



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 02:17 PM UTC

PDB ID : 8TL9 / pdb_00008tl9
EMDB ID : EMD-41365
Title : Human Type 3 IP3 Receptor - Resting State (+IP3/ATP)
Authors : Paknejad, N.; Sapuru, V.; Hite, R.K.
Deposited on : 2023-07-26
Resolution : 3.30 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

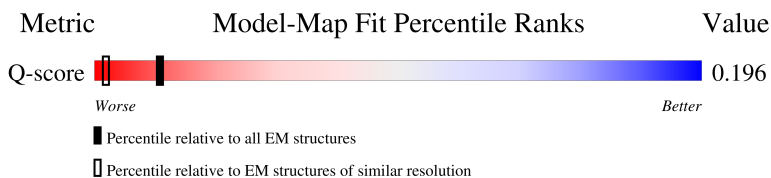
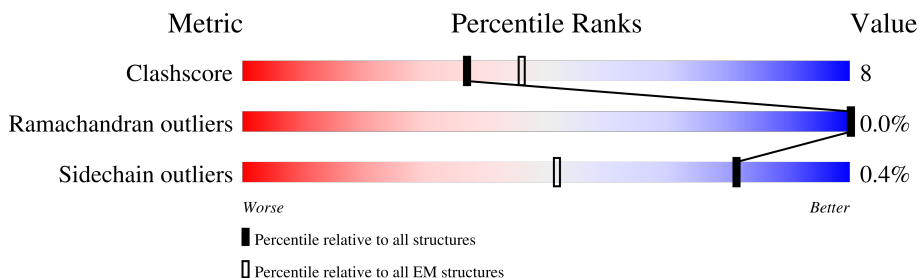
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	15087 (2.80 - 3.80)

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	2671	31% 60% 14% 26%
1	B	2671	35% 61% 13% 26%
1	C	2671	24% 63% 12% 25%
1	D	2671	9% 65% 11% 24%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 130518 atoms, of which 65442 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.

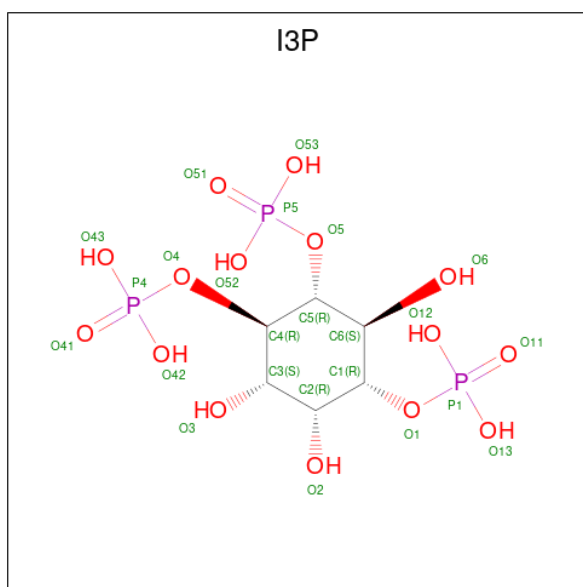
- Molecule 1 is a protein called Inositol 1,4,5-trisphosphate receptor type 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1989	Total	C	H	N	O	S	0	0
			32350	10293	16244	2749	2960	104		
1	B	1987	Total	C	H	N	O	S	0	0
			32312	10283	16225	2743	2957	104		
1	C	2005	Total	C	H	N	O	S	0	0
			32587	10375	16353	2768	2987	104		
1	D	2034	Total	C	H	N	O	S	0	0
			32957	10480	16536	2807	3029	105		

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Zn	0
			1	1	
2	B	1	Total	Zn	0
			1	1	
2	C	1	Total	Zn	0
			1	1	
2	D	1	Total	Zn	0
			1	1	

- Molecule 3 is D-MYO-INOSITOL-1,4,5-TRIPHOSPHATE (CCD ID: I3P) (formula: C₆H₁₅O₁₅P₃) (labeled as "Ligand of Interest" by depositor).

