



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 05:27 PM UTC

PDB ID : 9JW1 / pdb_00009jw1
EMDB ID : EMD-61848
Title : Cryo-EM structure of Human RNF213
Authors : Zhang, H.
Deposited on : 2024-10-09
Resolution : 3.46 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

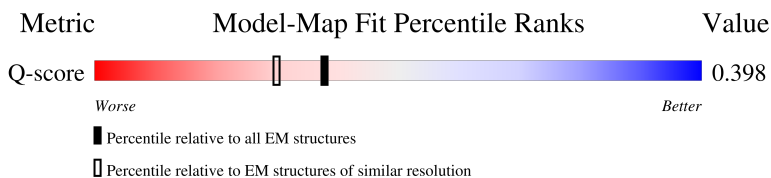
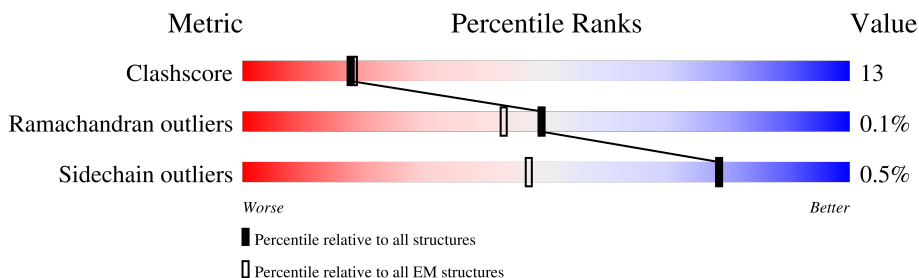
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.46 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13788 (2.96 - 3.96)

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	4841	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 35937 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.

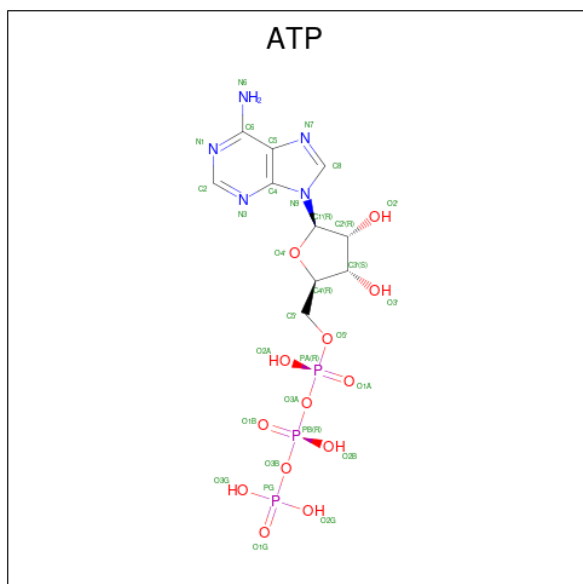
- Molecule 1 is a protein called Ring finger protein 213.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	4471	35905	22894	6203	6590	218	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	367	GLY	-	expression tag	UNP A0A0A0MTC1
A	368	PRO	-	expression tag	UNP A0A0A0MTC1
A	369	GLY	-	expression tag	UNP A0A0A0MTC1
A	370	THR	-	expression tag	UNP A0A0A0MTC1
A	2927	VAL	ARG	conflict	UNP A0A0A0MTC1
A	2928	ALA	VAL	conflict	UNP A0A0A0MTC1

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



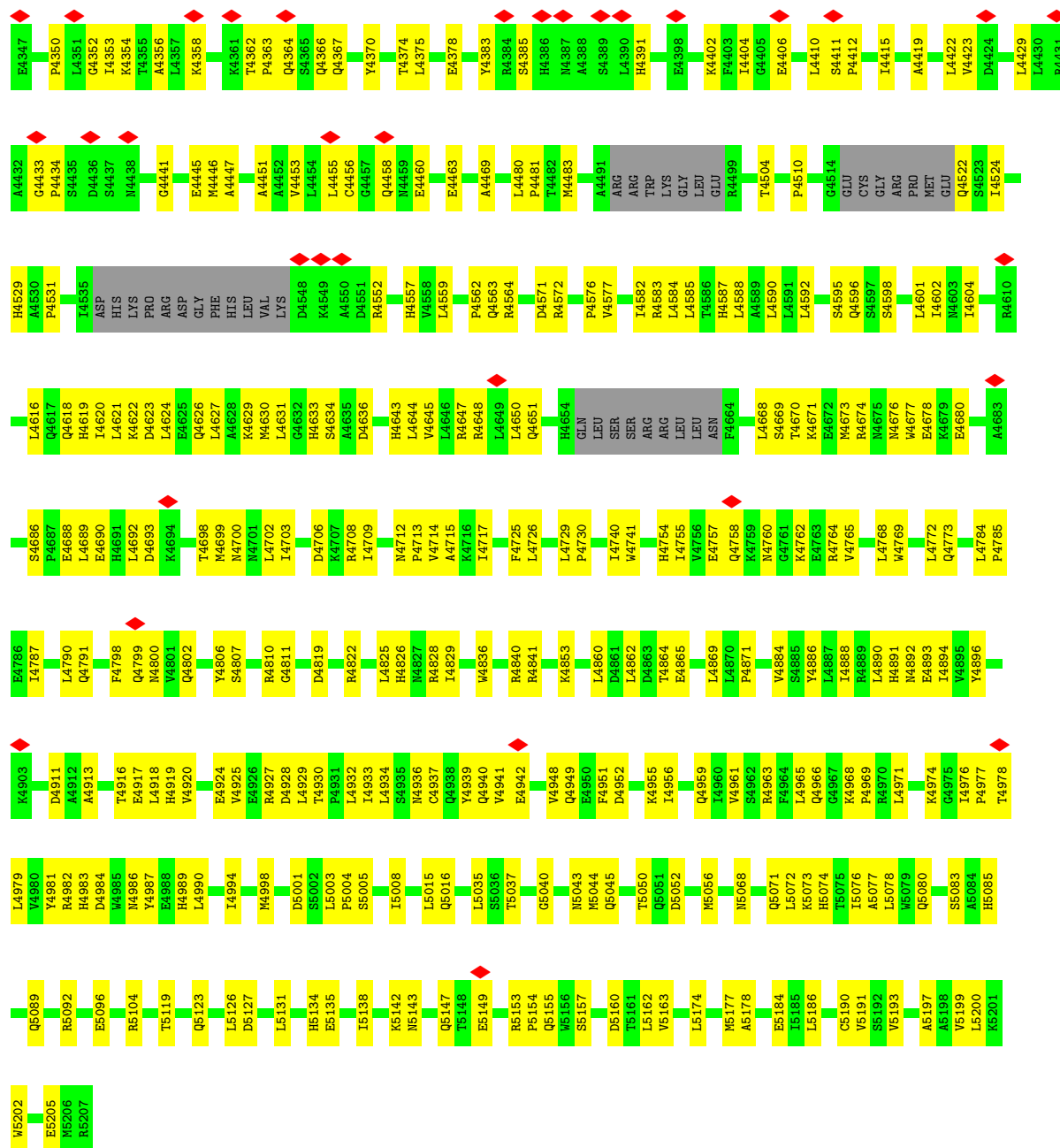
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Mg	0
			1	1	

V2906	N2761	E2421	P2304	L2215	E2098	Q1826	V1860	F1388	R1286	S1200
E2907	M2765	R2437	V2305	R2216	I2099	V1827	T1661	R1389	L1269	THR
L2910	L2910	F2437	V2306	F2221	K1997	Q1828	E1210	GLY	E1270	SER
L2911	E2760	L2448	F2307	L2222	K1998	Q1829	S1999	SER	L1271	SER
D2921	L2761	Y2461	N2309	Q2225	L2308	L1832	L2000	ASN	E1272	ASN
L2922	L2765	Y2461	N2309	Q2225	T2104	L1832	L2000	GLU	E1273	SER
L2923	L2765	Y2461	N2309	Q2225	T2104	L1832	L2000	GLU	E1274	SER
L2924	L2765	Y2461	N2309	Q2225	T2104	L1832	L2000	GLU	E1275	GLN
Q2925	L2765	Y2461	N2309	Q2225	T2104	L1832	L2000	GLU	E1276	R1207
Q2929	L2765	Y2461	N2309	Q2225	T2104	L1832	L2000	GLU	E1277	A1208
G2930	L2765	Y2461	N2309	Q2225	T2104	L1832	L2000	GLU	E1278	T1209
Y2931	L2765	Y2461	N2309	Q2225	T2104	L1832	L2000	GLU	E1279	H1210
F2932	L2765	Y2461	N2309	Q2225	T2104	L1832	L2000	GLU	E1280	Y1211
F2935	L2765	Y2461	N2309	Q2225	T2104	L1832	L2000	GLU	E1281	Q1216
Y2939	L2765	Y2461	N2309	Q2225	T2104	L1832	L2000	GLU	E1282	V1217
D2947	L2765	Y2461	N2309	Q2225	T2104	L1832	L2000	GLU	E1283	Q1218
F2951	L2765	Y2461	N2309	Q2225	T2104	L1832	L2000	GLU	E1284	E1219
D2955	L2765	Y2461	N2309	Q2225	T2104	L1832	L2000	GLU	E1285	M1220
S2958	L2765	Y2461	N2309	Q2225	T2104	L1832	L2000	GLU	E1286	A1221
M2962	L2765	Y2461	N2309	Q2225	T2104	L1832	L2000	GLU	E1287	G1222
V2963	L2765	Y2461	N2309	Q2225	T2104	L1832	L2000	GLU	E1288	K1223
K2968	L2765	Y2461	N2309	Q2225	T2104	L1832	L2000	GLU	E1289	I1224
P2976	L2765	Y2461	N2309	Q2225	T2104	L1832	L2000	GLU	E1290	K1225
L2979	L2765	Y2461	N2309	Q2225	T2104	L1832	L2000	GLU	E1291	R1228
L2984	L2765	Y2461	N2309	Q2225	T2104	L1832	L2000	GLU	E1292	I1303
P2987	L2765	Y2461	N2309	Q2225	T2104	L1832	L2000	GLU	E1293	S1230
D2992	L2765	Y2461	N2309	Q2225	T2104	L1832	L2000	GLU	E1294	H1231
L3000	L2765	Y2461	N2309	Q2225	T2104	L1832	L2000	GLU	E1295	I1232
A3001	L2765	Y2461	N2309	Q2225	T2104	L1832	L2000	GLU	E1296	F1233
P3004	L2765	Y2461	N2309	Q2225	T2104	L1832	L2000	GLU	E1297	F1236
A3006	L2765	Y2461	N2309	Q2225	T2104	L1832	L2000	GLU	E1298	W1237
K3007	L2765	Y2461	N2309	Q2225	T2104	L1832	L2000	GLU	E1299	R1238
S3013	L2765	Y2461	N2309	Q2225	T2104	L1832	L2000	GLU	E1300	E1239
F3014	L2765	Y2461	N2309	Q2225	T2104	L1832	L2000	GLU	E1301	E1242
K3015	L2765	Y2461	N2309	Q2225	T2104	L1832	L2000	GLU	E1302	S1245
K3019	L2765	Y2461	N2309	Q2225	T2104	L1832	L2000	GLU	E1303	GLU
									E1304	PRO
									E1305	LYS
									E1306	ASP
									E1307	GLN
									E1308	GLU
									E1309	ALA
									E1310	ALA
									E1311	GLU
									E1312	LEU
									E1313	LEU
									E1314	SER
									E1315	GLU
									E1316	PRO
									E1317	N1380
									E1318	F1381
									E1319	T1382
									E1320	GLU
									E1321	GLU
									E1322	SER
									E1323	GLU
									E1324	
									E1325	
									E1326	
									E1327	
									E1328	
									E1329	
									E1330	
									E1331	
									E1332	
									E1333	
									E1334	
									E1335	
									E1336	
									E1337	
									E1338	
									E1339	
									E1340	
									E1341	
									E1342	
									E1343	
									E1344	
									E1345	
									E1346	
									E1347	
									E1348	
									E1349	
									E1350	
									E1351	
									E1352	
									E1353	
									E1354	
									E1355	
									E1356	
									E1357	
									E1358	
									E1359	
									E1360	
									E1361	
									E1362	
									E1363	
									E1364	
									E1365	
									E1366	
									E1367	
									E1368	
									E1369	
									E1370	
									E1371	
									E1372	
									E1373	
									E1374	
									E1375	
									E1376	
									E1377	
									E1378	
									E1379	
									E1380	
									E1381	
									E1382	
									E1383	
									E1384	
									E1385	
									E1386	
									E1387	
									E1388	
									E1389	
									E1390	
									E1391	
									E1392	
									E1393	
									E1394	
									E1395	
									E1396	
									E1397	
									E1398	
									E1399	
									E1400	
									E1401	
									E1402	
									E1403	
									E1404	
									E1405	
									E1406	
									E1407	
									E1408	
									E1409	
									E1410	
									E1411	
									E1412	
									E1413	
									E1414	
									E1415	
									E1416	
									E1417	
									E1418	
									E1419	
									E1420	
									E1421	
									E1422	
									E1423	
									E1424	
									E1425	
									E1426	
									E1427	
									E1428	
									E1429	
									E1430	
									E1431	
									E1432	
									E1433	
									E1434	
									E1435	
									E1436	
									E1437	
									E1438	
									E1439	
									E1440	
									E1441	
									E1442	
									E1443	
									E1444	
									E1445	
									E1446	
									E1447	
									E1448	
									E1449	
									E1450	
									E1451	
									E1452	
									E1453	
									E1454	
									E1455	
									E1456	
									E1457	
									E1458	
									E1459	
									E1460	
									E1461	
									E1462	
									E1463	





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	179169	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49.41	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.518	Depositor
Minimum map value	-1.526	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.043	Depositor
Recommended contour level	0.25	Depositor
Map size ($\text{\AA}$)	527.5, 527.5, 527.5	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.055, 1.055, 1.055	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ATP

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	0.21	5/36657 (0.0%)	0.46	16/49608 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2134	PRO	CA-C	-12.01	1.41	1.52
1	A	1920	HIS	CA-C	-5.93	1.45	1.52
1	A	2002	VAL	CA-CB	-5.34	1.47	1.54
1	A	2000	LEU	CA-C	-5.18	1.46	1.52
1	A	1998	LYS	C-O	-5.01	1.17	1.24

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4969	PRO	O-C-N	16.86	145.41	122.64
1	A	2000	LEU	N-CA-C	-13.46	96.17	112.59
1	A	4969	PRO	CA-C-O	-13.22	96.53	120.60
1	A	1921	ARG	N-CA-C	-9.25	94.42	109.96
1	A	2785	ALA	N-CA-C	7.94	120.01	111.36
1	A	2134	PRO	CA-C-N	-7.27	110.75	119.84
1	A	2134	PRO	C-N-CA	-7.27	110.75	119.84
1	A	1281	PRO	N-CA-C	-6.09	105.59	113.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2001	TYR	N-CA-C	-5.96	103.96	112.13
1	A	2136	LYS	N-CA-C	-5.68	98.69	110.80
1	A	1829	GLN	CA-C-N	-5.57	114.19	119.76
1	A	1829	GLN	C-N-CA	-5.57	114.19	119.76
1	A	2414	ILE	CA-C-N	-5.43	114.33	119.76
1	A	2414	ILE	C-N-CA	-5.43	114.33	119.76
1	A	2134	PRO	CB-CA-C	-5.35	104.39	110.92
1	A	2790	ALA	N-CA-C	-5.05	100.04	110.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1719	GLN	Peptide
1	A	3058	THR	Peptide
1	A	895	GLY	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	35905	0	36077	966	0
2	A	31	0	12	1	0
3	A	1	0	0	0	0
All	All	35937	0	36089	966	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 13.

