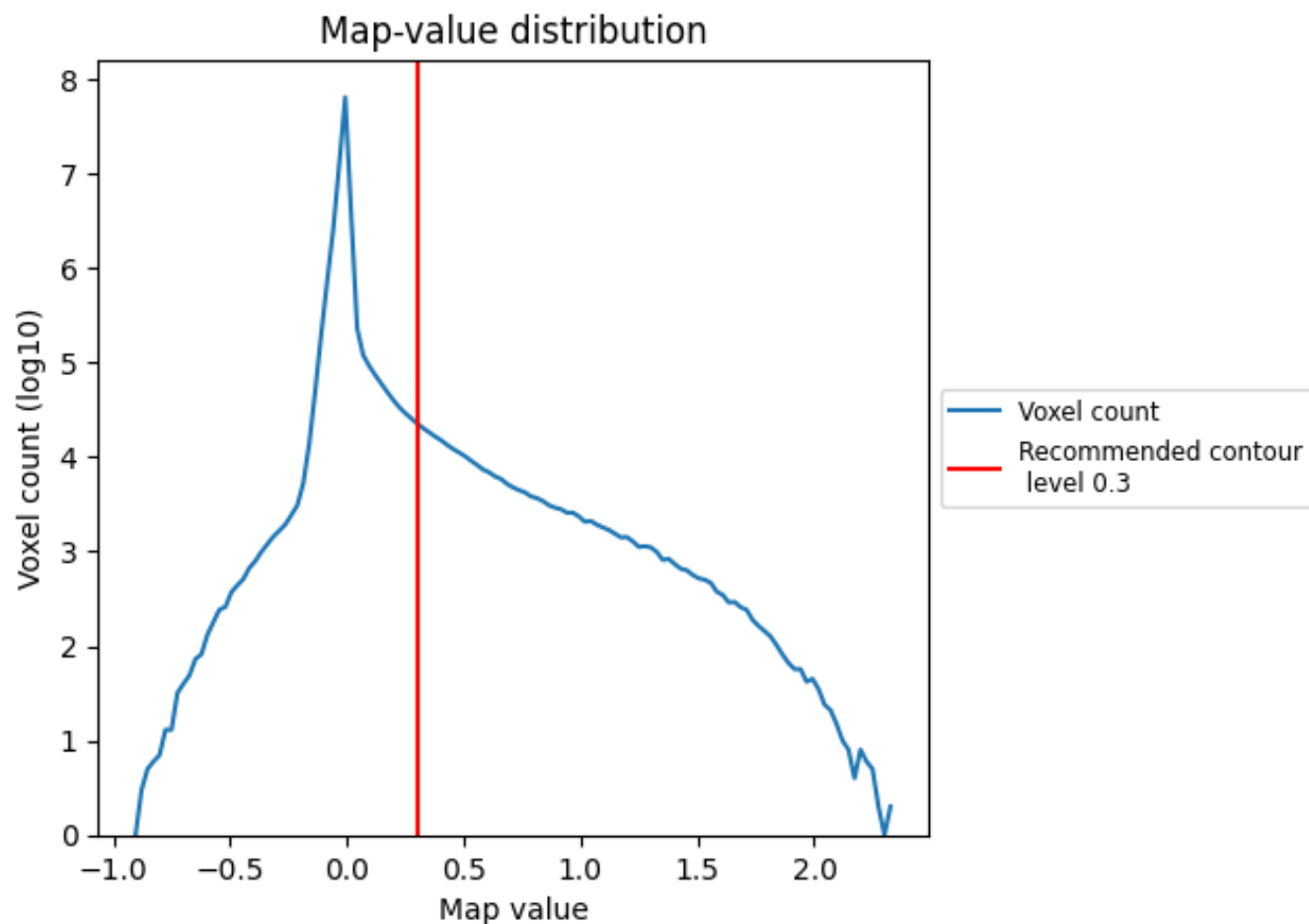
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