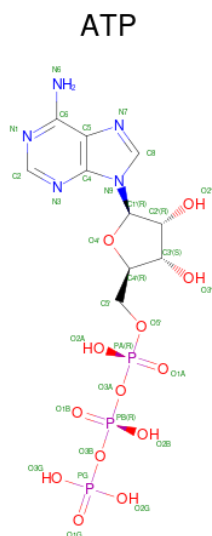


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	H	O	P	0
			33	6	9	15	3	
3	B	1	Total	C	H	O	P	0
			33	6	9	15	3	
3	C	1	Total	C	H	O	P	0
			33	6	9	15	3	
3	D	1	Total	C	H	O	P	0
			33	6	9	15	3	

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Ca	0
			1	1	
4	B	1	Total	Ca	0
			1	1	
4	C	1	Total	Ca	0
			1	1	
4	D	1	Total	Ca	0
			1	1	

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).

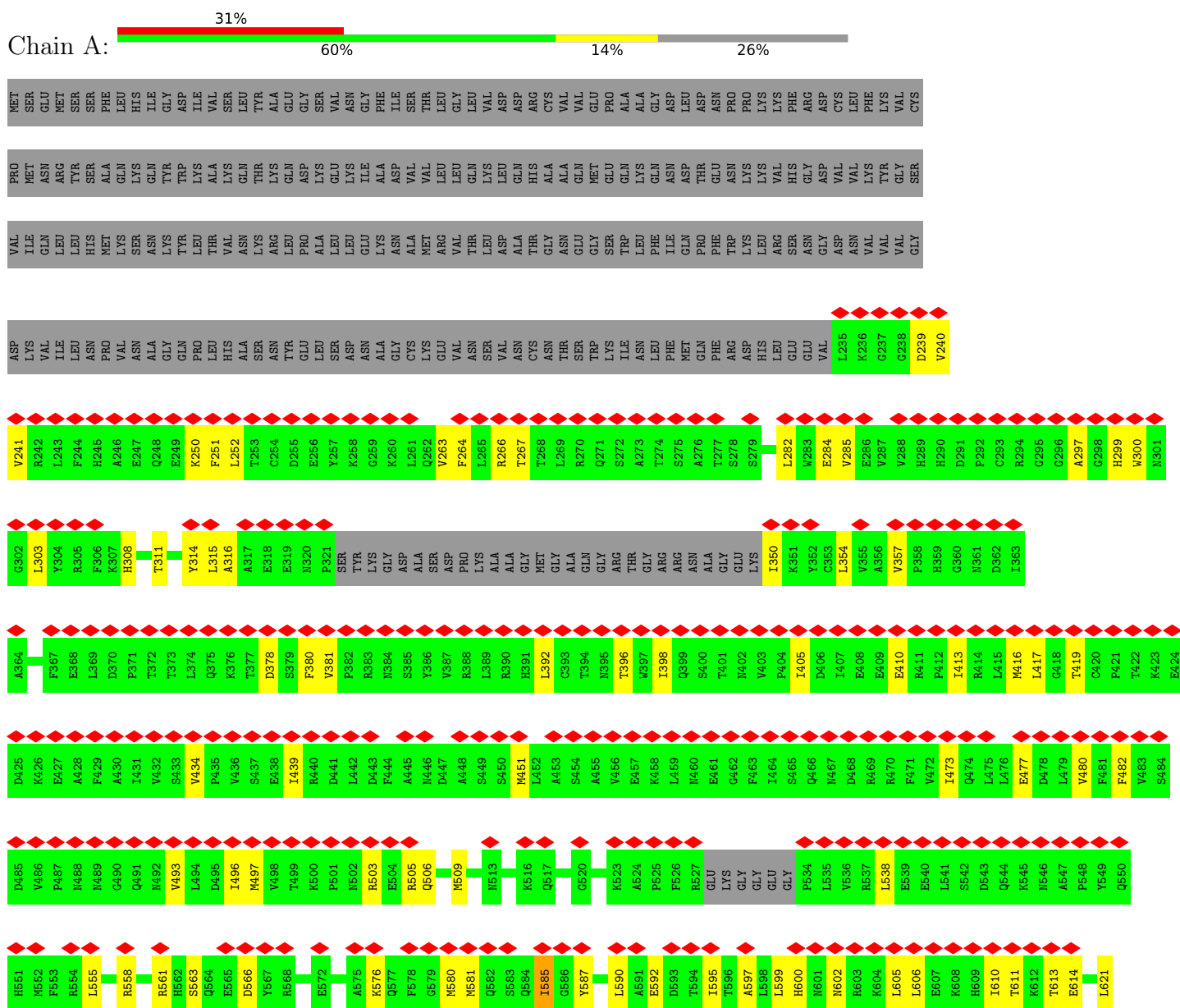


Mol	Chain	Residues	Atoms						AltConf
5	A	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
5	B	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
5	C	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
5	D	1	Total 43	C 10	H 12	N 5	O 13	P 3	0

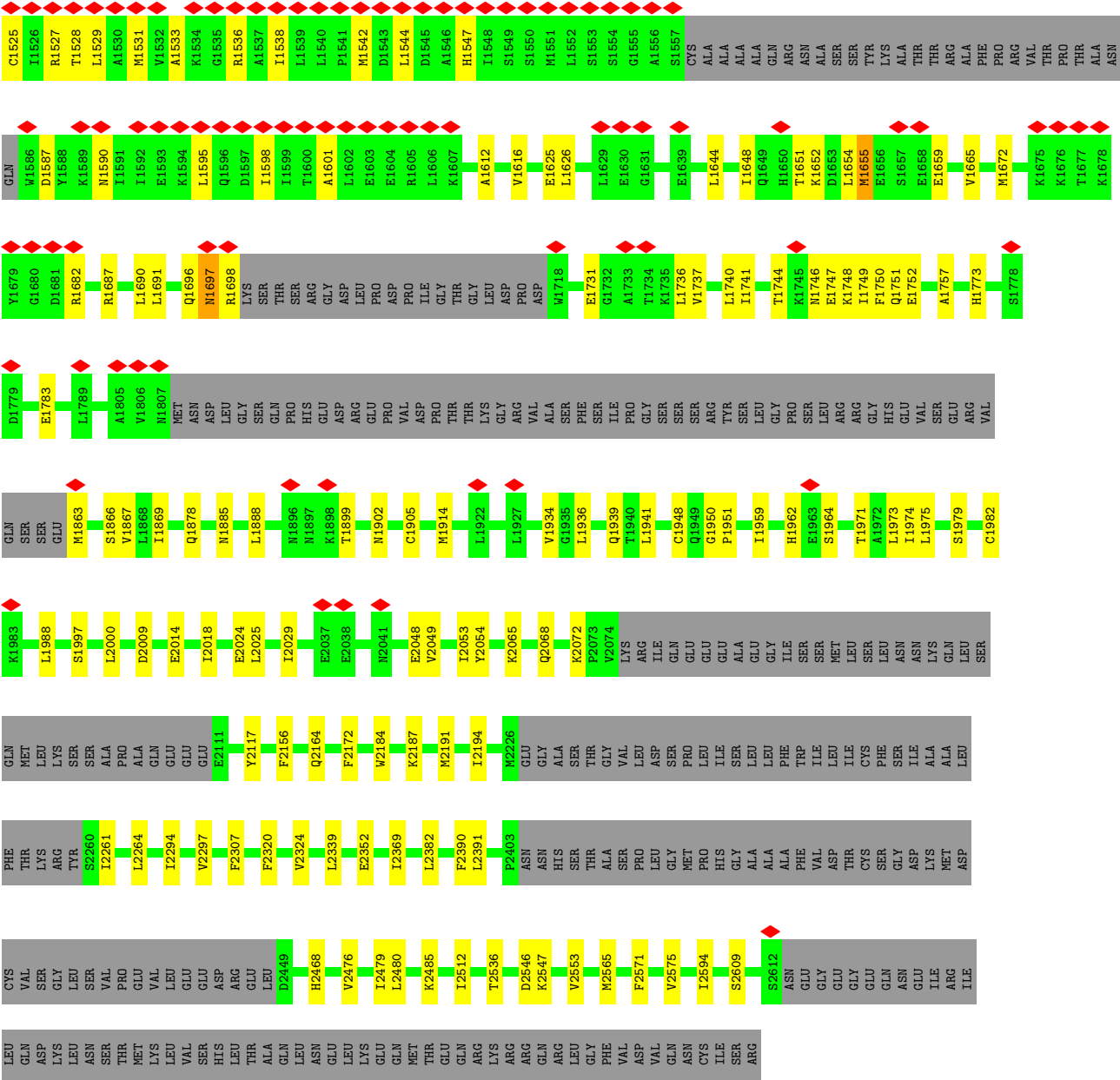
3 Residue-property plots

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.