All (966) 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:4084:PRO:HB2	1:A:4088:VAL:HG21	1.55	0.87
1:A:3832:LEU:HG	1:A:3838:VAL:HG11	1.58	0.84
1:A:731:ARG:HE	1:A:765:LEU:HG	1.43	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3934:LEU:O	1:A:3938:GLU:HB2	1.80	0.80
1:A:3199:ILE:HB	1:A:3217:VAL:HG21	1.63	0.80
1:A:719:TRP:O	1:A:759:ARG:NH1	2.15	0.80
1:A:764:LEU:O	1:A:798:ARG:NH2	2.17	0.78
1:A:692:LEU:HB2	1:A:743:PHE:HE2	1.49	0.78
1:A:1339:ARG:HH12	1:A:1393:LEU:HD23	1.49	0.76
1:A:4244:SER:HB3	1:A:4287:ARG:HH12	1.51	0.76
1:A:4802:GLN:HE22	1:A:4981:TYR:HB3	1.51	0.76
1:A:895:GLY:O	1:A:897:ASN:N	2.19	0.75
1:A:3932:HIS:HE2	1:A:4069:PHE:HD1	1.32	0.75
1:A:3066:PRO:HB3	1:A:3099:MET:HB3	1.68	0.75
1:A:1708:GLN:HE21	1:A:2084:GLY:HA2	1.53	0.74
1:A:4253:ALA:HA	1:A:4256:LYS:HB3	1.68	0.74
1:A:3891:MET:HE3	1:A:3895:LEU:HD21	1.69	0.74
1:A:2421:GLU:HG2	1:A:2526:PRO:HG3	1.70	0.74
1:A:3838:VAL:O	1:A:3842:LEU:HB2	1.88	0.73
1:A:2358:ARG:O	1:A:2358:ARG:NH1	2.21	0.73
1:A:4800:ASN:HB2	1:A:4979:LEU:HB3	1.71	0.73
1:A:2062:VAL:HG23	1:A:2066:ILE:HD11	1.70	0.72
1:A:2006:HIS:NE2	1:A:2018:VAL:HG23	2.04	0.72
1:A:2619:LEU:HD13	1:A:2641:VAL:HG13	1.70	0.72
1:A:1156:CYS:HB3	1:A:1221:ALA:HB1	1.71	0.72
1:A:1640:MET:HB2	1:A:1652:GLN:HB3	1.72	0.71
1:A:2704:ARG:HG2	1:A:2721:LEU:HD23	1.70	0.71
1:A:637:LEU:O	1:A:682:ARG:NH1	2.23	0.71
1:A:3057:GLN:HE21	1:A:3435:GLY:C	1.99	0.71
1:A:2365:PHE:O	1:A:2373:LYS:NZ	2.24	0.70
1:A:1103:VAL:HA	1:A:1106:LEU:HG	1.72	0.70
1:A:2018:VAL:HG23	1:A:2018:VAL:O	1.91	0.70
1:A:1632:MET:HE1	1:A:1710:VAL:HG13	1.73	0.70
1:A:1100:THR:HB	1:A:1190:ARG:HH21	1.57	0.70
1:A:2846:VAL:HG12	1:A:2885:SER:HB3	1.74	0.69
1:A:1351:GLN:HE22	1:A:1409:ASP:HB3	1.56	0.69
1:A:4483:MET:HE3	1:A:4557:HIS:HA	1.74	0.69
1:A:691:TRP:CD1	1:A:692:LEU:HD12	2.28	0.69
1:A:3330:CYS:SG	1:A:3343:LYS:NZ	2.61	0.69
1:A:4631:LEU:HD13	1:A:4754:HIS:HE1	1.58	0.68
1:A:2736:VAL:HG12	1:A:2785:ALA:HB2	1.74	0.68
1:A:3589:PHE:HZ	1:A:3677:ILE:HB	1.59	0.68
1:A:4624:LEU:HA	1:A:4627:LEU:HD12	1.76	0.68
1:A:4825:LEU:O	1:A:4829:ILE:HG12	1.94	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:840:LEU:HD13	1:A:882:LEU:HD22	1.75	0.68
1:A:3823:SER:O	1:A:3827:ASN:ND2	2.27	0.68
1:A:3922:ARG:NH1	1:A:3956:ASP:OD1	2.26	0.68
1:A:4201:GLU:OE1	1:A:4231:ARG:NH2	2.27	0.67
1:A:1105:GLN:O	1:A:1109:ILE:HG12	1.94	0.67
1:A:4058:HIS:HA	1:A:4061:PHE:HB2	1.75	0.67
1:A:4445:GLU:HB2	1:A:4446:MET:HE2	1.77	0.67
1:A:4893:GLU:O	1:A:4896:TYR:HB2	1.95	0.67
1:A:823:MET:HB2	1:A:826:ARG:HH12	1.60	0.67
1:A:3063:ASP:O	1:A:3406:ARG:NH1	2.28	0.66
1:A:849:LEU:HB2	1:A:902:VAL:HG23	1.75	0.66
1:A:2009:MET:HG2	1:A:2018:VAL:HG11	1.76	0.66
1:A:5003:LEU:HD23	1:A:5008:ILE:HG22	1.77	0.66
1:A:967:LYS:O	1:A:3248:GLN:NE2	2.23	0.66
1:A:1225:ASP:O	1:A:1228:ARG:NH1	2.28	0.66
1:A:1889:HIS:HA	1:A:1921:ARG:HH22	1.60	0.66
1:A:1651:LEU:HD21	1:A:1676:LEU:HD22	1.76	0.66
1:A:2550:GLU:O	1:A:2555:ARG:NH1	2.29	0.66
1:A:3934:LEU:HB3	1:A:3948:VAL:HG11	1.76	0.66
1:A:3539:CYS:O	1:A:3543:ALA:N	2.28	0.66
1:A:1225:ASP:OD1	1:A:1228:ARG:NH1	2.28	0.66
1:A:4924:GLU:HB2	1:A:4927:ARG:HB3	1.77	0.66
1:A:3674:LEU:O	1:A:3714:LYS:NZ	2.28	0.65
1:A:4894:ILE:HG12	1:A:4965:LEU:HD11	1.79	0.65
1:A:1854:GLN:O	1:A:1966:HIS:NE2	2.29	0.65
1:A:2686:MET:HE3	1:A:2721:LEU:HD12	1.79	0.65
1:A:1654:ASP:HB2	1:A:1662:GLU:HG3	1.79	0.64
1:A:3334:GLU:HA	1:A:3337:VAL:HG12	1.79	0.64
1:A:2300:SER:OG	1:A:2301:GLU:OE1	2.12	0.64
1:A:4324:MET:HG3	1:A:4709:ILE:HD13	1.79	0.64
1:A:1219:GLU:OE2	1:A:1275:TYR:OH	2.16	0.64
1:A:3556:ARG:HH22	1:A:3650:GLU:HG3	1.62	0.64
1:A:630:VAL:HG21	1:A:637:LEU:HD23	1.79	0.64
1:A:2733:LEU:HD22	1:A:2749:LYS:HG2	1.79	0.64
1:A:3884:GLN:HA	1:A:3887:LYS:HZ2	1.62	0.64
1:A:1030:SER:O	1:A:1034:THR:HG23	1.97	0.64
1:A:3882:TRP:O	1:A:3886:VAL:HG23	1.98	0.64
1:A:4098:VAL:HA	1:A:4115:LYS:HE2	1.80	0.63
1:A:4981:TYR:HE1	1:A:4984:ASP:H	1.46	0.63
1:A:1633:LEU:HD21	1:A:1655:PHE:HE2	1.63	0.63
1:A:2547:VAL:HG12	1:A:2548:SER:H	1.62	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:601:LEU:HD21	1:A:619:LYS:HG3	1.81	0.63
1:A:2534:MET:SD	1:A:2634:SER:OG	2.53	0.63
1:A:3461:VAL:HG13	1:A:3465:GLN:HB2	1.80	0.63
1:A:4062:ARG:O	1:A:4066:ASN:ND2	2.32	0.63
1:A:1472:TYR:HE2	1:A:1509:LEU:HD22	1.64	0.63
1:A:4616:LEU:O	1:A:4620:ILE:HG12	1.99	0.63
1:A:4911:ASP:HB3	1:A:4974:LYS:HZ1	1.64	0.63
1:A:1655:PHE:HB2	1:A:1660:VAL:HG21	1.80	0.63
1:A:3810:SER:HB3	1:A:3812:PRO:HD2	1.80	0.63
1:A:2172:ARG:HH21	1:A:2173:ARG:HE	1.46	0.62
1:A:2201:PHE:HB3	1:A:2215:LEU:HD11	1.82	0.62
1:A:2554:ASP:HB3	1:A:2561:LEU:HD12	1.80	0.62
1:A:3739:PHE:CE2	1:A:3812:PRO:HB3	2.33	0.62
1:A:4456:CYS:O	1:A:4458:GLN:NE2	2.32	0.62
1:A:2615:ILE:HD13	1:A:2685:LEU:HD13	1.82	0.62
1:A:3557:ASN:OD1	1:A:5037:THR:OG1	2.14	0.62
1:A:1610:SER:OG	1:A:3085:ARG:NH2	2.33	0.62
1:A:2647:VAL:HG22	1:A:2761:LEU:HD13	1.80	0.62
1:A:4173:LEU:HD11	1:A:4939:TYR:HB3	1.81	0.62
1:A:4891:HIS:NE2	1:A:4919:HIS:O	2.32	0.62
1:A:1652:GLN:NE2	1:A:1662:GLU:OE2	2.33	0.62
1:A:3828:PHE:HE2	1:A:3858:LEU:HG	1.65	0.62
1:A:4132:SER:OG	1:A:4939:TYR:O	2.16	0.62
1:A:5077:ALA:O	1:A:5080:GLN:HB3	2.00	0.62
1:A:684:MET:HE2	1:A:725:LEU:HD11	1.81	0.62
1:A:2315:MET:HE2	1:A:2315:MET:H	1.65	0.61
1:A:4481:PRO:HA	1:A:4674:ARG:HD2	1.81	0.61
1:A:4175:ILE:HD11	1:A:4226:LEU:HD22	1.80	0.61
1:A:4669:SER:OG	1:A:4673:MET:SD	2.57	0.61
1:A:620:LEU:HD23	1:A:620:LEU:H	1.66	0.61
1:A:1301:ALA:HB2	1:A:1389:ARG:HG2	1.82	0.61
1:A:1339:ARG:NH1	1:A:1342:GLN:OE1	2.32	0.61
1:A:2921:ASP:OD2	1:A:2968:LYS:NZ	2.33	0.61
1:A:805:VAL:HG23	1:A:813:ASP:HB3	1.82	0.61
1:A:1552:LYS:HA	1:A:1552:LYS:HE3	1.82	0.61
1:A:3057:GLN:HB3	1:A:3235:GLU:HG3	1.82	0.61
1:A:4583:ARG:HG3	1:A:4587:HIS:NE2	2.16	0.61
1:A:696:PRO:HG3	1:A:757:LEU:HD22	1.83	0.61
1:A:1858:THR:HG22	1:A:1859:TYR:H	1.65	0.61
1:A:3057:GLN:NE2	1:A:3435:GLY:O	2.30	0.61
1:A:2216:ARG:HD3	2:A:5301:ATP:H1'	1.81	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2791:ALA:HB3	1:A:2797:ARG:HG3	1.83	0.60
1:A:3265:ASP:OD1	1:A:3269:ARG:NH1	2.33	0.60
1:A:4252:MET:HE1	1:A:4256:LYS:HD3	1.83	0.60
1:A:886:ASP:O	1:A:891:ARG:NH1	2.34	0.60
1:A:1407:LEU:O	1:A:1414:ARG:NH2	2.34	0.60
1:A:3966:LYS:HD2	1:A:4084:PRO:HB3	1.82	0.60
1:A:1591:LYS:O	1:A:1595:MET:HG3	2.00	0.60
1:A:3900:GLU:HA	1:A:3903:GLN:HE22	1.66	0.60
1:A:3300:LEU:HD21	1:A:3374:ILE:HD13	1.84	0.60
1:A:1416:LYS:HA	1:A:1419:GLN:HB2	1.83	0.60
1:A:1610:SER:HG	1:A:3085:ARG:HH21	1.50	0.60
1:A:4647:ARG:O	1:A:4651:GLN:NE2	2.33	0.60
1:A:895:GLY:C	1:A:897:ASN:H	2.10	0.60
1:A:3746:THR:HG22	1:A:3748:LEU:H	1.67	0.60
1:A:4330:TYR:HD2	1:A:4370:TYR:HE1	1.47	0.60
1:A:744:MET:HB3	1:A:777:PHE:CZ	2.37	0.59
1:A:1280:GLN:HB2	1:A:1283:TYR:HB3	1.84	0.59
1:A:4836:TRP:HE1	1:A:4860:LEU:HD13	1.66	0.59
1:A:4768:LEU:O	1:A:4772:LEU:HD12	2.03	0.59
1:A:823:MET:O	1:A:827:LEU:HG	2.02	0.59
1:A:814:VAL:HG13	1:A:867:LEU:HD11	1.85	0.59
1:A:646:HIS:O	1:A:649:THR:OG1	2.20	0.59
1:A:1279:TYR:C	1:A:1281:PRO:HD3	2.27	0.59
1:A:2765:LEU:HB3	1:A:2882:VAL:HG23	1.83	0.59
1:A:3466:LEU:HD13	1:A:3530:LEU:HD22	1.84	0.59
1:A:939:TRP:O	1:A:943:VAL:HG23	2.01	0.59
1:A:3123:LEU:HB3	1:A:3128:TYR:HE2	1.67	0.59
1:A:4453:VAL:HG22	1:A:4650:LEU:HB2	1.85	0.59
1:A:1194:THR:HB	1:A:1210:HIS:HB2	1.85	0.58
1:A:4769:TRP:CD1	1:A:4773:GLN:HG2	2.37	0.58
1:A:2315:MET:HE2	1:A:2315:MET:N	2.18	0.58
1:A:4272:ASN:HD21	1:A:4274:TRP:HB2	1.66	0.58
1:A:3130:ASP:HA	1:A:3139:LYS:HA	1.83	0.58
1:A:3195:VAL:O	1:A:3199:ILE:HG23	2.02	0.58
1:A:649:THR:HG22	1:A:693:GLY:HA3	1.84	0.58
1:A:2736:VAL:HG12	1:A:2785:ALA:CB	2.32	0.58
1:A:4194:GLU:OE1	1:A:4238:ARG:NH1	2.34	0.58
1:A:3860:ALA:O	1:A:3864:MET:HG2	2.03	0.58
1:A:4977:PRO:O	1:A:4982:ARG:NH1	2.36	0.58
1:A:781:LEU:HD11	1:A:788:ILE:HB	1.84	0.58
1:A:1283:TYR:O	1:A:1287:ILE:HG12	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1467:ASP:OD2	1:A:1508:LYS:NZ	2.37	0.58
1:A:2958:SER:O	1:A:2962:MET:HG3	2.03	0.58
1:A:886:ASP:OD1	1:A:891:ARG:NH1	2.36	0.58
1:A:1625:ASP:OD1	1:A:1626:LEU:N	2.37	0.58
1:A:4072:LEU:O	1:A:4075:THR:OG1	2.19	0.58
1:A:965:LEU:O	1:A:973:GLN:NE2	2.36	0.58
1:A:2250:PHE:HD2	1:A:2346:MET:HB2	1.68	0.58
1:A:5153:ARG:HG3	1:A:5155:GLN:H	1.69	0.58
1:A:1076:GLU:HA	1:A:1079:LYS:HB2	1.86	0.58
1:A:3201:VAL:HG11	1:A:3274:SER:HB2	1.86	0.58
1:A:4563:GLN:O	1:A:4622:LYS:NZ	2.35	0.57
1:A:4714:VAL:HA	1:A:4717:ILE:HD12	1.84	0.57
1:A:1167:VAL:HG23	1:A:1172:GLN:HG3	1.85	0.57
1:A:1754:ARG:O	1:A:1758:ARG:HG2	2.04	0.57
1:A:3015:MET:HE3	1:A:3058:THR:HG21	1.85	0.57
1:A:4364:GLN:HA	1:A:4367:GLN:HB2	1.86	0.57
1:A:3162:PRO:HG2	1:A:3165:LEU:HB3	1.86	0.57
1:A:3764:LEU:HD12	1:A:3811:LEU:HD23	1.87	0.57
1:A:737:THR:HG22	1:A:740:LEU:HD21	1.85	0.57
1:A:3678:PRO:HG2	1:A:4799:GLN:HG3	1.86	0.57
1:A:3883:LEU:O	1:A:3887:LYS:HG3	2.05	0.57
1:A:4648:ARG:HG3	1:A:4688:GLU:HG3	1.86	0.57
1:A:4785:PRO:HD3	1:A:4920:VAL:HG11	1.85	0.57
1:A:4961:VAL:HA	1:A:4965:LEU:HB2	1.85	0.57
1:A:3664:LEU:HD23	1:A:3710:PRO:HD2	1.87	0.57
1:A:1157:VAL:HG11	1:A:1211:TYR:HE2	1.70	0.57
1:A:3462:THR:HG22	1:A:3601:LEU:HA	1.87	0.57
1:A:3951:HIS:NE2	1:A:3981:CYS:HB2	2.20	0.57
1:A:4172:MET:HB3	1:A:4740:ILE:HG12	1.86	0.57
1:A:4324:MET:HE2	1:A:4703:ILE:HG23	1.86	0.57
1:A:4529:HIS:HB2	1:A:4989:HIS:CD2	2.40	0.57
1:A:4892:ASN:O	1:A:4896:TYR:N	2.32	0.57
1:A:4994:ILE:HD12	1:A:5035:LEU:HD22	1.85	0.57
1:A:5153:ARG:HE	1:A:5154:PRO:HD2	1.69	0.57
1:A:1335:TRP:H	1:A:1335:TRP:CD1	2.22	0.56
1:A:1324:MET:HE2	1:A:1324:MET:HA	1.87	0.56
1:A:2661:GLN:NE2	1:A:2794:ASP:OD2	2.38	0.56
1:A:2755:MET:HE1	1:A:2779:LYS:HA	1.85	0.56
1:A:4415:ILE:HG12	1:A:4455:LEU:HD22	1.88	0.56
1:A:1047:ILE:O	1:A:1051:LEU:HG	2.05	0.56
1:A:2325:ASN:N	1:A:2329:SER:O	2.37	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2738:LEU:HD22	1:A:2742:ILE:HG21	1.87	0.56
1:A:2751:ASN:O	1:A:2755:MET:HG3	2.06	0.56
1:A:3686:HIS:HE1	1:A:5143:ASN:HB2	1.70	0.56
1:A:3893:LEU:HA	1:A:3896:ILE:HG22	1.85	0.56
1:A:4698:THR:O	1:A:4702:LEU:HG	2.05	0.56
1:A:4699:MET:HA	1:A:4702:LEU:HD12	1.88	0.56
1:A:1333:ARG:HB3	1:A:1335:TRP:HD1	1.69	0.56
1:A:788:ILE:O	1:A:791:CYS:HB2	2.06	0.56
1:A:4337:LEU:HG	1:A:4356:ALA:HB1	1.88	0.56
1:A:3922:ARG:HH22	1:A:3956:ASP:HA	1.70	0.56
1:A:4242:PHE:HZ	1:A:4256:LYS:HA	1.71	0.56
1:A:4864:THR:HG22	1:A:4865:GLU:H	1.70	0.56
1:A:923:LEU:HB2	1:A:968:GLU:HG3	1.88	0.56
1:A:1379:LEU:HA	1:A:1382:THR:HG22	1.88	0.56
1:A:4916:THR:HG23	1:A:4918:LEU:H	1.71	0.56
1:A:4228:GLU:O	1:A:4232:ILE:HG12	2.06	0.56
1:A:4620:ILE:HG22	1:A:4624:LEU:HD23	1.88	0.55
1:A:4940:GLN:HG3	1:A:4948:VAL:HB	1.87	0.55
1:A:558:GLN:O	1:A:562:VAL:HG23	2.06	0.55
1:A:2267:LEU:HD12	1:A:2576:ILE:HG23	1.86	0.55
1:A:4451:ALA:O	1:A:4455:LEU:HG	2.05	0.55
1:A:545:ASP:O	1:A:664:HIS:NE2	2.34	0.55
1:A:3840:HIS:H	1:A:3840:HIS:CD2	2.22	0.55
1:A:3000:LEU:HD22	1:A:3007:LYS:HG2	1.87	0.55
1:A:4018:LEU:HA	1:A:4021:LEU:HB2	1.89	0.55
1:A:5043:ASN:O	1:A:5071:GLN:NE2	2.35	0.55
1:A:1992:GLU:HA	1:A:2101:GLU:HB2	1.88	0.55
1:A:3675:LEU:O	1:A:3675:LEU:HD23	2.07	0.55
1:A:3956:ASP:O	1:A:3960:ARG:HD3	2.06	0.55
1:A:4341:VAL:HA	1:A:4353:ILE:HG12	1.89	0.55
1:A:4769:TRP:HD1	1:A:4773:GLN:HG2	1.71	0.55
1:A:540:ILE:C	1:A:542:GLN:H	2.14	0.55
1:A:3537:ARG:NH1	1:A:3565:LEU:O	2.39	0.55
1:A:3883:LEU:HD13	1:A:3930:VAL:HG13	1.89	0.55
1:A:676:LEU:HD23	1:A:679:LEU:HD21	1.87	0.55
1:A:762:PHE:HA	1:A:773:TYR:HE2	1.70	0.55
1:A:2025:LEU:HD21	1:A:2035:VAL:HG22	1.89	0.55
1:A:2309:ASN:ND2	1:A:2314:THR:OG1	2.40	0.55
1:A:4937:CYS:HA	1:A:4951:PHE:HD1	1.71	0.55
1:A:5157:SER:HA	1:A:5186:LEU:HA	1.88	0.55
1:A:1822:PRO:HG2	1:A:1825:LEU:HD13	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1095:ASP:HB3	1:A:1101:ILE:HB	1.89	0.55
1:A:2298:TRP:HB3	1:A:2583:GLY:HA2	1.89	0.55
1:A:2528:ARG:HE	1:A:2565:VAL:HG21	1.72	0.55
1:A:3015:MET:HG2	1:A:3179:VAL:HG23	1.89	0.55
1:A:3538:SER:OG	1:A:3629:GLN:OE1	2.21	0.55
1:A:3585:ARG:NH2	1:A:3671:ASP:O	2.40	0.55
1:A:744:MET:HB3	1:A:777:PHE:HZ	1.70	0.54
1:A:840:LEU:HD11	1:A:881:LEU:HG	1.89	0.54
1:A:1889:HIS:HA	1:A:1921:ARG:NH2	2.22	0.54
1:A:3721:GLU:O	1:A:3725:GLN:HG2	2.07	0.54
1:A:5052:ASP:OD1	1:A:5052:ASP:N	2.40	0.54
1:A:1623:PHE:HB2	1:A:1637:TRP:HZ3	1.72	0.54
1:A:3797:LYS:HD2	1:A:3855:GLU:HG2	1.89	0.54
1:A:5162:LEU:HD23	1:A:5177:MET:SD	2.47	0.54
1:A:2048:GLN:HG3	1:A:2049:LYS:HG2	1.89	0.54
1:A:4936:ASN:HD22	1:A:4956:ILE:HG13	1.72	0.54
1:A:883:SER:O	1:A:887:SER:OG	2.25	0.54
1:A:2690:GLY:HA2	1:A:2694:HIS:HB3	1.88	0.54
1:A:4239:ALA:HB2	1:A:4263:VAL:HG21	1.90	0.54
1:A:913:TRP:O	1:A:917:VAL:HG12	2.07	0.54
1:A:3624:LEU:O	1:A:3628:VAL:HG23	2.07	0.54
1:A:3950:GLU:O	1:A:3954:LEU:HG	2.08	0.54
1:A:4004:ALA:HA	1:A:4017:CYS:HB2	1.88	0.54
1:A:2654:HIS:HB3	1:A:2658:LEU:HD23	1.90	0.54
1:A:3913:ILE:HA	1:A:3916:VAL:HG12	1.89	0.54
1:A:4363:PRO:HD2	1:A:4366:GLN:HE22	1.71	0.54
1:A:1139:ALA:O	1:A:1143:ARG:HG2	2.08	0.54
1:A:1157:VAL:O	1:A:1161:LEU:HD22	2.06	0.54
1:A:3560:ARG:NE	1:A:3644:ASP:OD2	2.29	0.54
1:A:2905:PRO:HB2	1:A:2910:LEU:HG	1.88	0.54
1:A:4270:VAL:HG21	1:A:4275:HIS:CE1	2.42	0.54
1:A:932:TYR:HB2	1:A:935:GLU:HB2	1.90	0.54
1:A:1101:ILE:HD12	1:A:1102:LEU:H	1.72	0.54
1:A:2556:LEU:HD23	1:A:2556:LEU:O	2.08	0.54
1:A:4385:SER:O	1:A:4391:HIS:NE2	2.32	0.54
1:A:1537:ALA:HB2	1:A:1592:LEU:HD11	1.89	0.53
1:A:3128:TYR:HD1	1:A:3141:ARG:HA	1.72	0.53
1:A:1657:LEU:HB2	1:A:1660:VAL:HG22	1.90	0.53
1:A:3221:TYR:OH	1:A:3226:CYS:SG	2.66	0.53
1:A:4676:ASN:O	1:A:4680:GLU:HG2	2.08	0.53
1:A:1037:TRP:HZ2	1:A:1085:ALA:HB2	1.73	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1216:GLN:HG3	1:A:1217:VAL:N	2.23	0.53
1:A:1998:LYS:HE2	1:A:2100:LEU:HD12	1.91	0.53
1:A:1424:ARG:NH2	1:A:1510:CYS:SG	2.82	0.53
1:A:1493:LYS:O	1:A:1497:LYS:NZ	2.41	0.53
1:A:2448:LEU:HA	1:A:2485:PHE:HB3	1.88	0.53
1:A:4062:ARG:HH22	1:A:4123:VAL:HG13	1.74	0.53
1:A:4913:ALA:HB2	1:A:4974:LYS:HD2	1.90	0.53
1:A:5083:SER:O	1:A:5134:HIS:NE2	2.42	0.53
1:A:1719:GLN:HB3	1:A:1720:PRO:HD2	1.90	0.53
1:A:2076:LEU:HD23	1:A:2078:TYR:HE1	1.74	0.53
1:A:3943:GLU:N	1:A:3943:GLU:OE1	2.42	0.53
1:A:4333:GLU:O	1:A:4337:LEU:HD12	2.08	0.53
1:A:940:ARG:NH2	1:A:983:ASP:OD1	2.41	0.53
1:A:1283:TYR:CE1	1:A:1287:ILE:HD11	2.44	0.53
1:A:728:SER:HB2	1:A:765:LEU:HD13	1.91	0.53
1:A:996:GLU:O	1:A:1000:ILE:HG22	2.09	0.53
1:A:1046:ASP:OD1	1:A:1047:ILE:N	2.41	0.53
1:A:1232:ILE:HG22	1:A:1236:PHE:CE2	2.43	0.53
1:A:2294:LEU:HD22	1:A:2581:ASP:HB2	1.90	0.53
1:A:691:TRP:HD1	1:A:692:LEU:N	2.06	0.53
1:A:1733:LYS:HG2	1:A:1813:GLY:HA2	1.91	0.53
1:A:3665:TRP:CD1	1:A:3710:PRO:HB3	2.44	0.53
1:A:923:LEU:HD23	1:A:927:GLY:HA2	1.92	0.53
1:A:1329:HIS:O	1:A:1332:GLN:NE2	2.38	0.53
1:A:4446:MET:HE2	1:A:4446:MET:N	2.24	0.53
1:A:660:ARG:HA	1:A:663:SER:HB3	1.92	0.52
1:A:3086:ASN:HB3	1:A:3108:LEU:HD21	1.91	0.52
1:A:4175:ILE:HG23	1:A:4230:ALA:HB2	1.91	0.52
1:A:4179:GLU:OE1	1:A:4233:ARG:NH2	2.42	0.52
1:A:4238:ARG:O	1:A:4242:PHE:HB3	2.08	0.52
1:A:1631:ASN:OD1	1:A:1633:LEU:N	2.42	0.52