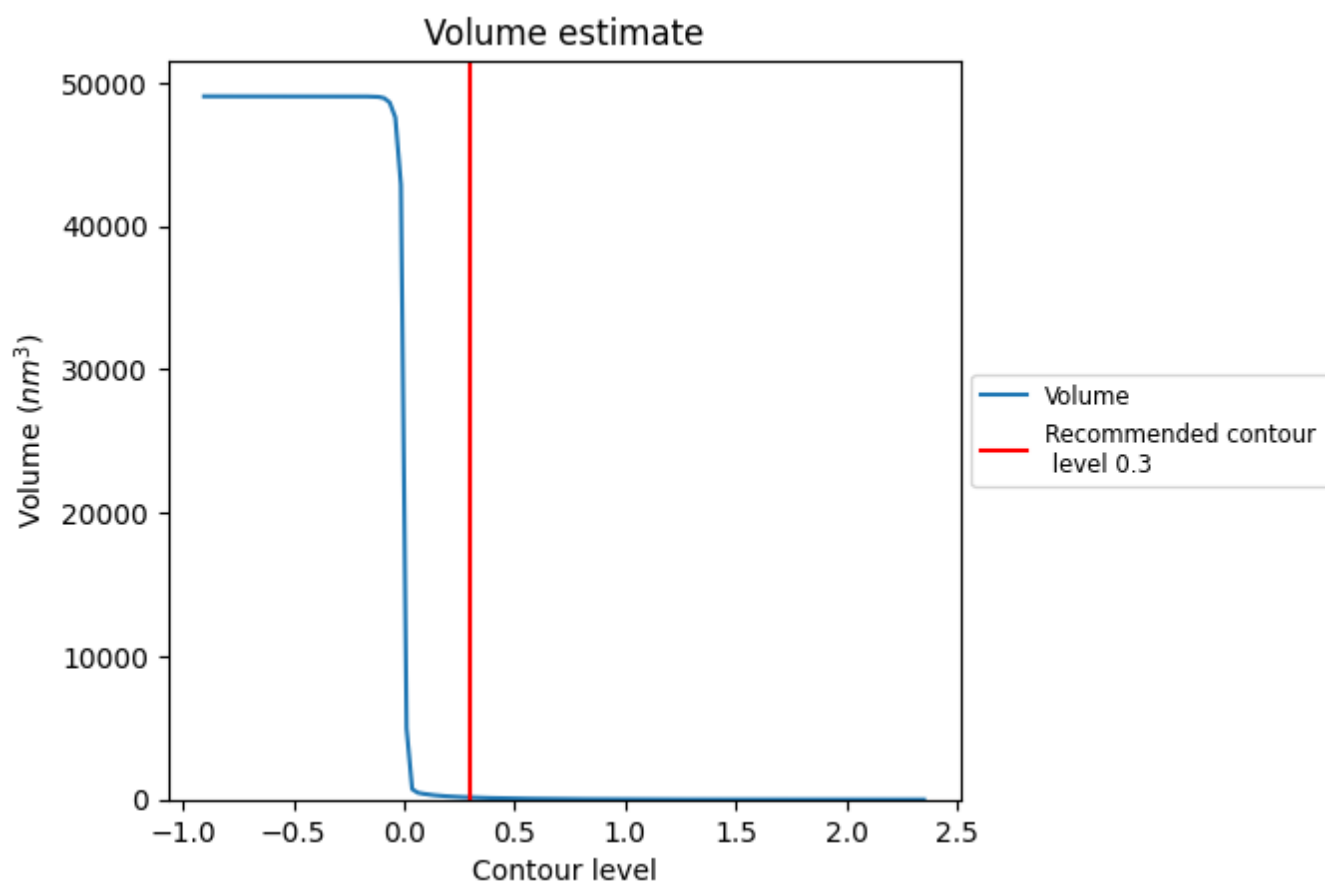
This section contains the results of statistical analysis of the map.

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.