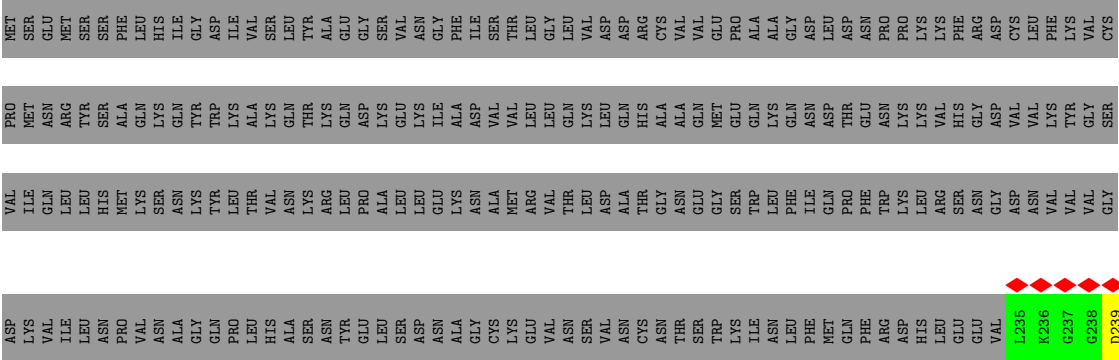
- Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3