1:A:1821:LEU:HD12	1:A:1827:VAL:HG12	1.91	0.52
1:A:2043:LEU:HD12	1:A:2087:TRP:HE3	1.74	0.52
1:A:1844:ALA:HB2	1:A:1895:LEU:HD11	1.90	0.52
1:A:803:GLU:O	1:A:807:ASN:N	2.42	0.52
1:A:1236:PHE:CZ	1:A:1286:PHE:HB3	2.45	0.52
1:A:1345:GLU:OE1	1:A:1405:LYS:NZ	2.30	0.52
1:A:1700:TYR:C	1:A:1702:ASN:H	2.17	0.52
1:A:2590:GLU:O	1:A:2594:ILE:HG12	2.08	0.52
1:A:620:LEU:HD12	1:A:662:LEU:HG	1.91	0.52
1:A:1480:ASP:OD1	1:A:1480:ASP:N	2.41	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4017:CYS:O	1:A:4021:LEU:N	2.42	0.52
1:A:1545:ILE:HB	1:A:1566:ILE:HB	1.92	0.52
1:A:1988:ILE:HD13	1:A:2097:VAL:HB	1.91	0.52
1:A:4330:TYR:CD2	1:A:4370:TYR:HE1	2.26	0.52
1:A:1239:GLU:HA	1:A:1242:GLU:HG2	1.91	0.52
1:A:1335:TRP:HE3	1:A:1339:ARG:HG3	1.74	0.52
1:A:4807:SER:HB2	1:A:4865:GLU:HA	1.91	0.52
1:A:2951:PHE:HB3	1:A:2987:PHE:CD2	2.45	0.52
1:A:3979:CYS:HA	1:A:4120:PHE:CE2	2.45	0.52
1:A:4798:PHE:HB3	1:A:4979:LEU:HD21	1.92	0.52
1:A:1380:ASN:O	1:A:1384:ASN:ND2	2.43	0.52
1:A:3222:HIS:H	1:A:3222:HIS:CD2	2.28	0.52
1:A:1052:LEU:HD12	1:A:1112:HIS:HB2	1.92	0.52
1:A:2167:PRO:HA	1:A:2170:TYR:CD1	2.45	0.52
1:A:4469:ALA:O	1:A:4596:GLN:NE2	2.43	0.52
1:A:624:LEU:HA	1:A:627:LEU:HG	1.92	0.51
1:A:645:CYS:O	1:A:649:THR:HG23	2.09	0.51
1:A:692:LEU:HA	1:A:695:LEU:HD12	1.91	0.51
1:A:697:VAL:O	1:A:700:CYS:HB2	2.10	0.51
1:A:752:SER:OG	1:A:783:ARG:NH1	2.41	0.51
1:A:2018:VAL:O	1:A:2018:VAL:CG2	2.58	0.51
1:A:4584:LEU:HD22	1:A:4627:LEU:HD11	1.92	0.51
1:A:550:ASN:OD1	1:A:551:SER:N	2.43	0.51
1:A:1594:LEU:HD23	1:A:3138:VAL:HG12	1.92	0.51
1:A:3686:HIS:CE1	1:A:5143:ASN:HB2	2.45	0.51
1:A:1276:ASP:OD1	1:A:1277:TYR:N	2.44	0.51
1:A:2547:VAL:HG12	1:A:2548:SER:N	2.26	0.51
1:A:3828:PHE:CE2	1:A:3858:LEU:HG	2.43	0.51
1:A:691:TRP:HD1	1:A:692:LEU:HD12	1.75	0.51
1:A:696:PRO:HG2	1:A:750:LEU:HD11	1.91	0.51
1:A:801:GLY:O	1:A:804:GLN:HB3	2.10	0.51
1:A:3052:LEU:HD22	1:A:3103:LEU:HD21	1.91	0.51
1:A:4644:LEU:O	1:A:4647:ARG:HG2	2.11	0.51
1:A:765:LEU:HD23	1:A:765:LEU:H	1.74	0.51
1:A:1381:PHE:HA	1:A:1384:ASN:HD21	1.75	0.51
1:A:3163:ILE:O	1:A:3167:ASN:ND2	2.43	0.51
1:A:3265:ASP:OD2	1:A:3422:ARG:NH1	2.39	0.51
1:A:5074:HIS:O	1:A:5078:LEU:N	2.34	0.51
1:A:4884:VAL:O	1:A:4888:ILE:HG12	2.10	0.51
1:A:1879:ARG:O	1:A:1883:THR:OG1	2.23	0.51
1:A:2055:HIS:HE2	1:A:2098:GLU:HB3	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1149:LEU:HD21	1:A:1209:THR:HG22	1.93	0.51
1:A:2059:THR:O	1:A:2062:VAL:HG22	2.11	0.51
1:A:2760:GLU:O	1:A:2800:LYS:NZ	2.44	0.51
1:A:4292:VAL:O	1:A:4296:SER:OG	2.21	0.51
1:A:977:TYR:CG	1:A:999:ILE:HG13	2.46	0.51
1:A:1174:ASP:HB2	1:A:1269:LEU:H	1.74	0.51
1:A:1723:ASP:OD2	1:A:2045:ALA:N	2.44	0.51
1:A:3924:PHE:O	1:A:3928:LEU:HG	2.11	0.51
1:A:3971:PHE:HZ	1:A:4092:LEU:HG	1.76	0.51
1:A:590:LEU:HD22	1:A:635:LEU:HB3	1.92	0.50
1:A:3885:LEU:O	1:A:3889:LEU:HG	2.11	0.50
1:A:3951:HIS:ND1	1:A:3954:LEU:HD12	2.25	0.50
1:A:4618:GLN:HA	1:A:4621:LEU:HB2	1.94	0.50
1:A:4787:ILE:O	1:A:4791:GLN:HG2	2.11	0.50
1:A:1233:PHE:HA	1:A:1236:PHE:CZ	2.46	0.50
1:A:3645:ARG:HD2	1:A:3713:TRP:CE2	2.46	0.50
1:A:766:PRO:HB2	1:A:769:HIS:HB2	1.94	0.50
1:A:3958:CYS:HB3	1:A:3959:LEU:HD22	1.93	0.50
1:A:803:GLU:OE2	1:A:854:ALA:HB1	2.11	0.50
1:A:1632:MET:HB2	1:A:1789:LEU:HD11	1.93	0.50
1:A:1637:TRP:CZ2	1:A:1639:ALA:HB2	2.46	0.50
1:A:2786:MET:O	1:A:2788:GLY:N	2.45	0.50
1:A:2976:PRO:HA	1:A:2979:ILE:HG22	1.92	0.50
1:A:3718:TYR:HE2	1:A:3746:THR:HG21	1.75	0.50
1:A:4585:LEU:HA	1:A:4588:LEU:HG	1.93	0.50
1:A:1026:GLY:HA3	1:A:1073:ASN:HB3	1.94	0.50
1:A:2346:MET:SD	1:A:2347:THR:N	2.85	0.50
1:A:899:VAL:HA	1:A:902:VAL:HG12	1.93	0.50
1:A:3040:ARG:HH21	1:A:3170:GLU:HA	1.77	0.50
1:A:4259:TYR:O	1:A:4262:GLN:HG2	2.11	0.50
1:A:2378:CYS:SG	1:A:2383:ILE:HG13	2.52	0.50
1:A:4007:PRO:O	1:A:4048:SER:OG	2.30	0.50
1:A:4686:SER:O	1:A:4690:GLU:HG3	2.12	0.50
1:A:4769:TRP:CD1	1:A:4769:TRP:C	2.90	0.50
1:A:4886:TYR:O	1:A:4890:LEU:N	2.45	0.50
1:A:4927:ARG:HG3	1:A:4928:ASP:OD1	2.12	0.50
1:A:760:SER:O	1:A:764:LEU:HD22	2.11	0.49
1:A:3310:GLU:OE1	1:A:3310:GLU:N	2.45	0.49
1:A:4073:VAL:HA	1:A:4076:ILE:HG22	1.93	0.49
1:A:1335:TRP:O	1:A:1339:ARG:HG2	2.11	0.49
1:A:1546:TYR:HB2	1:A:1641:ALA:HB3	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2201:PHE:O	1:A:2205:CYS:HB2	2.13	0.49
1:A:3271:SER:HA	1:A:3280:ALA:HB1	1.95	0.49
1:A:4447:ALA:HB1	1:A:4592:LEU:HD21	1.93	0.49
1:A:1223:LYS:HD2	1:A:1283:TYR:CE2	2.47	0.49
1:A:2243:THR:HG21	1:A:2245:ARG:HE	1.76	0.49
1:A:4623:ASP:HA	1:A:4626:GLN:HE21	1.75	0.49
1:A:681:GLN:HA	1:A:684:MET:HG2	1.94	0.49
1:A:1216:GLN:O	1:A:1275:TYR:OH	2.28	0.49
1:A:4819:ASP:HA	1:A:4822:ARG:HB2	1.93	0.49
1:A:3164:PRO:HA	1:A:3167:ASN:HD22	1.76	0.49
1:A:3971:PHE:HE1	1:A:3975:MET:HE2	1.78	0.49
1:A:4096:LEU:HG	1:A:4113:HIS:NE2	2.27	0.49
1:A:766:PRO:O	1:A:770:LEU:N	2.46	0.49
1:A:1592:LEU:HD22	1:A:1606:VAL:HG22	1.94	0.49
1:A:1753:ALA:O	1:A:1757:MET:HG2	2.13	0.49
1:A:2589:ALA:O	1:A:2593:TYR:HD1	1.95	0.49
1:A:2947:ASP:HB3	1:A:2993:ILE:HG13	1.94	0.49
1:A:3063:ASP:OD1	1:A:3063:ASP:N	2.45	0.49
1:A:4480:LEU:HD22	1:A:4483:MET:HE2	1.94	0.49
1:A:4582:ILE:HA	1:A:4585:LEU:HG	1.93	0.49
1:A:4755:ILE:HG13	1:A:4951:PHE:HE2	1.77	0.49
1:A:4810:ARG:HH21	1:A:4862:LEU:HD21	1.78	0.49
1:A:758:PHE:CE2	1:A:787:HIS:HB3	2.48	0.49
1:A:591:TRP:HZ3	1:A:637:LEU:HB2	1.78	0.49
1:A:676:LEU:O	1:A:679:LEU:HG	2.13	0.49
1:A:2390:ASP:OD1	1:A:2391:LYS:N	2.46	0.49
1:A:4350:PRO:HG3	1:A:4402:LYS:NZ	2.28	0.49
1:A:4590:LEU:HG	1:A:4601:LEU:HD23	1.95	0.49
1:A:1633:LEU:HD21	1:A:1655:PHE:CE2	2.46	0.49
1:A:3332:ILE:O	1:A:3335:SER:OG	2.25	0.49
1:A:3989:LEU:HD22	1:A:4058:HIS:HB2	1.94	0.49
1:A:4228:GLU:HA	1:A:4231:ARG:HG2	1.94	0.49
1:A:1502:ASP:N	1:A:1502:ASP:OD1	2.45	0.48
1:A:831:TYR:HA	1:A:834:LYS:HZ3	1.78	0.48
1:A:3322:SER:OG	1:A:3323:ARG:N	2.45	0.48
1:A:4321:PRO:HG2	1:A:4323:GLN:HG3	1.94	0.48
1:A:3068:ILE:HG23	1:A:3103:LEU:HD13	1.95	0.48
1:A:3665:TRP:HD1	1:A:3710:PRO:HB3	1.79	0.48
1:A:3928:LEU:HD22	1:A:4072:LEU:HD13	1.96	0.48
1:A:4089:ILE:HD12	1:A:4149:TYR:CZ	2.48	0.48
1:A:5184:GLU:CD	1:A:5184:GLU:H	2.20	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1236:PHE:CD1	1:A:1282:SER:HB3	2.47	0.48
1:A:1283:TYR:HA	1:A:1286:PHE:CE2	2.49	0.48
1:A:2167:PRO:HA	1:A:2170:TYR:CE1	2.48	0.48
1:A:2461:TYR:O	1:A:2465:ARG:HG2	2.13	0.48
1:A:4089:ILE:HD12	1:A:4149:TYR:CE1	2.49	0.48
1:A:794:GLY:O	1:A:798:ARG:HG2	2.14	0.48
1:A:2388:ASP:OD1	1:A:2388:ASP:N	2.42	0.48
1:A:636:LEU:HB3	1:A:682:ARG:HH22	1.79	0.48
1:A:1283:TYR:HD1	1:A:1286:PHE:CE2	2.31	0.48
1:A:3793:SER:HB2	1:A:3856:MET:HB2	1.95	0.48
1:A:4966:GLN:O	1:A:4968:LYS:HG2	2.13	0.48
1:A:2221:PHE:CZ	1:A:2258:MET:HE2	2.48	0.48
1:A:2381:LEU:HD21	1:A:2437:ARG:NE	2.29	0.48
1:A:3090:VAL:HG11	1:A:3112:LEU:HD21	1.96	0.48
1:A:3382:GLU:HB3	1:A:3386:ARG:HH22	1.77	0.48
1:A:3687:LYS:HD2	1:A:5142:LYS:HE2	1.95	0.48
1:A:876:CYS:HA	1:A:879:ILE:HD12	1.96	0.48
1:A:1384:ASN:HB2	1:A:1387:ASP:HB2	1.94	0.48
1:A:1849:MET:HE1	1:A:1959:ILE:HG12	1.94	0.48
1:A:1969:VAL:HG12	1:A:1983:ARG:HB3	1.96	0.48
1:A:2207:VAL:HB	1:A:2210:PRO:HG3	1.96	0.48
1:A:2309:ASN:ND2	1:A:2315:MET:O	2.47	0.48
1:A:2385:GLN:OE1	1:A:2387:THR:N	2.47	0.48
1:A:2976:PRO:HG3	1:A:3006:ALA:HA	1.96	0.48
1:A:3164:PRO:O	1:A:3168:ARG:HG3	2.14	0.48
1:A:5119:THR:O	1:A:5123:GLN:HG2	2.13	0.48
1:A:2176:GLN:HA	1:A:2180:LEU:HD22	1.96	0.48
1:A:3425:ARG:NH2	1:A:5016:GLN:OE1	2.47	0.48
1:A:3585:ARG:HH22	1:A:3672:THR:HA	1.79	0.48
1:A:4441:GLY:O	1:A:4445:GLU:HG3	2.14	0.48
1:A:4524:ILE:HD12	1:A:4529:HIS:HD2	1.79	0.48
1:A:4871:PRO:HG2	1:A:4977:PRO:HD3	1.95	0.48
1:A:676:LEU:HD22	1:A:698:LEU:HD22	1.96	0.48
1:A:4706:ASP:OD2	1:A:4708:ARG:NH1	2.46	0.48
1:A:831:TYR:HD2	1:A:834:LYS:HD2	1.77	0.47
1:A:1158:ASP:HB3	1:A:1182:HIS:NE2	2.29	0.47
1:A:4089:ILE:O	1:A:4093:LEU:HG	2.14	0.47
1:A:962:GLU:HG3	1:A:998:CYS:SG	2.55	0.47
1:A:1236:PHE:CE1	1:A:1282:SER:HB3	2.49	0.47
1:A:1274:VAL:HG13	1:A:1279:TYR:HB3	1.97	0.47
1:A:1275:TYR:HA	1:A:1279:TYR:CE1	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2849:ALA:HB1	1:A:2856:PRO:HG2	1.95	0.47
1:A:4725:PHE:CD1	1:A:4725:PHE:C	2.92	0.47
1:A:687:ARG:NH2	1:A:734:MET:SD	2.88	0.47
1:A:3171:LYS:HE2	1:A:3171:LYS:HB2	1.71	0.47
1:A:3830:ARG:HH11	1:A:3892:PRO:HB3	1.78	0.47
1:A:3895:LEU:HB3	1:A:3901:HIS:CE1	2.49	0.47
1:A:859:THR:OG1	1:A:913:TRP:NE1	2.47	0.47
1:A:1054:LEU:HD23	1:A:1057:VAL:HG13	1.97	0.47
1:A:1996:VAL:HA	1:A:2212:TRP:HB2	1.95	0.47
1:A:2601:LEU:HD21	1:A:2648:PHE:HE2	1.79	0.47
1:A:2925:GLN:HG2	1:A:2929:GLN:HG2	1.96	0.47
1:A:3091:LYS:NZ	1:A:3095:GLU:OE2	2.47	0.47
1:A:3971:PHE:CD2	1:A:4088:VAL:HG12	2.49	0.47
1:A:536:SER:O	1:A:540:ILE:HG13	2.14	0.47
1:A:2225:GLN:HE21	1:A:2255:MET:HE1	1.78	0.47
1:A:1120:TRP:O	1:A:1124:GLU:HG2	2.14	0.47
1:A:1333:ARG:HB3	1:A:1335:TRP:CD1	2.48	0.47
1:A:1870:THR:N	1:A:1873:GLU:OE1	2.47	0.47
1:A:3300:LEU:HD23	1:A:3333:LEU:HD21	1.95	0.47
1:A:3382:GLU:HB2	1:A:3386:ARG:HH12	1.80	0.47
1:A:3716:LYS:NZ	1:A:3720:GLU:OE2	2.48	0.47
1:A:4354:LYS:O	1:A:4358:LYS:HG2	2.15	0.47
1:A:539:SER:O	1:A:542:GLN:HG3	2.14	0.47
1:A:792:LEU:HD23	1:A:792:LEU:HA	1.74	0.47
1:A:845:LEU:HD13	1:A:902:VAL:HG11	1.96	0.47
1:A:933:VAL:HG23	1:A:934:LYS:HG2	1.96	0.47
1:A:1171:ILE:HG22	1:A:1266:ARG:N	2.29	0.47
1:A:2408:MET:HE3	1:A:2412:CYS:SG	2.54	0.47
1:A:3076:LYS:HD3	1:A:3076:LYS:HA	1.61	0.47
1:A:3592:LYS:HA	1:A:3592:LYS:HD3	1.67	0.47
1:A:4344:ALA:HB2	1:A:4352:GLY:HA3	1.97	0.47
1:A:4936:ASN:HD21	1:A:4952:ASP:HB3	1.80	0.47
1:A:5015:LEU:HD23	1:A:5085:HIS:HD1	1.79	0.47
1:A:590:LEU:O	1:A:594:LEU:HG	2.15	0.47
1:A:687:ARG:NH2	1:A:730:PHE:O	2.47	0.47
1:A:880:ARG:O	1:A:883:SER:OG	2.32	0.47
1:A:978:CYS:SG	1:A:1024:LYS:HB2	2.55	0.47
1:A:1404:LYS:HA	1:A:1404:LYS:HE2	1.97	0.47
1:A:1819:ARG:HD2	1:A:1891:VAL:H	1.80	0.47
1:A:2323:GLN:NE2	1:A:2324:PRO:O	2.47	0.47
1:A:2561:LEU:HD13	1:A:2567:ARG:HH21	1.80	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2733:LEU:O	1:A:2736:VAL:HG22	2.15	0.47
1:A:3123:LEU:HB3	1:A:3128:TYR:CE2	2.49	0.47
1:A:3873:ASN:HB2	1:A:3876:LYS:HE3	1.96	0.47
1:A:4325:ASP:H	1:A:4708:ARG:HD2	1.79	0.47
1:A:4362:THR:HB	1:A:4366:GLN:NE2	2.29	0.47
1:A:4576:PRO:HD2	1:A:4757:GLU:HG3	1.96	0.47
1:A:4693:ASP:OD1	1:A:4693:ASP:N	2.47	0.47
1:A:5177:MET:HE3	1:A:5178:ALA:N	2.29	0.47
1:A:1351:GLN:NE2	1:A:1409:ASP:HB3	2.27	0.47
1:A:543:THR:OG1	1:A:548:ASN:ND2	2.48	0.47
1:A:699:HIS:CE1	1:A:756:PRO:HB2	2.50	0.47
1:A:3546:MET:O	1:A:3692:TYR:HB3	2.16	0.47
1:A:744:MET:HG2	1:A:761:TRP:CZ3	2.50	0.46
1:A:2354:LEU:HD22	1:A:2359:VAL:HG11	1.97	0.46
1:A:3934:LEU:HG	1:A:3935:LEU:HD23	1.97	0.46
1:A:1052:LEU:HD11	1:A:1116:PHE:HB2	1.98	0.46
1:A:1778:LEU:HA	1:A:1781:ILE:HD12	1.97	0.46
1:A:3614:LEU:HD23	1:A:3623:THR:HG21	1.96	0.46
1:A:4066:ASN:OD1	1:A:4067:SER:N	2.48	0.46
1:A:4338:ARG:CZ	1:A:4708:ARG:HH12	2.28	0.46
1:A:4383:TYR:HA	1:A:4391:HIS:CD2	2.50	0.46
1:A:527:GLN:HB3	1:A:589:TYR:HE2	1.80	0.46
1:A:673:ARG:HD2	1:A:702:MET:HA	1.97	0.46
1:A:1093:VAL:HG21	1:A:1120:TRP:CD2	2.50	0.46
1:A:1782:MET:HE2	1:A:1782:MET:HB2	1.86	0.46
1:A:3824:ARG:HA	1:A:3827:ASN:HD21	1.81	0.46
1:A:4623:ASP:OD1	1:A:4626:GLN:NE2	2.48	0.46
1:A:3379:THR:HG21	1:A:3391:ILE:HG12	1.97	0.46
1:A:3718:TYR:O	1:A:3721:GLU:HG2	2.16	0.46
1:A:4281:ARG:NH1	1:A:4741:TRP:O	2.48	0.46
1:A:4976:ILE:HG22	1:A:4978:THR:HG23	1.96	0.46
1:A:5149:GLU:HB2	1:A:5153:ARG:HD2	1.97	0.46
1:A:1419:GLN:HA	1:A:1422:SER:HB3	1.97	0.46
1:A:2225:GLN:OE1	1:A:2408:MET:HE1	2.15	0.46
1:A:3830:ARG:HA	1:A:3833:THR:HG22	1.98	0.46
1:A:4068:PHE:CZ	1:A:4072:LEU:HD12	2.51	0.46
1:A:4326:ARG:NH2	1:A:4636:ASP:O	2.49	0.46
1:A:4983:HIS:CG	1:A:4983:HIS:O	2.69	0.46
1:A:5004:PRO:O	1:A:5008:ILE:HG23	2.16	0.46
1:A:5138:ILE:O	1:A:5142:LYS:HD3	2.15	0.46
1:A:1233:PHE:HA	1:A:1236:PHE:CE1	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2865:GLU:OE1	1:A:2895:ASN:ND2	2.47	0.46
1:A:4167:LYS:O	1:A:4171:TYR:HB2	2.15	0.46
1:A:3971:PHE:HD2	1:A:4088:VAL:HG12	1.80	0.46
1:A:4650:LEU:HD23	1:A:4651:GLN:HE22	1.81	0.46
1:A:4677:TRP:CZ3	1:A:4678:GLU:HG3	2.50	0.46
1:A:757:LEU:HD11	1:A:761:TRP:CE2	2.51	0.46
1:A:837:GLU:HG3	1:A:885:VAL:HG22	1.96	0.46
1:A:1401:ILE:HA	1:A:1405:LYS:HB3	1.97	0.46
1:A:1860:ASP:HA	1:A:1880:ARG:NH2	2.31	0.46
1:A:3688:GLY:HA3	1:A:4983:HIS:O	2.16	0.46
1:A:4071:ASP:O	1:A:4075:THR:HG23	2.16	0.46
1:A:4313:GLN:HG3	1:A:4713:PRO:HG2	1.98	0.46
1:A:5045:GLN:NE2	1:A:5068:ASN:O	2.44	0.46
1:A:5193:VAL:O	1:A:5197:ALA:N	2.44	0.46
1:A:627:LEU:HD12	1:A:628:PHE:N	2.31	0.46
1:A:1154:LYS:O	1:A:1158:ASP:OD1	2.34	0.46
1:A:2243:THR:HG21	1:A:2245:ARG:NE	2.31	0.46
1:A:2931:TYR:CG	1:A:2932:PHE:N	2.84	0.46
1:A:3088:ASN:O	1:A:3092:ILE:HG12	2.16	0.46
1:A:4068:PHE:HA	1:A:4071:ASP:OD2	2.16	0.46
1:A:4093:LEU:O	1:A:4096:LEU:HB3	2.16	0.46
1:A:1719:GLN:O	1:A:1720:PRO:C	2.58	0.46
1:A:3325:LEU:HB2	1:A:3378:GLN:HE22	1.81	0.46
1:A:3835:TYR:CD1	1:A:3838:VAL:HG12	2.50	0.46
1:A:3956:ASP:HB3	1:A:3957:LYS:HE2	1.98	0.46
1:A:3982:LYS:HZ1	1:A:4066:ASN:HB3	1.79	0.46
1:A:712:TRP:CZ3	1:A:850:LYS:HE2	2.51	0.45
1:A:1410:ILE:HB	1:A:1414:ARG:HD3	1.98	0.45
1:A:1923:ASP:OD1	1:A:1923:ASP:N	2.44	0.45
1:A:2165:GLN:O	1:A:2168:TYR:HB2	2.15	0.45
1:A:3055:LEU:O	1:A:3058:THR:C	2.59	0.45
1:A:3924:PHE:CE1	1:A:3928:LEU:HD21	2.51	0.45
1:A:4253:ALA:HB1	1:A:4257:GLN:HG3	1.98	0.45
1:A:779:GLU:CD	1:A:783:ARG:HH21	2.25	0.45
1:A:829:ASP:OD1	1:A:830:THR:N	2.50	0.45
1:A:1022:LEU:HD11	1:A:1069:LYS:HE3	1.97	0.45
1:A:2501:VAL:HG12	1:A:2520:ILE:HD13	1.98	0.45
1:A:4987:TYR:CD1	1:A:4990:LEU:HD23	2.51	0.45
1:A:748:GLN:HB3	1:A:783:ARG:HH22	1.81	0.45
1:A:1236:PHE:HA	1:A:1239:GLU:HG2	1.97	0.45
1:A:3869:MET:C	1:A:3869:MET:HE2	2.40	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4119:PRO:HD2	1:A:4120:PHE:CE1	2.51	0.45
1:A:964:ARG:HD2	1:A:3278:PHE:CE2	2.50	0.45
1:A:1210:HIS:CD2	1:A:1211:TYR:H	2.34	0.45
1:A:1743:ARG:HH21	1:A:1812:MET:HE3	1.81	0.45
1:A:2028:PRO:HA	1:A:2062:VAL:HA	1.99	0.45
1:A:2992:ASP:C	1:A:2992:ASP:OD1	2.60	0.45
1:A:3640:ILE:HA	1:A:3643:ILE:HG12	1.97	0.45
1:A:564:GLN:NE2	1:A:565:GLN:HG2	2.31	0.45
1:A:3540:VAL:HA	1:A:3543:ALA:HB3	1.98	0.45
1:A:2166:ARG:N	1:A:2167:PRO:HD2	2.31	0.45
1:A:2955:ASP:OD1	1:A:3040:ARG:NH2	2.49	0.45
1:A:3091:LYS:HE2	1:A:3140:CYS:HB3	1.98	0.45
1:A:3163:ILE:HG22	1:A:3167:ASN:HD21	1.81	0.45
1:A:3971:PHE:CZ	1:A:4092:LEU:HG	2.52	0.45
1:A:4335:LYS:HG3	1:A:4338:ARG:NH1	2.31	0.45
1:A:4790:LEU:HD22	1:A:4828:ARG:HB3	1.98	0.45
1:A:4829:ILE:HG22	1:A:4869:LEU:HD21	1.98	0.45
1:A:1695:ARG:NH1	1:A:1701:LEU:O	2.50	0.45
1:A:2925:GLN:O	1:A:2929:GLN:N	2.50	0.45
1:A:3866:CYS:HA	1:A:3869:MET:SD	2.57	0.45
1:A:4419:ALA:O	1:A:4423:VAL:HG13	2.17	0.45
1:A:714:GLN:O	1:A:797:TYR:OH	2.28	0.45
1:A:1101:ILE:HD11	1:A:1105:GLN:HG2	1.98	0.45
1:A:2235:CYS:C	1:A:2237:PRO:HD3	2.42	0.45
1:A:2932:PHE:CE2	1:A:2963:VAL:HG21	2.52	0.45
1:A:4183:LEU:HD11	1:A:4934:LEU:HD13	1.99	0.45
1:A:4629:LYS:HD3	1:A:4629:LYS:HA	1.59	0.45