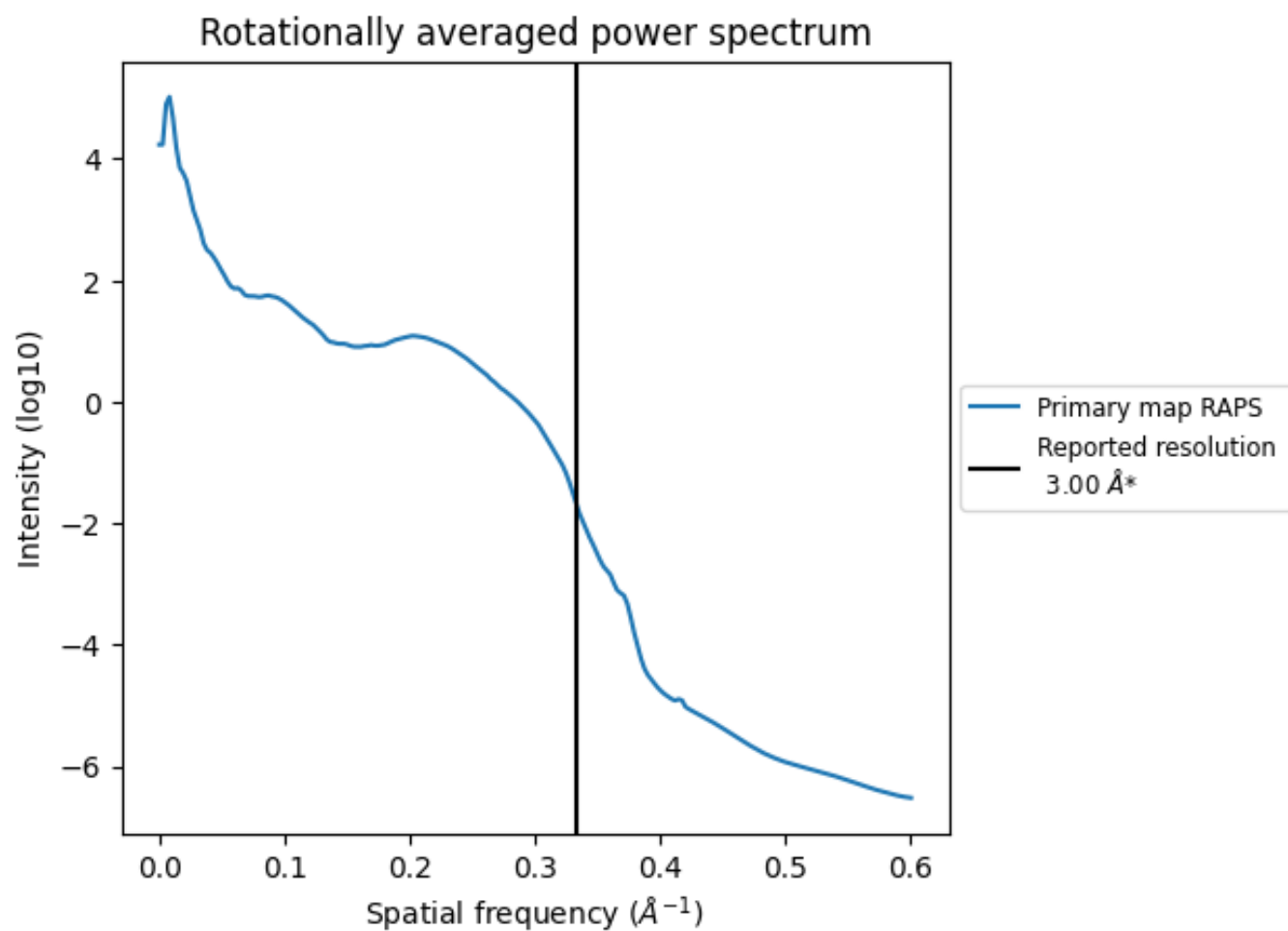
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 149 nm³; this corresponds to an approximate mass of 134 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 ⓘ