T1463	L1464	E1465	K1466	V1467	V1468	L1469	S1470	D1474	T1475	I1476	N1477	A1478	F1479	F1480	S1481	S1482	P1483	F1484	S1485	E1486	N1487	S1488	T1489	S1490	L1491	Q1492	T1493	H1494	Q1495	T1496	L1497	V1498	V1499	Q1500	L1501	L1502	Q1503	S1504	T1505	T1506	R1507	L1508	L1509	E1510	C1511	P1512	W1513	L1514	Q1515	Q1516	Q1517	H1518	K1519	L1520	S1521	V1522	E1523	A1524
T1401	H1402	E1403	D1404	C1405	T1406	T1407	E1408	M1411	T1475	T1476	N1477	A1478	F1479	F1480	S1481	S1482	P1483	F1484	S1485	E1486	N1487	S1488	T1489	S1490	L1491	Q1492	T1493	H1494	Q1495	T1496	L1497	V1498	V1499	Q1500	L1501	L1502	Q1503	S1504	T1505	T1506	T1445	L1446	D1447	M1448	A1449	R14450	V1451	C1452	S1453	K1454	R1455	E1456	K1457	R1458	V1459	S1460	V1461	P1462
S1341	L1342	A1343	H1344	L1345	L1346	D1347	M1348	M1349	K1350	A1351	A1352	R1353	D1354	G1355	V1356	E1357	D1358	H1359	S1360	P1361	L1362	M1363	Y1364	H1365	T1366	S1367	L1368	V1369	D1370	L1371	L1372	A1373	A1374	K1375	A1376	E1377	G1378	K1379	N1380	V1381	Y1382	T1383	I1385	K1386	C1387	T1388	S1389	L1390	L1391	P1392	L1393	E1394	D1395	V1396	V1397	S1398	V1399	V1400
S1279	E1280	P1281	V1282	L1283	Q1284	H1285	F1286	V1287	H1288	L1289	L1290	A1291	T1292	H1293	G1294	R1295	H1296	V1297	Q1298	D1301	F1302	L1303	H1304	T1305	V1306	K1307	L1308	A1309	E1310	G1311	K1312	Y1313	V1314	K1315	K1316	D1319	M1320	L1321	M1322	T1323	E1324	L1325	T1326	N1327	A1328	G1329	D1330	D1331	V1332	V1333	V1334	F1335	V1336	N1337	D1338	K1339	A1340	
I1212	P1213	Y1214	D1215	K1216	G1217	D1218	A1219	K1220	M1221	M1222	E1223	R1226	Y1227	Q1230	F1231	A1237	G1238	N1239	P1240	G1241	N1242	Q1243	A1244	L1245	H1247	K1248	H1249	K1250	H1251	L1252	F1253	L1254	T1255	P1256	G1257	L1258	L1259	E1262	T1263	M1264	Q1265	I1267	F1268	L1269	N1270	N1271	Y1272	Q1273	L1274	C1275	E1277	I1278						
LYS	GLU	ARG	PRO	THR	ASP	GLU	GLU	PHE	LEU	HIS	PRO	PRO	GLY	GLY	LYS	SER	S1166	E1167	M1168	Y1169	Q1170	I1171	V1172	K1173	G1174	I1175	E1177	R1178	L1179	M1180	K1181	M1182	C1183	G1184	V1185	G1186	E1187	Q1188	M1189	R1190	K1191	K1192	R1195	M1199	M1200	H1203	K1204	V1205	M1206	L1207	D1208	L1209	L1210	Q1211				
D1066	Y1067	A1068	P1069	L1070	V1071	F1079	H1090	T1091	F1092	K1093	Q1094	V1095	Q1096	L1097	L1098	I1099	S1100	A1101	Q1102	D1103	V1104	E1105	N1106	D1115	R1116	L1117	R1118	T1119	M1120	V1121	S1124	E1125	L1126	W1127	V1128	D1129	LYS	LYS	GLY	LYS	GLY	GLU	VAL	GLU	ALA	GLY	ALA	ASP	LYS									
V1001	F1002	P1003	M1004	GLN	ASP	SER	GLY	ALA	ASP	GLY	THR	ALA	PRO	ALA	PHE	ASP	SER	THR	ALA	N1022	M1023	N1024	L1025	D1026	R1027	I1028	G1029	E1030	Q1031	R1032	E1033	A1034	M1035	F1036	G1037	VAL	GLY	LYS	THR	SER	S1043	M1044	L1045	PRO	PRO	ALA	ASP	M1054	F1055	L1056	R1057	I1060	H1061	L1062				
ARG	SER	ILE	GLN	GLY	VAL	GLY	HIS	MET	MET	GLY	GLY	ASP	VAL	LEU	LEU	VAL	PHE	SER	ALA	PRO	SER	LEU	ALA	ALA	GLY	ALA	ALA	GLU	PRO	LEU	ASP	ARG	ASP	SER	LYS	PHE	GLY	ASN	D961	M965	Y974	I978	D984	E997	F998	V999	E1000											
L841	N842	N843	V844	V845	S846	E847	V848	V849	P850	F851	A852	N853	E854	E855	T860	F861	V863	V864	H868	I871	Y872	L881	L882	R883	L884	T885	R886	L889	G890	I891	D893	C894	VAL	GLN	GLY	PRO	PRO	ALA	ALA	MET	TRP	GLU	ASP	F830	V831	N832	T833	M834	E835	F836	D839	Y840						
L769	P770	E771	D772	L773	R774	A775	S776	F777	C778	H779	L780	M781	D787	R788	D789	E792	L793	K798	F799	V800	W803	T804	E805	I806	P807	T808	T811	I812	K813	D814	S817	N818	L819	N820	A821	S822	R823	D824	D825	K826	K827	N828	K829	A831	L759	N832	T833	M834	E835	F836	D839	Y840						
N701	E702	H703	H704	E705	K706	S707	V708	R709	Q710	L711	A712	Q713	E714	A715	R716	A717	G718	N719	H720	H721	D722	E723	N724	V725	Y729	L733	K734	L735	M739	D742	R743	Q744	Y745	L746	P747	I748	D749	E750	I751	S752	Q753	Q754	V757	D758	I760	F761	L762	M764	A765	D766	E767	M768						
V622	R623	K624	F630	L631	D636	V639	S640	N641	H642	I643	A644	I645	P646	V647	E650	L651	K654	L657	D658	P659	K660	N661	S662	D663	R667	T668	E669	L670	R671	P672	V673	LYS	GLU	MET	ALA	GLN	SER	HIS	TRP	LEU	SER	ILE	GLU	TRP	SER	E689	C763	E690	D698	K699	N700							