1:A:4955:LYS:HE2	1:A:4959:GLN:HE21	1.82	0.45
1:A:2047:TYR:HA	1:A:2050:VAL:HG22	1.99	0.45
1:A:2575:LEU:HD23	1:A:2578:LEU:HD12	1.98	0.45
1:A:3004:PRO:HA	1:A:3007:LYS:HG3	1.99	0.45
1:A:5174:LEU:H	1:A:5174:LEU:HD23	1.82	0.45
1:A:722:LEU:HD21	1:A:760:SER:OG	2.17	0.44
1:A:1274:VAL:HA	1:A:1278:LEU:HB2	1.99	0.44
1:A:1435:LEU:HD23	1:A:1477:PHE:HZ	1.82	0.44
1:A:3159:LYS:HB3	1:A:3159:LYS:HE2	1.63	0.44
1:A:4324:MET:HA	1:A:4708:ARG:HD3	1.98	0.44
1:A:4433:GLY:N	1:A:4434:PRO:HD3	2.32	0.44
1:A:4598:SER:O	1:A:4602:ILE:HG13	2.17	0.44
1:A:4755:ILE:HD13	1:A:4758:GLN:OE1	2.17	0.44
1:A:1057:VAL:HA	1:A:1060:VAL:HG12	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2257:PHE:HB2	1:A:2342:LYS:NZ	2.32	0.44
1:A:3745:GLN:O	1:A:3750:ARG:NH2	2.50	0.44
1:A:687:ARG:HH12	1:A:730:PHE:HD2	1.64	0.44
1:A:1472:TYR:CD2	1:A:1509:LEU:HD13	2.52	0.44
1:A:3982:LYS:HE2	1:A:4120:PHE:CE2	2.51	0.44
1:A:4272:ASN:ND2	1:A:4274:TRP:HB2	2.32	0.44
1:A:4285:SER:HA	1:A:4634:SER:HB2	2.00	0.44
1:A:4445:GLU:HB2	1:A:4446:MET:CE	2.45	0.44
1:A:4762:LYS:HG2	1:A:4769:TRP:CZ3	2.52	0.44
1:A:4942:GLU:N	1:A:4942:GLU:OE1	2.50	0.44
1:A:3105:LEU:O	1:A:3107:ASN:N	2.51	0.44
1:A:3830:ARG:NH1	1:A:3892:PRO:HB3	2.33	0.44
1:A:4689:LEU:HA	1:A:4692:LEU:HG	1.98	0.44
1:A:1826:GLN:OE1	1:A:1826:GLN:N	2.47	0.44
1:A:2623:GLN:OE1	1:A:2641:VAL:HG23	2.18	0.44
1:A:3099:MET:HG3	1:A:3147:ARG:HB2	2.00	0.44
1:A:3723:TRP:HE1	1:A:3735:LEU:HD21	1.82	0.44
1:A:4080:ASP:OD1	1:A:4080:ASP:N	2.51	0.44
1:A:4173:LEU:HD13	1:A:4941:VAL:HG23	2.00	0.44
1:A:4202:GLY:O	1:A:4206:LYS:HG2	2.17	0.44
1:A:5050:THR:O	1:A:5056:MET:HB2	2.17	0.44
1:A:694:ALA:O	1:A:697:VAL:HG12	2.18	0.44
1:A:892:ASP:OD1	1:A:892:ASP:N	2.51	0.44
1:A:1080:ARG:HG2	1:A:1081:LEU:HD22	1.99	0.44
1:A:2686:MET:CE	1:A:2721:LEU:HD12	2.48	0.44
1:A:3610:ASN:HB3	1:A:3613:ALA:HB3	1.99	0.44
1:A:1789:LEU:HB3	1:A:1790:PRO:HD3	1.99	0.44
1:A:3849:HIS:HB3	1:A:3861:PHE:HE2	1.82	0.44
1:A:4249:GLY:N	1:A:4250:PRO:HD3	2.33	0.44
1:A:4341:VAL:HG22	1:A:4353:ILE:HG23	1.99	0.44
1:A:4483:MET:SD	1:A:4559:LEU:HG	2.57	0.44
1:A:4806:TYR:HE1	1:A:4811:GLY:HA3	1.83	0.44
1:A:4826:HIS:HA	1:A:4829:ILE:HD11	2.00	0.44
1:A:4998:MET:HE1	1:A:5040:GLY:H	1.82	0.44
1:A:591:TRP:CZ3	1:A:637:LEU:HB2	2.53	0.44
1:A:1029:LEU:HD22	1:A:1060:VAL:HG23	1.99	0.44
1:A:1819:ARG:HA	1:A:1851:THR:HG21	2.00	0.44
1:A:2100:LEU:HB3	1:A:2102:ARG:HH12	1.83	0.44
1:A:5126:LEU:HD11	1:A:5200:LEU:HD23	2.00	0.44
1:A:5160:ASP:HA	1:A:5163:VAL:HG22	2.00	0.44
1:A:1059:HIS:O	1:A:1063:LEU:HD23	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2251:VAL:O	1:A:2255:MET:HG3	2.16	0.44
1:A:3300:LEU:HD23	1:A:3333:LEU:HD11	2.00	0.44
1:A:3729:ILE:HG23	1:A:3730:THR:HG23	2.00	0.44
1:A:4990:LEU:O	1:A:4994:ILE:HG12	2.17	0.44
1:A:1035:LYS:HA	1:A:1035:LYS:HE3	2.00	0.43
1:A:3115:ALA:HA	1:A:3129:VAL:HG21	2.00	0.43
1:A:3920:TRP:HE3	1:A:3923:ILE:HD11	1.82	0.43
1:A:4014:HIS:HE2	1:A:4035:CYS:HB3	1.82	0.43
1:A:4631:LEU:HD13	1:A:4754:HIS:CE1	2.46	0.43
1:A:668:ILE:HG21	1:A:672:TRP:HZ2	1.83	0.43
1:A:994:THR:HA	1:A:997:LYS:HD3	2.00	0.43
1:A:2172:ARG:NH2	1:A:2173:ARG:HE	2.13	0.43
1:A:3060:PHE:HB3	1:A:3065:GLN:HA	2.00	0.43
1:A:3101:LEU:HD23	1:A:3149:ILE:HB	2.00	0.43
1:A:3864:MET:SD	1:A:3916:VAL:HB	2.58	0.43
1:A:4925:VAL:HA	1:A:4929:LEU:HD12	2.01	0.43
1:A:553:PHE:HE1	1:A:628:PHE:CD2	2.36	0.43
1:A:619:LYS:HE2	1:A:619:LYS:HB2	1.90	0.43
1:A:3089:ARG:HA	1:A:3089:ARG:HD3	1.83	0.43
1:A:3645:ARG:HD3	1:A:3698:HIS:NE2	2.33	0.43
1:A:4971:LEU:HD23	1:A:4971:LEU:HA	1.79	0.43
1:A:2855:MET:HG2	1:A:2858:LYS:HG2	1.99	0.43
1:A:2992:ASP:OD1	1:A:2993:ILE:HG12	2.18	0.43
1:A:4153:TYR:CE1	1:A:4157:LEU:HD11	2.53	0.43
1:A:4341:VAL:HG22	1:A:4353:ILE:HG12	1.99	0.43
1:A:5190:CYS:SG	1:A:5191:VAL:N	2.91	0.43
1:A:692:LEU:HB2	1:A:743:PHE:CE2	2.41	0.43
1:A:764:LEU:C	1:A:766:PRO:HD3	2.44	0.43
1:A:3211:LYS:HB3	1:A:3211:LYS:HE3	1.88	0.43
1:A:3435:GLY:C	1:A:3437:TRP:H	2.27	0.43
1:A:3689:GLU:HA	1:A:4986:ASN:HB3	2.00	0.43
1:A:4274:TRP:HA	1:A:4277:VAL:HG12	2.01	0.43
1:A:4712:ASN:OD1	1:A:4715:ALA:N	2.43	0.43
1:A:1819:ARG:HG3	1:A:1891:VAL:HG23	2.01	0.43
1:A:2307:PHE:CZ	1:A:2404:LEU:HD12	2.53	0.43
1:A:2461:TYR:HA	1:A:2464:VAL:HG12	2.01	0.43
1:A:4668:LEU:HD22	1:A:4674:ARG:HA	2.01	0.43
1:A:4930:THR:HA	1:A:4933:ILE:HG22	2.01	0.43
1:A:584:LYS:HB2	1:A:584:LYS:HE2	1.76	0.43
1:A:912:ARG:HG3	1:A:912:ARG:HH11	1.84	0.43
1:A:1337:LYS:HA	1:A:1337:LYS:HD3	1.79	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4088:VAL:HG23	1:A:4089:ILE:HG13	2.00	0.43
1:A:4522:GLN:NE2	1:A:4531:PRO:O	2.48	0.43
1:A:4562:PRO:HB3	1:A:4619:HIS:CD2	2.54	0.43
1:A:1231:HIS:NE2	1:A:1309:ASP:OD2	2.33	0.43
1:A:1625:ASP:OD1	1:A:1625:ASP:C	2.61	0.43
1:A:1881:CYS:SG	1:A:1924:TYR:HB2	2.59	0.43
1:A:4007:PRO:HB2	1:A:4051:HIS:HD2	1.84	0.43
1:A:4411:SER:OG	1:A:4412:PRO:HD3	2.19	0.43
1:A:4932:LEU:HD12	1:A:4963:ARG:NH2	2.34	0.43
1:A:940:ARG:NE	1:A:989:ASP:OD2	2.51	0.43
1:A:1499:LEU:HD11	1:A:1506:PRO:HD3	2.01	0.43
1:A:2590:GLU:OE2	1:A:2623:GLN:NE2	2.51	0.43
1:A:2650:TRP:HB2	1:A:2761:LEU:HD21	2.00	0.43
1:A:3220:GLY:CA	1:A:3431:GLY:H	2.32	0.43
1:A:3699:MET:SD	1:A:3701:LEU:HG	2.59	0.43
1:A:3734:GLY:O	1:A:3738:LYS:HB2	2.19	0.43
1:A:4822:ARG:HH11	1:A:4822:ARG:HG2	1.83	0.43
1:A:5127:ASP:OD1	1:A:5127:ASP:N	2.44	0.43
1:A:644:LEU:O	1:A:648:LEU:HD22	2.18	0.42
1:A:741:LEU:O	1:A:745:ARG:HG2	2.19	0.42
1:A:1238:ARG:O	1:A:1242:GLU:HG2	2.19	0.42
1:A:1380:ASN:HA	1:A:1383:ASP:OD2	2.19	0.42
1:A:2846:VAL:HG13	1:A:2889:LEU:HD21	2.01	0.42
1:A:2935:PHE:HD1	1:A:2935:PHE:O	2.02	0.42
1:A:2987:PHE:HD1	1:A:2987:PHE:O	2.01	0.42
1:A:3682:ASN:HA	1:A:4981:TYR:HE2	1.85	0.42
1:A:4374:THR:O	1:A:4378:GLU:HG2	2.19	0.42
1:A:4460:GLU:HA	1:A:4463:GLU:HB2	2.00	0.42
1:A:4644:LEU:HA	1:A:4647:ARG:HG2	2.01	0.42
1:A:4726:LEU:HD23	1:A:4726:LEU:HA	1.92	0.42
1:A:4890:LEU:HD23	1:A:4890:LEU:HA	1.90	0.42
1:A:1121:GLN:HB3	1:A:1125:LYS:NZ	2.34	0.42
1:A:1934:TRP:HB3	1:A:1937:CYS:SG	2.59	0.42
1:A:4618:GLN:HA	1:A:4621:LEU:HD12	2.00	0.42
1:A:4784:LEU:HD21	1:A:4888:ILE:HD13	2.01	0.42
1:A:877:ARG:HD3	1:A:880:ARG:NH2	2.35	0.42
1:A:1816:PRO:HB3	1:A:1887:LEU:HD12	2.02	0.42
1:A:2094:LEU:HG	1:A:2096:ILE:HG13	2.01	0.42
1:A:2302:PRO:HB3	1:A:2335:HIS:HE1	1.84	0.42
1:A:2302:PRO:HB3	1:A:2335:HIS:CE1	2.54	0.42
1:A:2490:ASN:ND2	1:A:2524:CYS:HB3	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2896:ARG:HD3	1:A:2896:ARG:HA	1.58	0.42
1:A:2907:GLU:O	1:A:2911:ILE:HG13	2.19	0.42
1:A:3959:LEU:HD12	1:A:3962:ASN:O	2.20	0.42
1:A:3971:PHE:CD1	1:A:3971:PHE:C	2.97	0.42
1:A:545:ASP:OD1	1:A:545:ASP:N	2.51	0.42
1:A:2230:GLU:HA	1:A:2234:PHE:CD2	2.54	0.42
1:A:3929:PHE:CE2	1:A:3951:HIS:HB3	2.54	0.42
1:A:5131:LEU:O	1:A:5135:GLU:HG2	2.19	0.42
1:A:540:ILE:C	1:A:542:GLN:N	2.78	0.42
1:A:1158:ASP:OD1	1:A:1158:ASP:N	2.52	0.42
1:A:2935:PHE:CZ	1:A:3003:LEU:HB2	2.54	0.42
1:A:3689:GLU:OE1	1:A:4983:HIS:NE2	2.53	0.42
1:A:4552:ARG:HG2	1:A:4853:LYS:NZ	2.34	0.42
1:A:643:TRP:O	1:A:647:LEU:HG	2.19	0.42
1:A:737:THR:O	1:A:740:LEU:HG	2.19	0.42
1:A:796:TYR:HB2	1:A:847:VAL:HG13	2.00	0.42
1:A:1037:TRP:CD1	1:A:1050:HIS:HE2	2.38	0.42
1:A:2019:PRO:HB2	1:A:2052:VAL:HG13	2.02	0.42
1:A:2300:SER:HG	1:A:2301:GLU:CD	2.21	0.42
1:A:2495:ILE:HD12	1:A:2498:ILE:HD13	2.00	0.42
1:A:2739:ARG:HB3	1:A:2742:ILE:HG12	2.00	0.42
1:A:4134:ILE:O	1:A:4137:LEU:HG	2.20	0.42
1:A:4295:LEU:HA	1:A:4300:ARG:NH2	2.34	0.42
1:A:831:TYR:O	1:A:835:ILE:HG12	2.20	0.42
1:A:2421:GLU:OE2	1:A:2528:ARG:NH1	2.53	0.42
1:A:2575:LEU:HD23	1:A:2575:LEU:HA	1.87	0.42
1:A:3714:LYS:HD2	1:A:3714:LYS:HA	1.83	0.42
1:A:3947:LEU:O	1:A:3951:HIS:HB2	2.20	0.42
1:A:3979:CYS:O	1:A:3983:GLU:HG2	2.20	0.42
1:A:4264:LYS:HE3	1:A:4305:VAL:HG12	2.02	0.42
1:A:4601:LEU:HA	1:A:4604:ILE:HG22	2.01	0.42
1:A:1754:ARG:HA	1:A:1757:MET:HG2	2.01	0.42
1:A:2772:GLY:C	1:A:2774:SER:H	2.26	0.42
1:A:3953:PHE:O	1:A:3957:LYS:HG2	2.20	0.42
1:A:4446:MET:HE1	1:A:4643:HIS:HE2	1.85	0.42
1:A:915:ARG:NH1	1:A:3276:GLY:O	2.44	0.42
1:A:1025:PHE:HD1	1:A:1025:PHE:O	2.03	0.42
1:A:1313:LYS:NZ	1:A:2923:LEU:HD21	2.35	0.42
1:A:4987:TYR:HD1	1:A:4990:LEU:HD23	1.85	0.42
1:A:759:ARG:O	1:A:763:SER:OG	2.28	0.42
1:A:1304:ASP:OD1	1:A:1304:ASP:C	2.63	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1516:LEU:HD12	1:A:1516:LEU:HA	1.91	0.42
1:A:1567:LEU:HA	1:A:1568:PRO:HD3	1.93	0.42
1:A:1598:LYS:HA	1:A:1598:LYS:HD2	1.84	0.42
1:A:2234:PHE:CE2	1:A:2248:LYS:HD3	2.55	0.42
1:A:4258:CYS:SG	1:A:4262:GLN:NE2	2.93	0.42
1:A:4263:VAL:HG12	1:A:4264:LYS:HE2	2.01	0.42
1:A:4404:ILE:HG13	1:A:4410:LEU:HD12	2.00	0.42
1:A:4760:ASN:C	1:A:4762:LYS:H	2.28	0.42
1:A:4764:ARG:HG3	1:A:4765:VAL:HG13	2.01	0.42
1:A:2657:MET:HE1	1:A:2795:LEU:HD12	2.02	0.41
1:A:3187:ILE:HA	1:A:3190:GLU:HB3	2.02	0.41
1:A:3652:LEU:HD23	1:A:3662:ARG:HG3	2.02	0.41
1:A:4670:THR:OG1	1:A:4671:LYS:N	2.53	0.41
1:A:4840:ARG:HG3	1:A:4841:ARG:N	2.35	0.41
1:A:4940:GLN:CG	1:A:4948:VAL:HB	2.50	0.41
1:A:5001:ASP:N	1:A:5073:LYS:O	2.45	0.41
1:A:5092:ARG:NH2	1:A:5205:GLU:OE1	2.51	0.41
1:A:5104:ARG:HH22	1:A:5147:GLN:HA	1.85	0.41
1:A:5153:ARG:HG3	1:A:5155:GLN:N	2.33	0.41
1:A:751:LEU:HD22	1:A:758:PHE:HB2	2.02	0.41
1:A:1759:ARG:O	1:A:1763:GLU:HB2	2.20	0.41
1:A:3709:VAL:HG11	1:A:3767:TYR:HD1	1.85	0.41
1:A:5044:MET:HB3	1:A:5072:LEU:HD12	2.01	0.41
1:A:1061:PHE:CD2	1:A:1119:ILE:HD11	2.55	0.41
1:A:1120:TRP:CD1	1:A:1136:VAL:HG11	2.55	0.41
1:A:1294:LYS:HE2	1:A:1331:ASP:OD2	2.20	0.41
1:A:2172:ARG:HE	1:A:2173:ARG:HG3	1.84	0.41
1:A:2585:LEU:HD23	1:A:2585:LEU:HA	1.87	0.41
1:A:3019:LYS:HG3	1:A:3059:PHE:CE1	2.55	0.41
1:A:3253:GLU:OE2	1:A:3253:GLU:HA	2.21	0.41
1:A:3859:ASP:OD2	1:A:3896:ILE:HD11	2.21	0.41
1:A:4577:VAL:HG22	1:A:4630:MET:HE2	2.03	0.41
1:A:4631:LEU:HD12	1:A:4633:HIS:CD2	2.54	0.41
1:A:4729:LEU:HD13	1:A:4730:PRO:HD2	2.03	0.41
1:A:5160:ASP:N	1:A:5160:ASP:OD1	2.51	0.41
1:A:1884:LEU:HD11	1:A:1919:GLN:HB3	2.02	0.41
1:A:2303:HIS:HB3	1:A:2305:TYR:CE1	2.56	0.41
1:A:2662:LEU:HB2	1:A:2731:LEU:HD22	2.02	0.41
1:A:2813:SER:O	1:A:2856:PRO:HG3	2.20	0.41
1:A:3776:MET:HE2	1:A:3818:TYR:OH	2.20	0.41
1:A:4069:PHE:O	1:A:4073:VAL:HG22	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4375:LEU:HG	1:A:4422:LEU:HD22	2.01	0.41
1:A:4673:MET:HA	1:A:4676:ASN:HD22	1.86	0.41
1:A:4911:ASP:HB3	1:A:4974:LYS:NZ	2.32	0.41
1:A:1160:LEU:HA	1:A:1224:ILE:HD11	2.01	0.41
1:A:2180:LEU:HD23	1:A:2181:ASP:H	1.85	0.41
1:A:2527:TYR:OH	1:A:2569:HIS:O	2.25	0.41
1:A:3130:ASP:HB3	1:A:3139:LYS:HG2	2.02	0.41
1:A:3648:ASN:HD21	1:A:3711:PHE:HA	1.86	0.41
1:A:3776:MET:HE1	1:A:3825:LEU:HB3	2.02	0.41
1:A:3922:ARG:HH21	1:A:3959:LEU:C	2.28	0.41
1:A:4072:LEU:HD23	1:A:4072:LEU:HA	1.82	0.41
1:A:4242:PHE:CZ	1:A:4256:LYS:HA	2.54	0.41
1:A:4504:THR:HA	1:A:4510:PRO:HA	2.03	0.41
1:A:5138:ILE:HD12	1:A:5138:ILE:HA	1.90	0.41
1:A:691:TRP:CD1	1:A:692:LEU:N	2.87	0.41
1:A:1029:LEU:HD23	1:A:1029:LEU:HA	1.86	0.41
1:A:2419:MET:HE2	1:A:2579:VAL:HG11	2.02	0.41
1:A:3325:LEU:HB2	1:A:3378:GLN:NE2	2.36	0.41
1:A:3571:ASP:OD1	1:A:3571:ASP:N	2.53	0.41
1:A:3773:LEU:HD23	1:A:3773:LEU:HA	1.94	0.41
1:A:4148:ASP:OD1	1:A:4148:ASP:N	2.52	0.41
1:A:4312:LYS:HD2	1:A:4312:LYS:HA	1.76	0.41
1:A:4326:ARG:CZ	1:A:4636:ASP:HB3	2.50	0.41
1:A:4916:THR:OG1	1:A:4917:GLU:N	2.51	0.41
1:A:588:ARG:HE	1:A:588:ARG:HB3	1.73	0.41
1:A:969:GLU:H	1:A:969:GLU:CD	2.29	0.41
1:A:1022:LEU:HB3	1:A:1073:ASN:OD1	2.21	0.41
1:A:1270:GLU:HG2	1:A:1271:LEU:H	1.86	0.41
1:A:1438:ILE:HD13	1:A:1438:ILE:HA	1.92	0.41
1:A:2309:ASN:HB2	1:A:2314:THR:O	2.21	0.41
1:A:3272:ALA:HB2	1:A:3605:ALA:HB1	2.02	0.41
1:A:3786:PHE:CZ	1:A:3842:LEU:HB3	2.56	0.41
1:A:2562:ARG:HE	1:A:2562:ARG:HB2	1.60	0.41
1:A:2594:ILE:HD12	1:A:2641:VAL:HG21	2.02	0.41
1:A:3106:GLN:NE2	1:A:3160:HIS:O	2.51	0.41
1:A:3687:LYS:HB2	1:A:5143:ASN:HB3	2.03	0.41
1:A:3708:ASN:HB3	1:A:3766:CYS:HB3	2.03	0.41
1:A:3846:ARG:O	1:A:3846:ARG:NH1	2.53	0.41
1:A:4564:ARG:HH11	1:A:4564:ARG:HA	1.85	0.41
1:A:4647:ARG:C	1:A:4651:GLN:HE21	2.28	0.41
1:A:731:ARG:O	1:A:731:ARG:NH1	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:753:ILE:HD12	1:A:753:ILE:HA	1.92	0.41
1:A:831:TYR:HA	1:A:834:LYS:NZ	2.35	0.41
1:A:895:GLY:C	1:A:897:ASN:N	2.75	0.41
1:A:1179:ALA:O	1:A:1183:SER:N	2.50	0.41
1:A:1764:LEU:HA	1:A:1767:MET:SD	2.60	0.41
1:A:1799:LEU:HD23	1:A:1799:LEU:HA	1.79	0.41
1:A:2056:LEU:HB2	1:A:2097:VAL:HG22	2.03	0.41
1:A:2222:LEU:HD12	1:A:2222:LEU:HA	1.92	0.41
1:A:3218:PHE:O	1:A:3221:TYR:HB2	2.21	0.41
1:A:3425:ARG:HD3	1:A:5089:GLN:HE22	1.85	0.41
1:A:3550:GLN:HB2	1:A:3696:GLN:HA	2.03	0.41
1:A:3707:ASN:OD1	1:A:3707:ASN:N	2.53	0.41
1:A:3884:GLN:HA	1:A:3887:LYS:NZ	2.34	0.41
1:A:3942:PRO:HA	1:A:3945:GLN:HG2	2.02	0.41
1:A:4083:PRO:HA	1:A:4084:PRO:HD3	1.97	0.41
1:A:4699:MET:SD	1:A:4700:ASN:N	2.94	0.41
1:A:4800:ASN:HA	1:A:4979:LEU:HD23	2.03	0.41
1:A:4937:CYS:SG	1:A:4949:GLN:NE2	2.94	0.41
1:A:5005:SER:HA	1:A:5008:ILE:HG12	2.03	0.41
1:A:692:LEU:HD21	1:A:744:MET:HE2	2.03	0.41
1:A:2822:PHE:CE2	1:A:2863:LEU:HB3	2.57	0.41
1:A:2984:LEU:HD23	1:A:2984:LEU:HA	1.87	0.41
1:A:3577:SER:O	1:A:3581:VAL:HG22	2.21	0.41
1:A:4328:LEU:HD12	1:A:4703:ILE:HA	2.02	0.41
1:A:4402:LYS:O	1:A:4406:GLU:HB2	2.21	0.41
1:A:4571:ASP:C	1:A:4572:ARG:HG2	2.46	0.41
1:A:751:LEU:HD13	1:A:780:HIS:CD2	2.56	0.40
1:A:826:ARG:O	1:A:830:THR:OG1	2.31	0.40
1:A:1618:ARG:HG2	1:A:1677:CYS:SG	2.61	0.40
1:A:4053:GLU:O	1:A:4057:LYS:HG2	2.21	0.40
1:A:4151:GLN:O	1:A:4154:LEU:HG	2.21	0.40
1:A:587:LYS:HD3	1:A:590:LEU:HD21	2.03	0.40
1:A:1229:ASP:OD1	1:A:1229:ASP:N	2.46	0.40
1:A:2359:VAL:HG23	1:A:2361:PHE:HB2	2.02	0.40
1:A:3013:SER:C	1:A:3015:MET:H	2.28	0.40
1:A:3257:ILE:O	1:A:3260:ASN:HB2	2.21	0.40
1:A:3973:ALA:O	1:A:3977:THR:OG1	2.37	0.40
1:A:4367:GLN:HA	1:A:4370:TYR:CD2	2.56	0.40
1:A:4645:VAL:HG22	1:A:4689:LEU:HD11	2.04	0.40
1:A:5143:ASN:OD1	1:A:5143:ASN:N	2.55	0.40
1:A:934:LYS:HB3	1:A:934:LYS:HE3	1.87	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1695:ARG:HG2	1:A:1701:LEU:O	2.21	0.40
1:A:2038:ALA:O	1:A:2041:PRO:HD2	2.21	0.40
1:A:2322:LEU:HB2	1:A:2361:PHE:HZ	1.87	0.40
1:A:2644:CYS:HA	1:A:2692:CYS:SG	2.61	0.40
1:A:4429:LEU:HA	1:A:4595:SER:HB3	2.03	0.40
1:A:4982:ARG:O	1:A:4983:HIS:ND1	2.54	0.40
1:A:5199:VAL:O	1:A:5202:TRP:HB3	2.21	0.40
1:A:552:PHE:HA	1:A:555:GLN:CD	2.46	0.40
1:A:553:PHE:CE2	1:A:668:ILE:HD13	2.56	0.40
1:A:751:LEU:HA	1:A:751:LEU:HD23	1.83	0.40
1:A:1452:ALA:HB1	1:A:1458:ASP:O	2.22	0.40
1:A:2862:PRO:HG2	1:A:2869:ILE:HD13	2.04	0.40
1:A:3753:ALA:O	1:A:3756:HIS:NE2	2.54	0.40
1:A:4175:ILE:HG12	1:A:4226:LEU:HB3	2.04	0.40
1:A:5096:GLU:OE1	1:A:5096:GLU:N	2.46	0.40
1:A:964:ARG:HD2	1:A:3278:PHE:HE2	1.86	0.40
1:A:1407:LEU:HD12	1:A:1407:LEU:HA	1.95	0.40
1:A:2173:ARG:O	1:A:2180:LEU:HB2	2.22	0.40
1:A:2221:PHE:CE1	1:A:2258:MET:HE2	2.56	0.40
1:A:4994:ILE:HG21	1:A:5076:ILE:HD11	2.04	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	4439/4841 (92%)	4117 (93%)	316 (7%)	6 (0%)	48 79