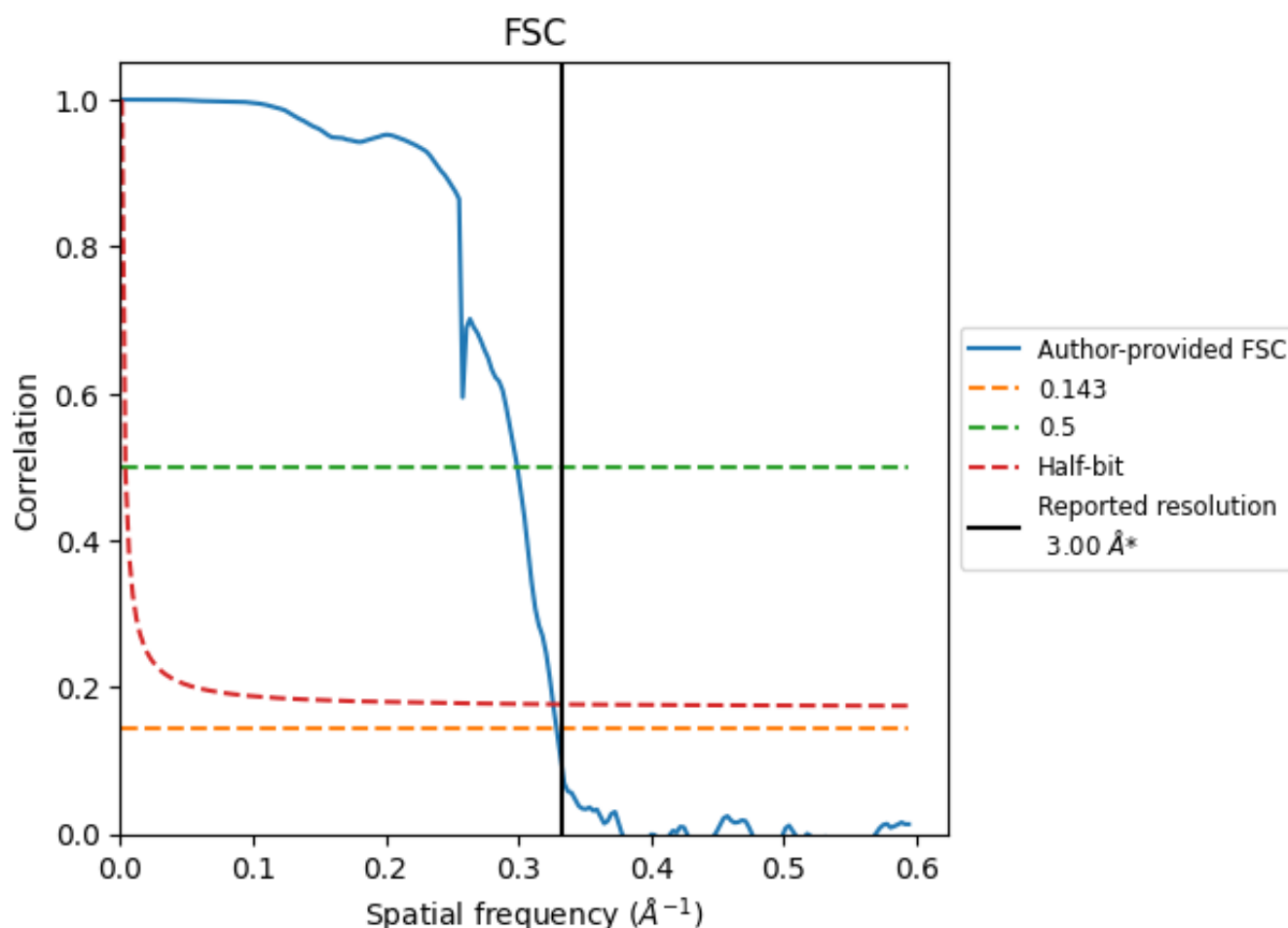


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

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 0.333 Å⁻¹

8.2 Resolution estimates [i](#)

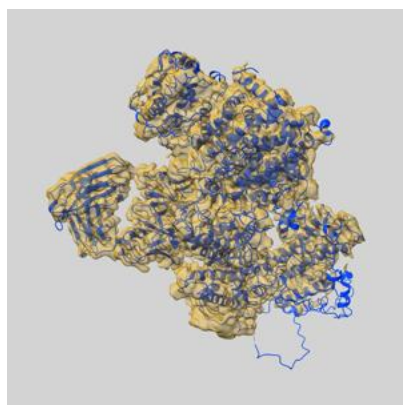
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.04	3.34	3.06
Unmasked-calculated*	-	-	-

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

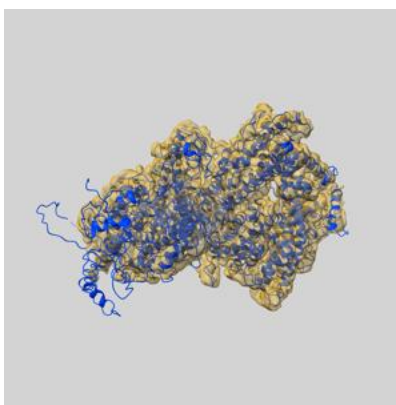
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14438 and PDB model 7Z12. Per-residue inclusion information can be found in section [3](#) on page [4](#).