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	896	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2787	GLN
1	A	2922	ILE
1	A	541	LEU
1	A	2790	ALA
1	A	1423	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	3999/4329 (92%)	3978 (100%)	21 (0%)	81	81

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	899	VAL
1	A	1220	MET
1	A	1632	MET
1	A	1832	LEU
1	A	1890	LYS
1	A	1919	GLN
1	A	1999	SER
1	A	2026	ILE
1	A	2058	VAL
1	A	2134	PRO
1	A	2136	LYS
1	A	2418	ILE
1	A	2721	LEU
1	A	2939	TYR
1	A	3059	PHE
1	A	3161	PHE
1	A	3258	LEU
1	A	3316	THR
1	A	3379	THR
1	A	3728	TYR
1	A	3951	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	548	ASN
1	A	597	HIS
1	A	678	ASN
1	A	780	HIS
1	A	852	HIS
1	A	904	GLN
1	A	973	GLN
1	A	1121	GLN
1	A	1166	ASN
1	A	1210	HIS
1	A	1312	ASN
1	A	1350	HIS
1	A	1351	GLN
1	A	1384	ASN
1	A	1574	HIS
1	A	1590	ASN
1	A	1889	HIS
1	A	1907	GLN
1	A	1919	GLN
1	A	2223	ASN
1	A	2399	ASN
1	A	2584	GLN
1	A	2599	GLN
1	A	2623	GLN
1	A	2652	HIS
1	A	2661	GLN
1	A	2803	HIS
1	A	3057	GLN
1	A	3177	ASN
1	A	3378	GLN
1	A	3433	HIS
1	A	3551	ASN
1	A	3611	GLN
1	A	3615	GLN
1	A	3682	ASN
1	A	3697	ASN
1	A	3744	GLN
1	A	3761	GLN
1	A	3826	GLN
1	A	3827	ASN
1	A	3840	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	3848	ASN
1	A	3901	HIS
1	A	3995	GLN
1	A	4066	ASN
1	A	4099	GLN
1	A	4196	ASN
1	A	4197	HIS
1	A	4262	GLN
1	A	4275	HIS
1	A	4286	GLN
1	A	4293	GLN
1	A	4314	GLN
1	A	4366	GLN
1	A	4386	HIS
1	A	4529	HIS
1	A	4563	GLN
1	A	4619	HIS
1	A	4651	GLN
1	A	4653	GLN
1	A	4676	ASN
1	A	4728	HIS
1	A	4754	HIS
1	A	4802	GLN
1	A	4816	HIS
1	A	4837	ASN
1	A	4850	ASN
1	A	4936	ASN
1	A	4959	GLN
1	A	4996	ASN
1	A	5059	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ATP	A	5301	3	32,33,33	1.45	5 (15%)	48,52,52	1.85	12 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	A	5301	3	-	3/22/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	5301	ATP	C5-C4	3.61	1.45	1.39
2	A	5301	ATP	C5-N7	-2.83	1.33	1.39
2	A	5301	ATP	C4-N9	-2.75	1.32	1.37
2	A	5301	ATP	PB-O3B	-2.42	1.56	1.59
2	A	5301	ATP	C8-N9	-2.03	1.34	1.37

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5301	ATP	C5-C4-N3	-5.33	119.38	126.72
2	A	5301	ATP	N3-C4-N9	4.82	135.37	127.17
2	A	5301	ATP	C4-N9-C8	3.74	109.67	105.74
2	A	5301	ATP	C2-N3-C4	3.46	120.28	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5301	ATP	N3-C2-N1	-3.08	123.92	128.58
2	A	5301	ATP	O5'-C5'-C4'	-2.85	99.30	108.99
2	A	5301	ATP	N9-C8-N7	-2.38	110.56	113.94
2	A	5301	ATP	C4-C5-N7	-2.38	107.86	110.58
2	A	5301	ATP	O2B-PB-O1B	2.35	123.38	112.44
2	A	5301	ATP	O2A-PA-O1A	2.30	123.15	112.44
2	A	5301	ATP	C5'-C4'-C3'	-2.25	107.10	115.21
2	A	5301	ATP	C5-N7-C8	2.04	106.66	103.45

There are no chirality outliers.

All (3) torsion outliers are listed below:

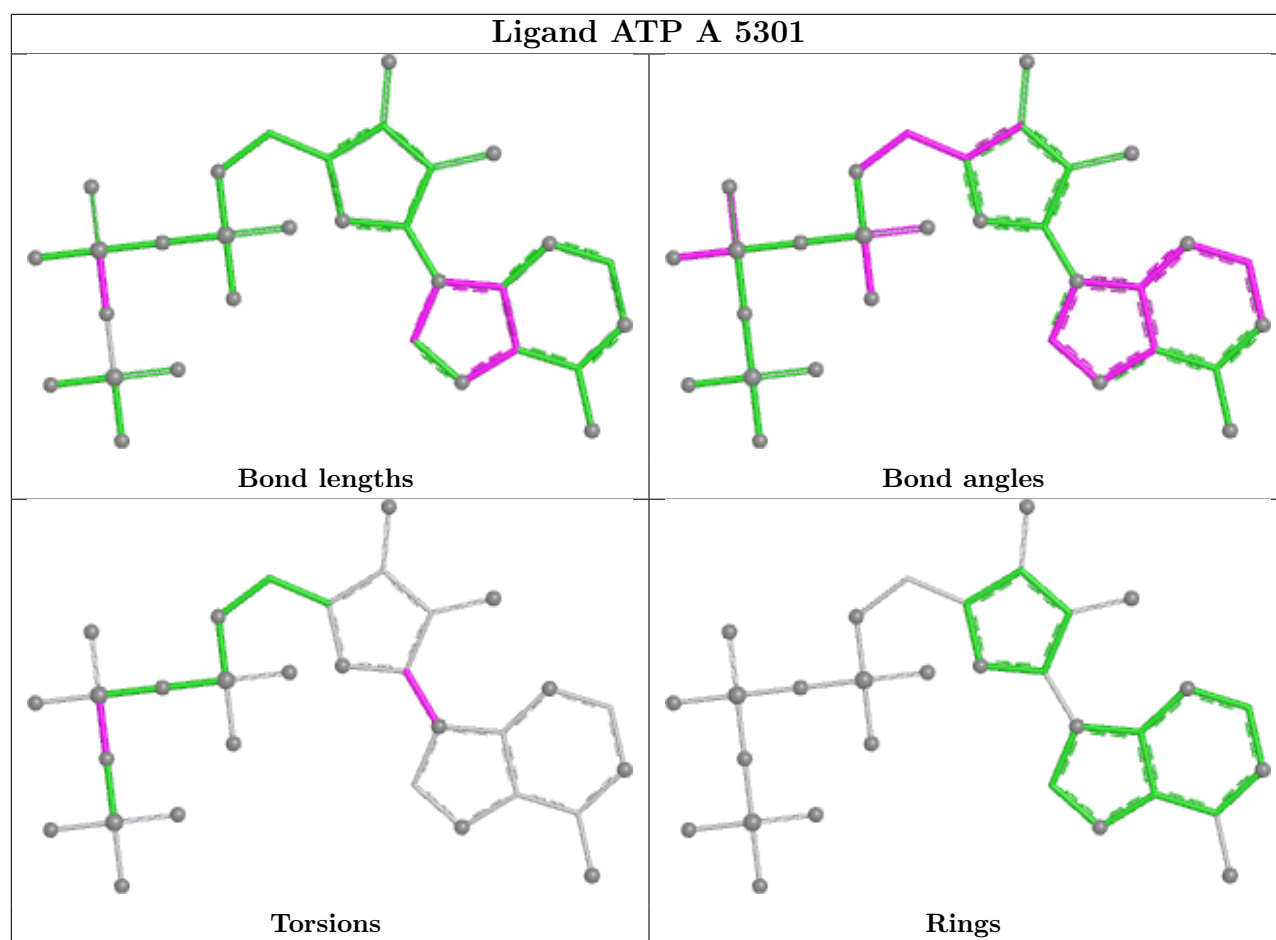
Mol	Chain	Res	Type	Atoms
2	A	5301	ATP	O4'-C1'-N9-C4
2	A	5301	ATP	O4'-C1'-N9-C8
2	A	5301	ATP	PG-O3B-PB-O2B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5301	ATP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

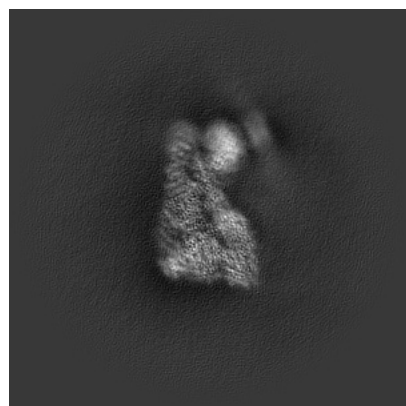
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61848. These allow visual inspection of the internal detail of the map and identification of artifacts.