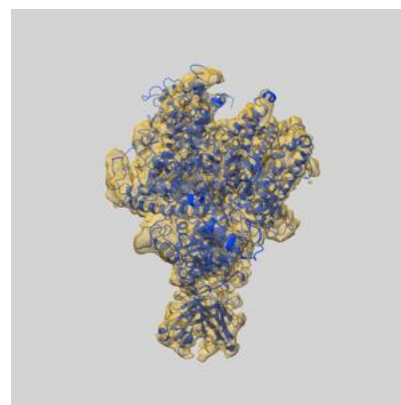
9.1 Map-model overlay [i](#)



X



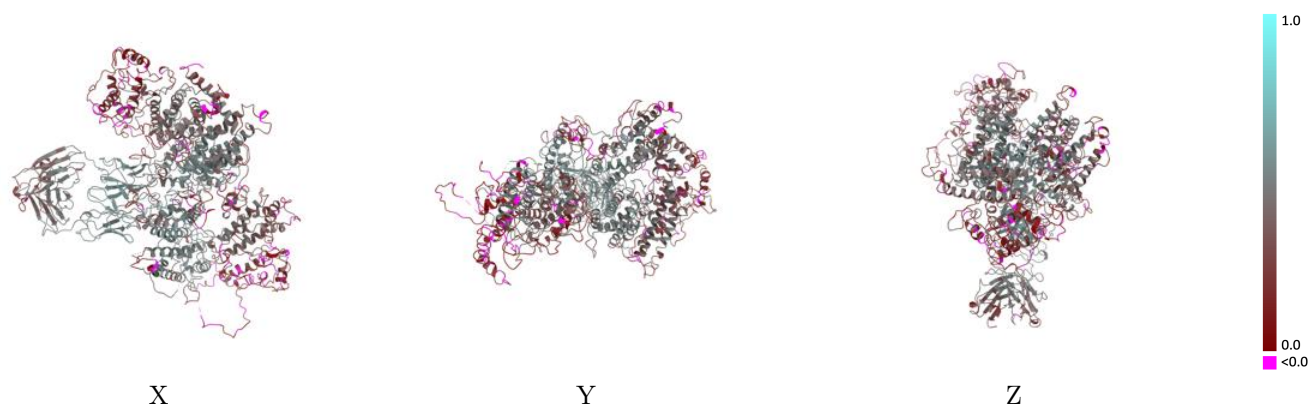
Y



Z

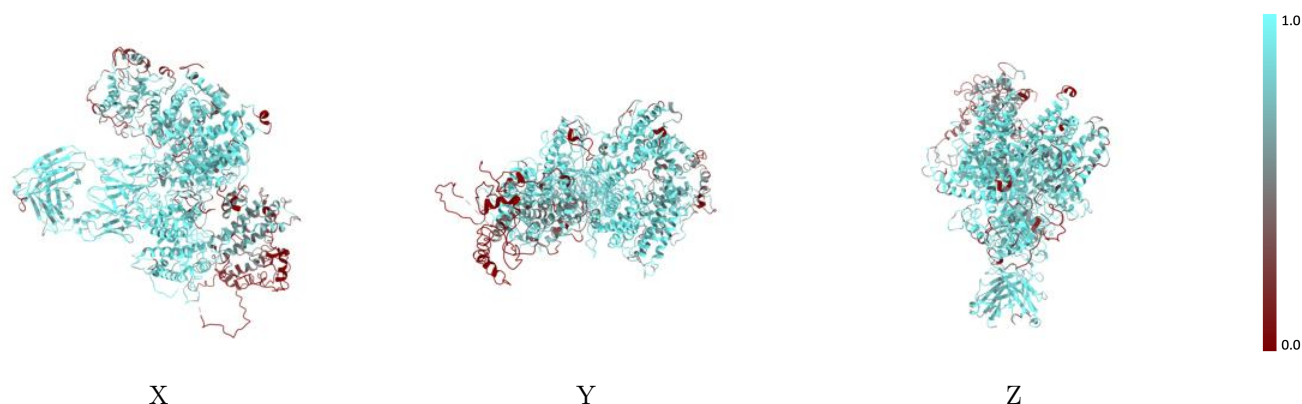
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



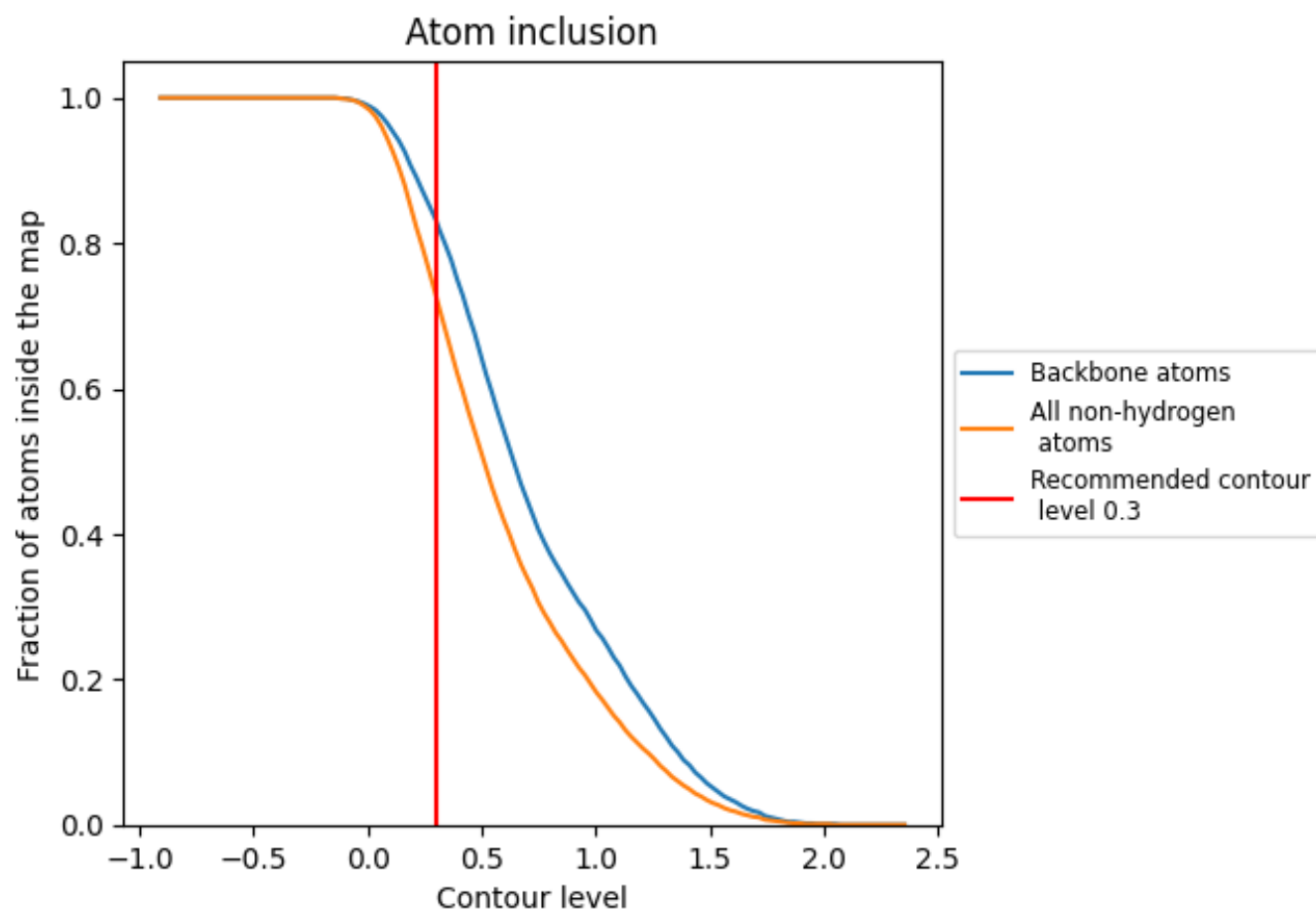
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.3).

9.4 Atom inclusion ⓘ



At the recommended contour level, 83% of all backbone atoms, 73% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7280	<div></div> 0.3620
A	<div></div> 0.6940	<div></div> 0.3360
B	<div></div> 0.8900	<div></div> 0.4880
C	<div></div> 0.8770	<div></div> 0.4750