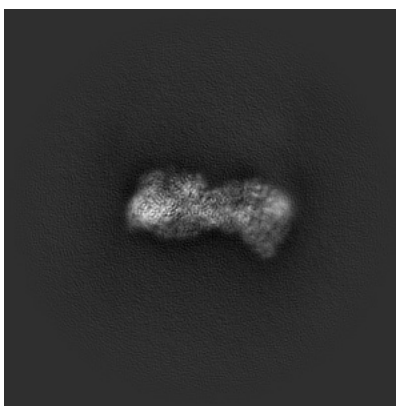
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

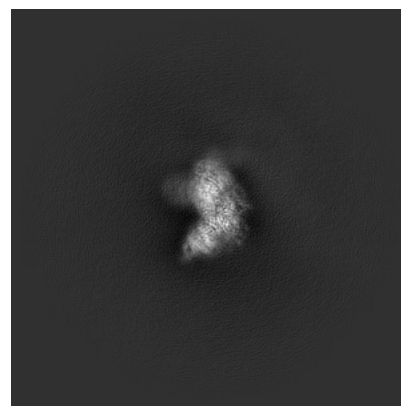
6.1.1 Primary map



X

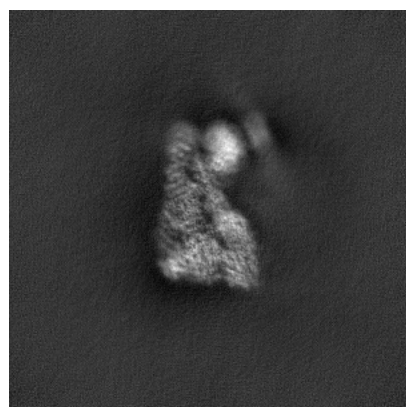


Y

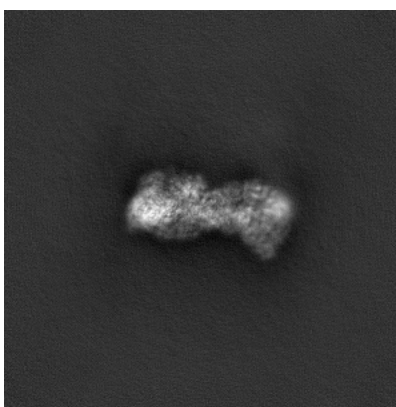


Z

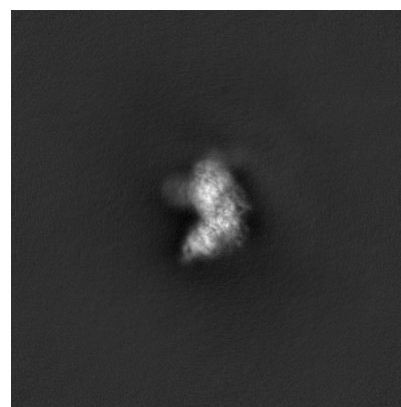
6.1.2 Raw map



X



Y

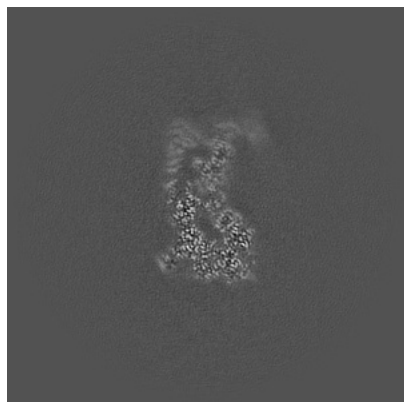


Z

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

6.2 Central slices [i](#)

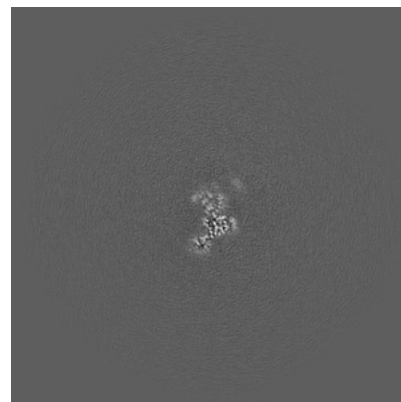
6.2.1 Primary map



X Index: 250

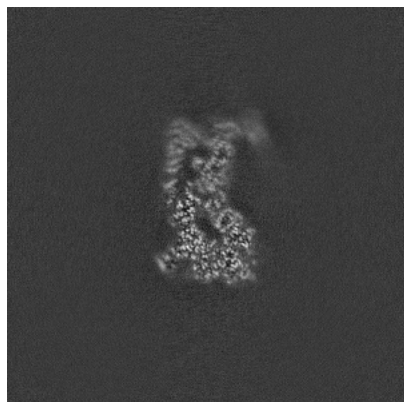


Y Index: 250

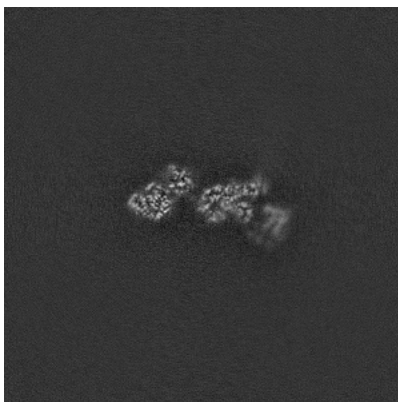


Z Index: 250

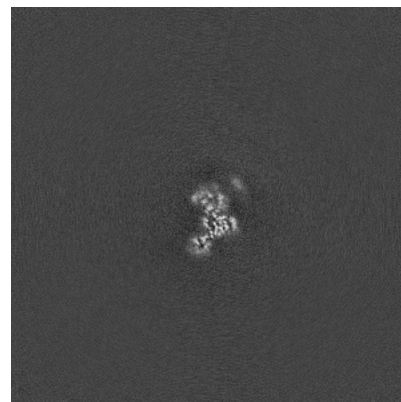
6.2.2 Raw map



X Index: 250



Y Index: 250

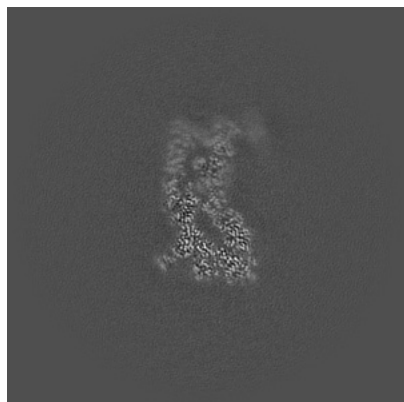


Z Index: 250

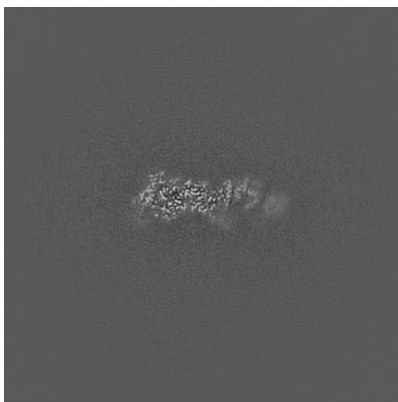
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

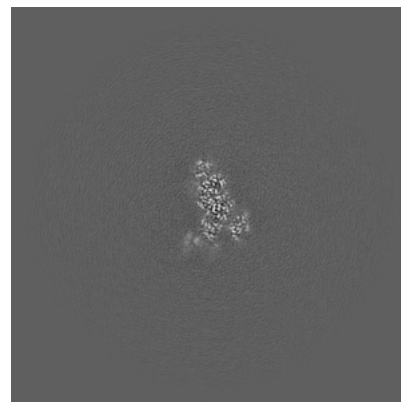
6.3.1 Primary map



X Index: 248

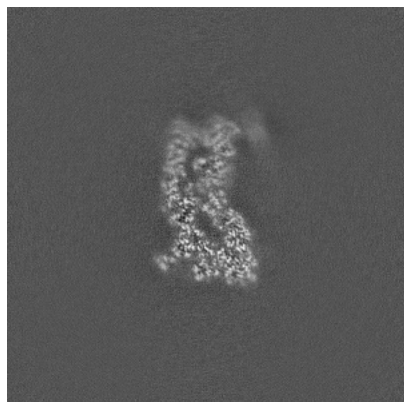


Y Index: 232

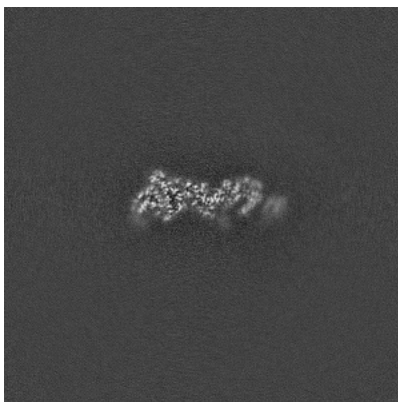


Z Index: 191

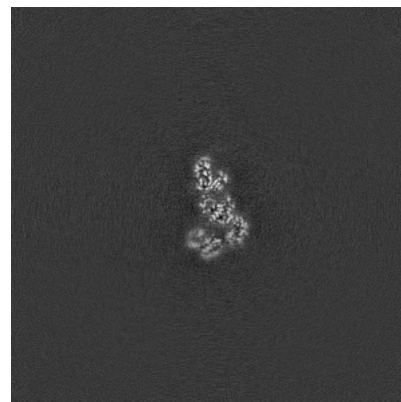
6.3.2 Raw map



X Index: 247



Y Index: 235

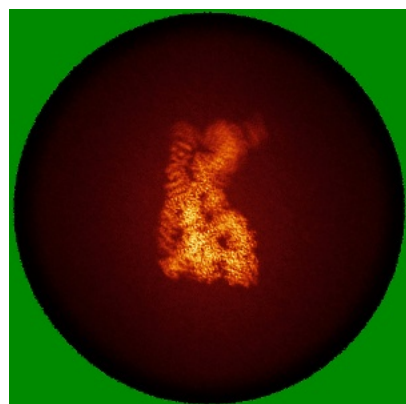


Z Index: 184

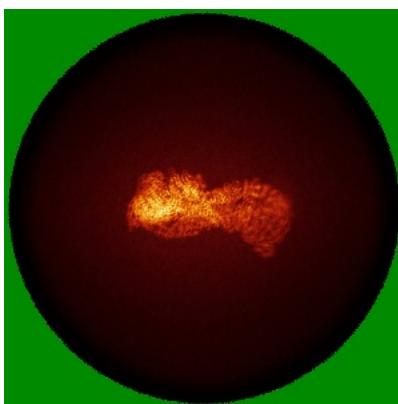
The images above show the largest variance slices of the map in three orthogonal directions.

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

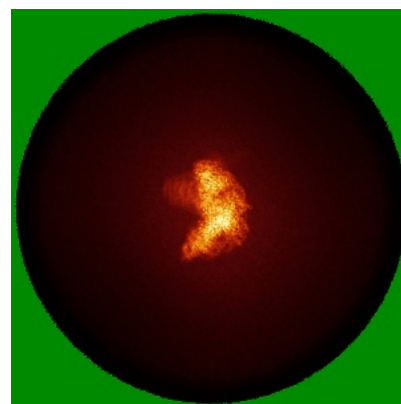
6.4.1 Primary map



X

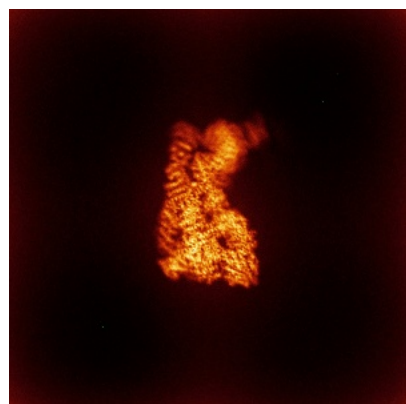


Y

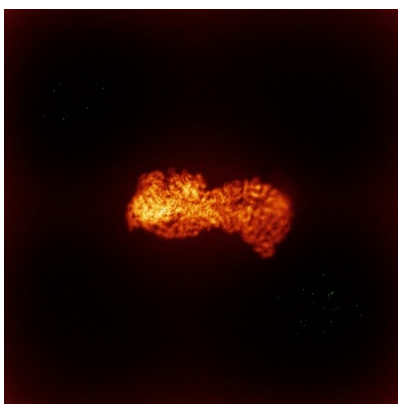


Z

6.4.2 Raw map



X



Y

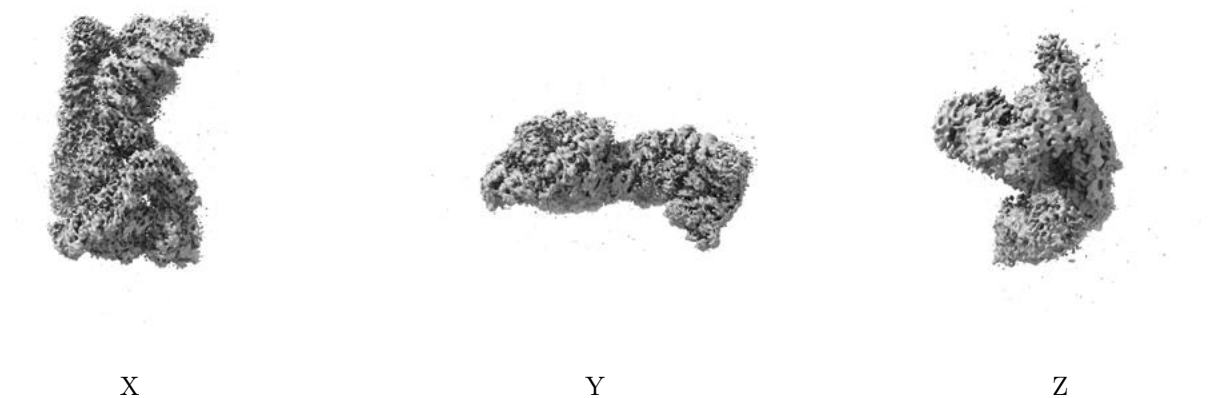


Z

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

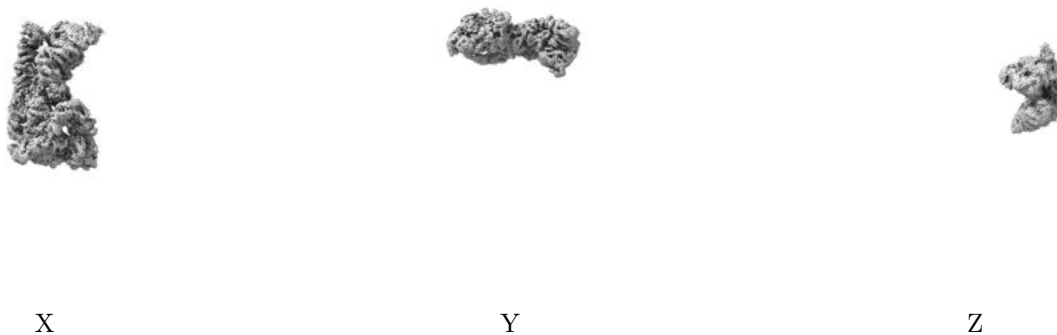
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

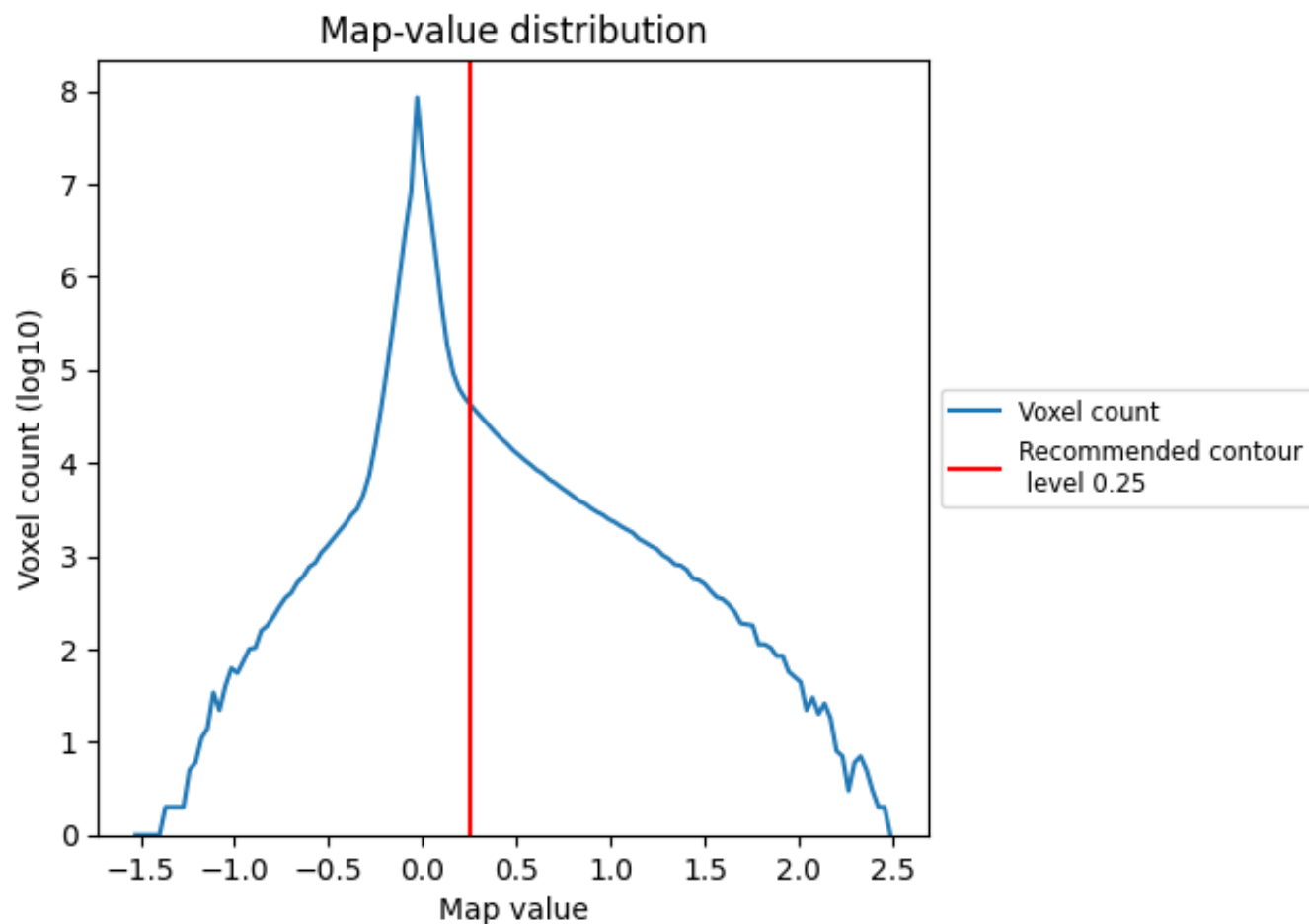
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

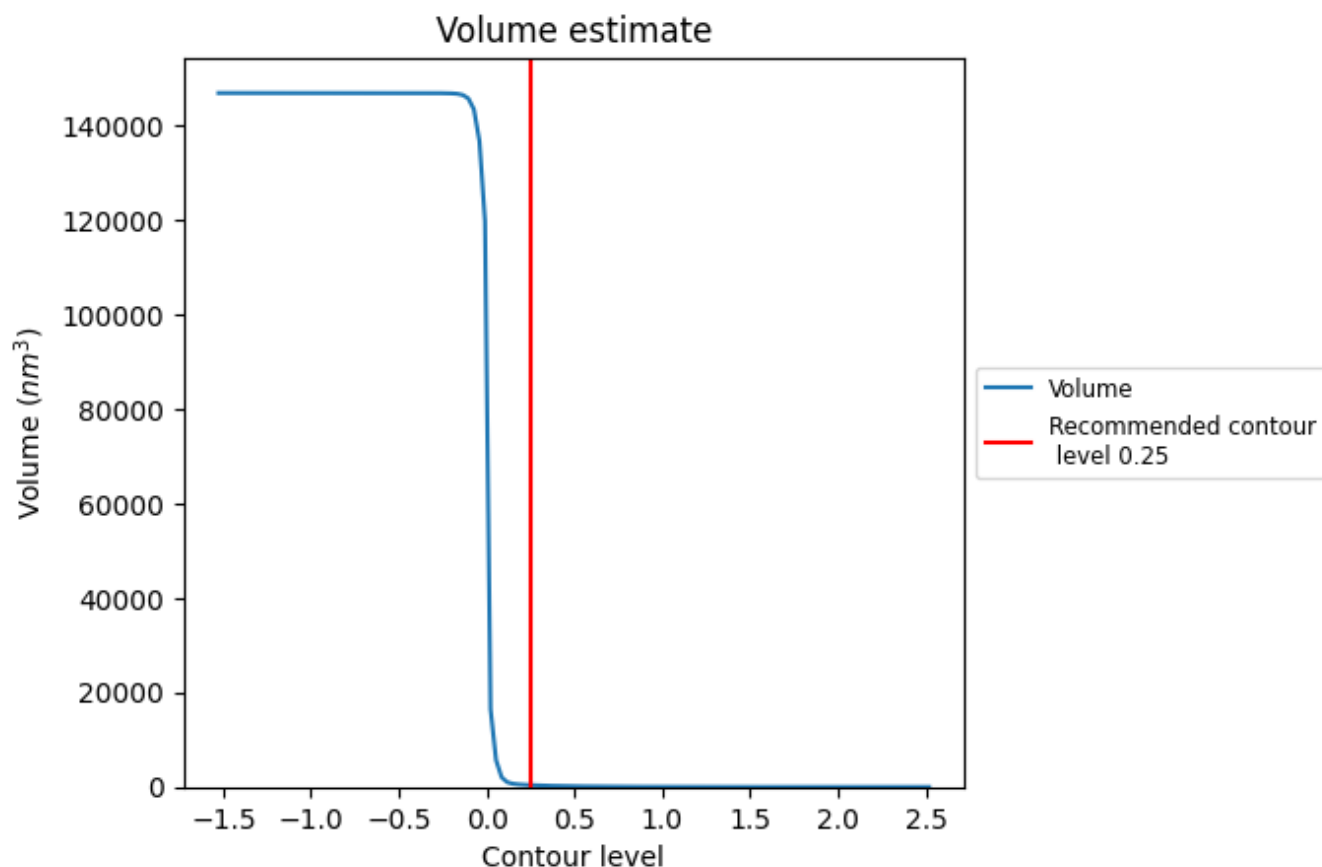
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

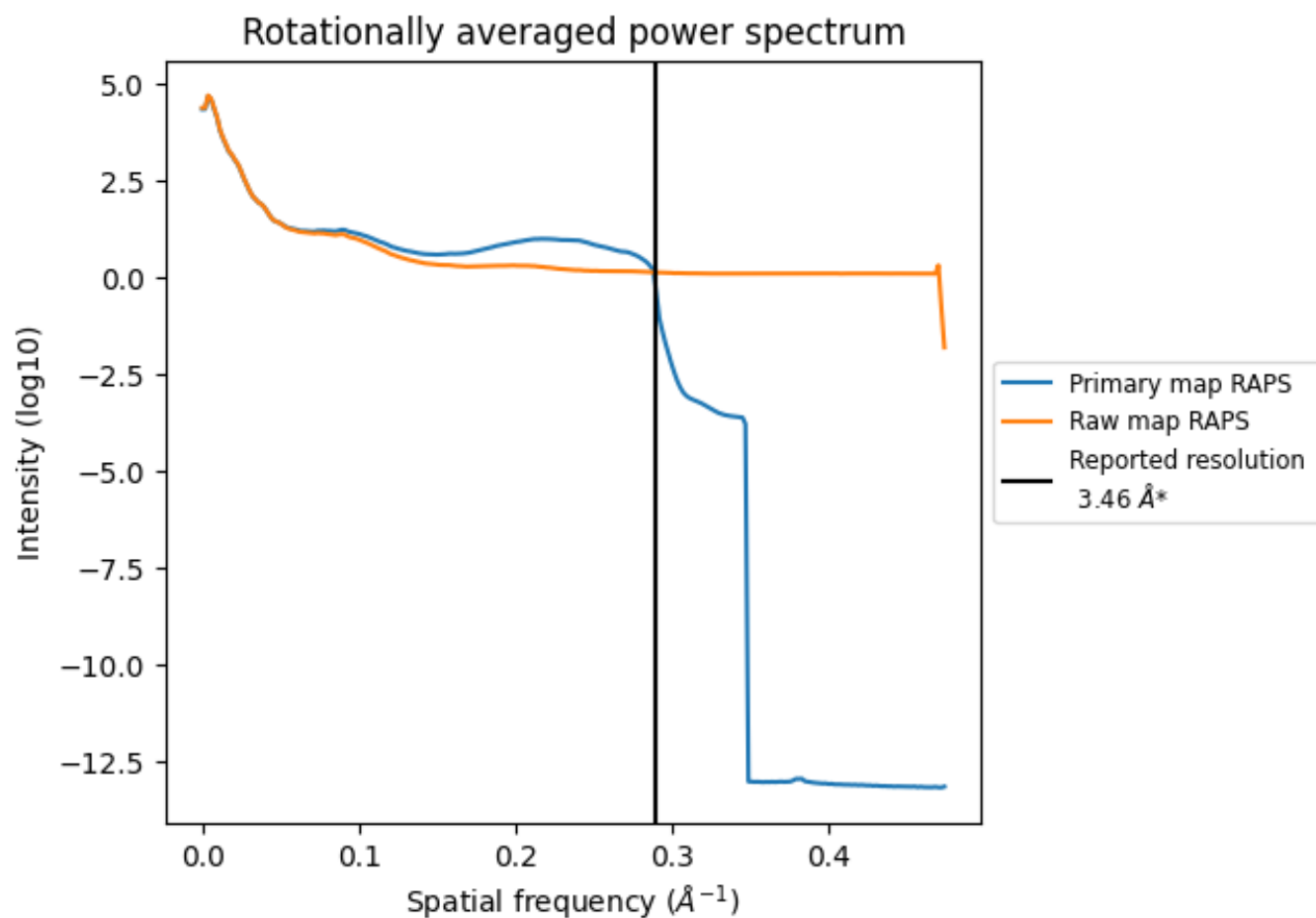
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 386 nm³; this corresponds to an approximate mass of 349 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 ⓘ

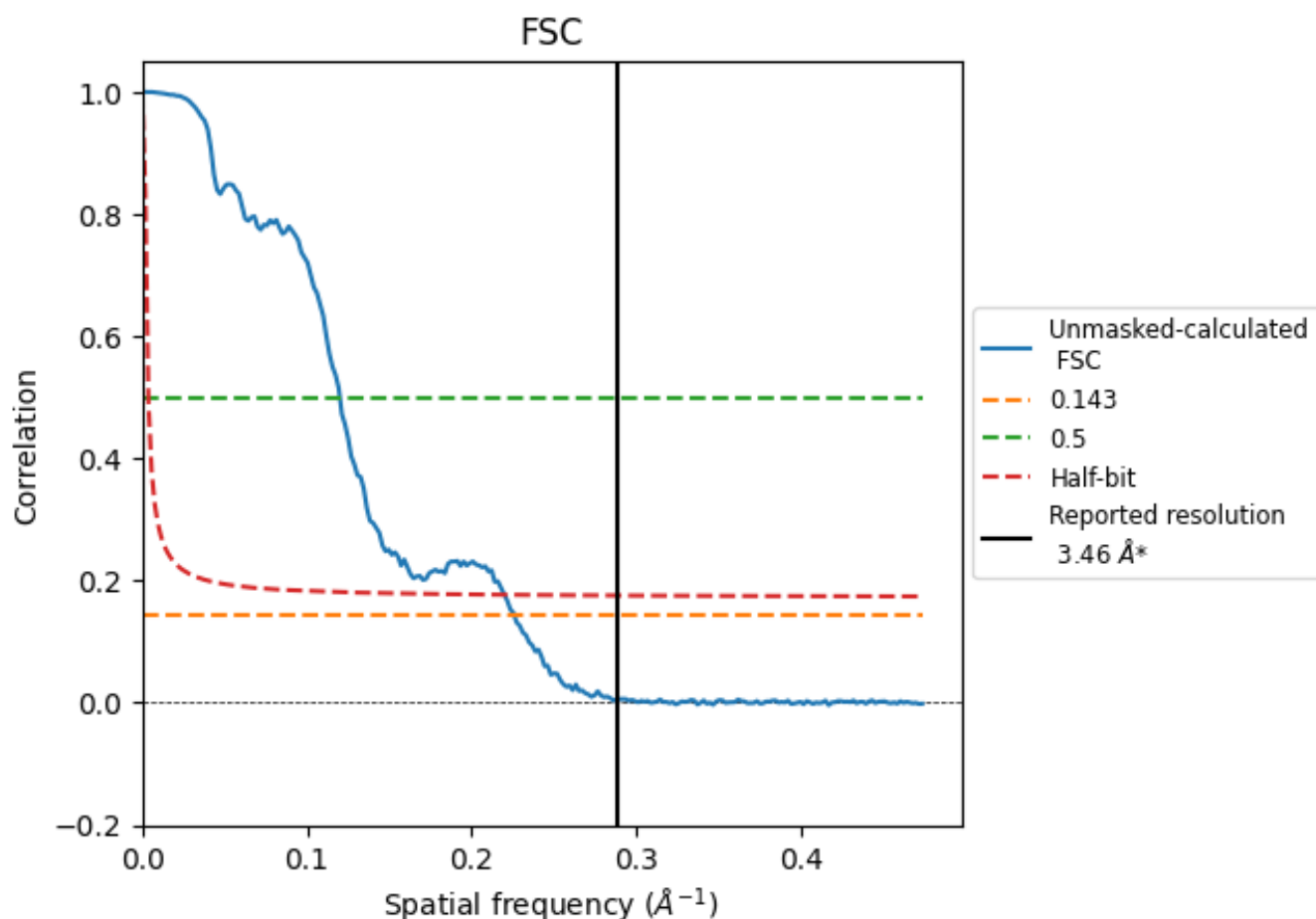


*Reported resolution corresponds to spatial frequency of 0.289 Å⁻¹

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 0.289 Å⁻¹

8.2 Resolution estimates [i](#)

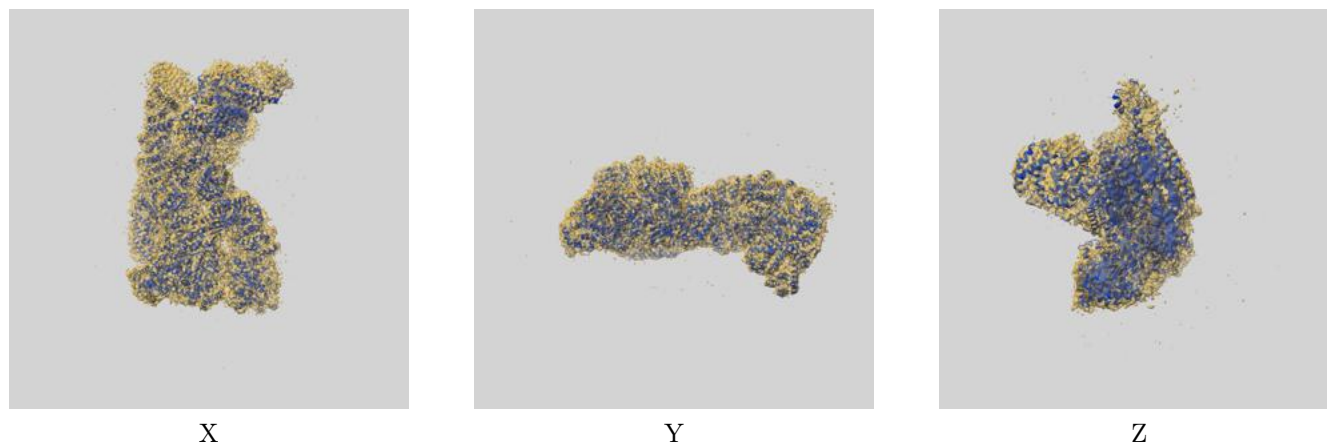
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.46	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.42	8.33	4.54

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.42 differs from the reported value 3.46 by more than 10 %

9 Map-model fit [i](#)

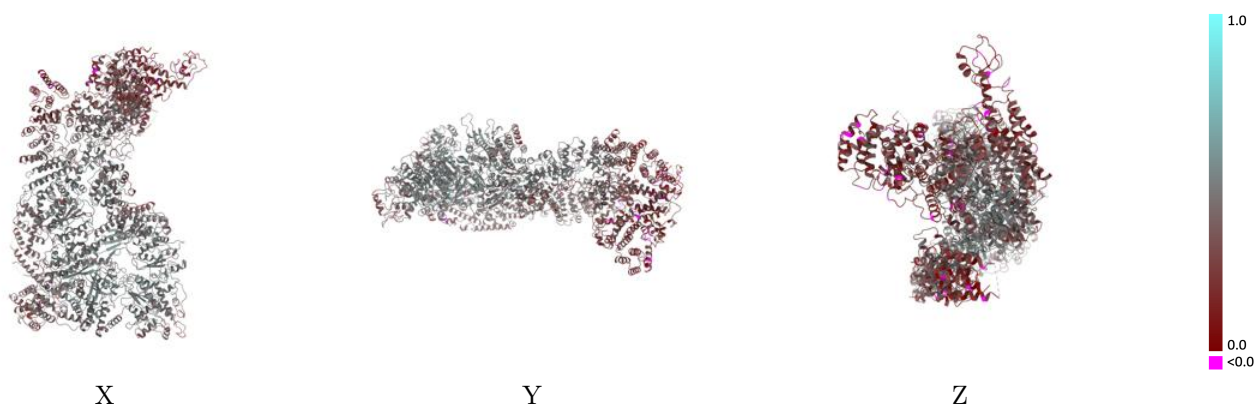
This section contains information regarding the fit between EMDB map EMD-61848 and PDB model 9JW1. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



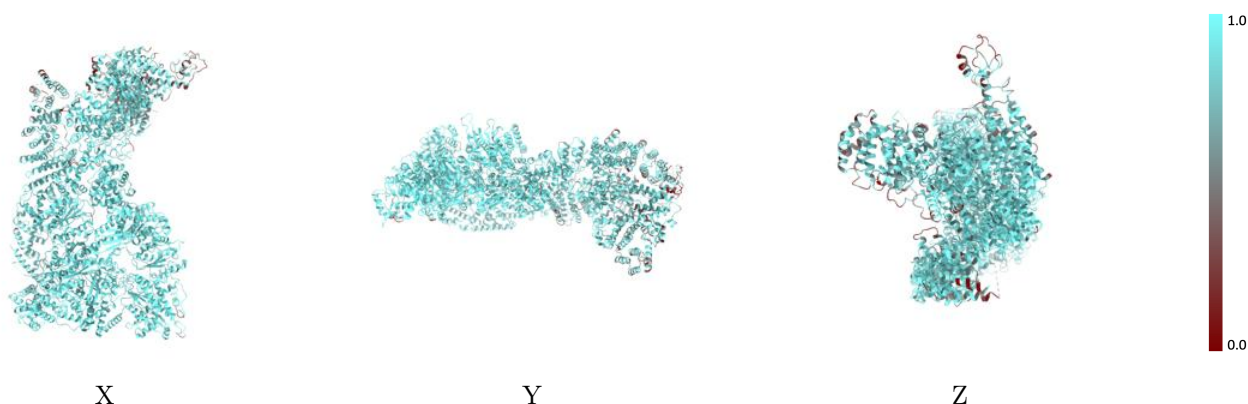
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



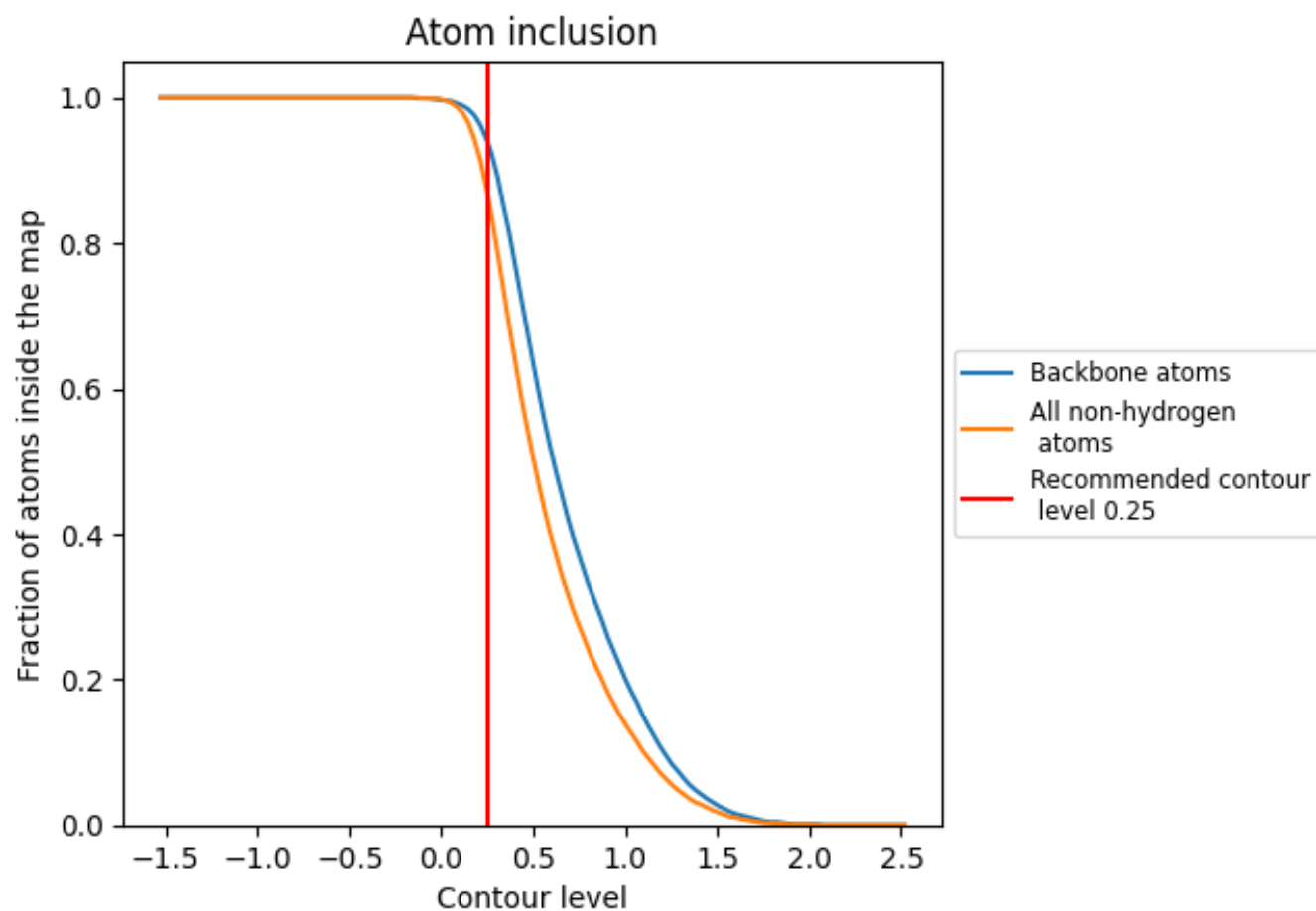
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.25).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 87% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8700	0.3980
A	0.8700	0.3980