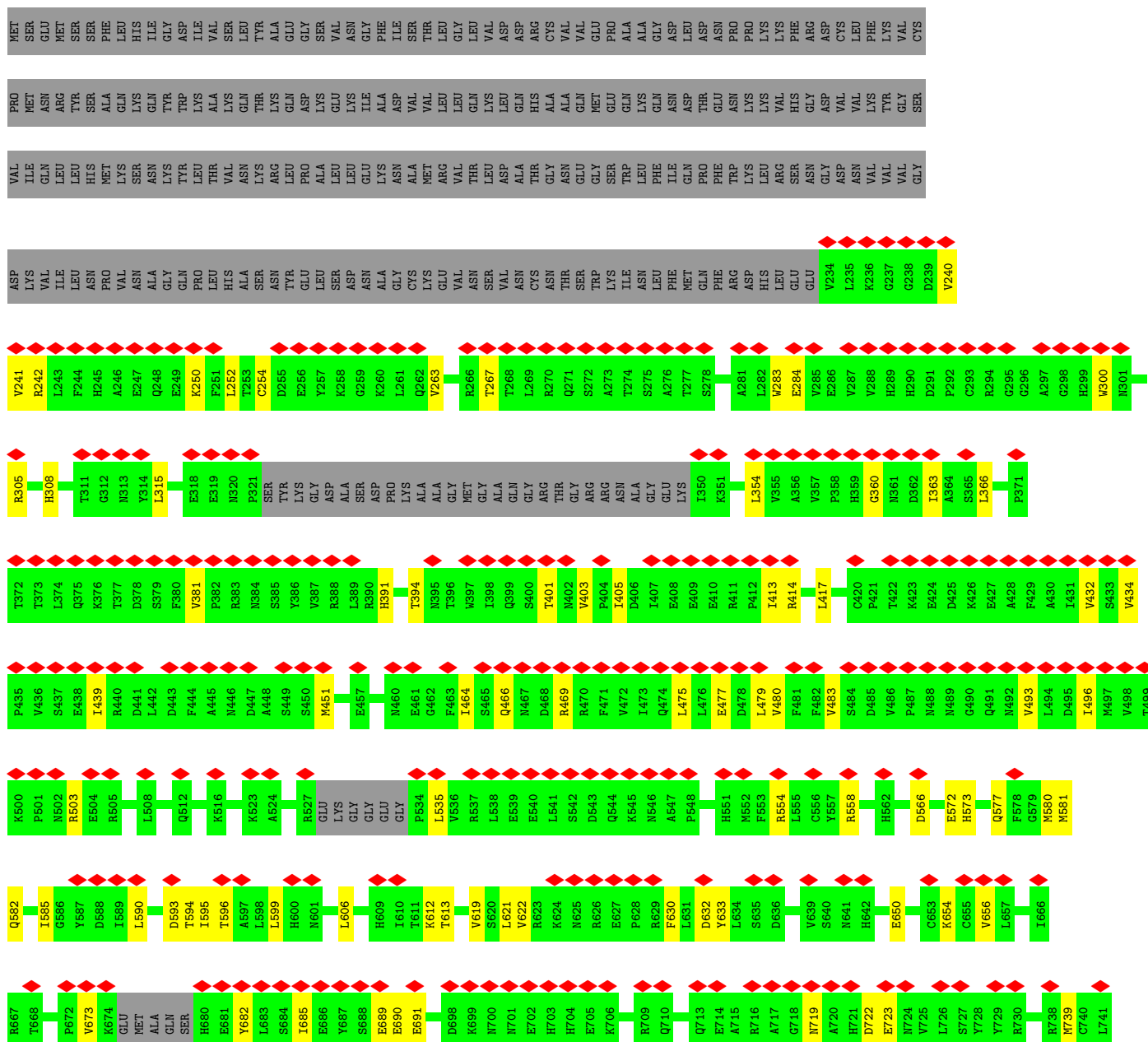
● Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3



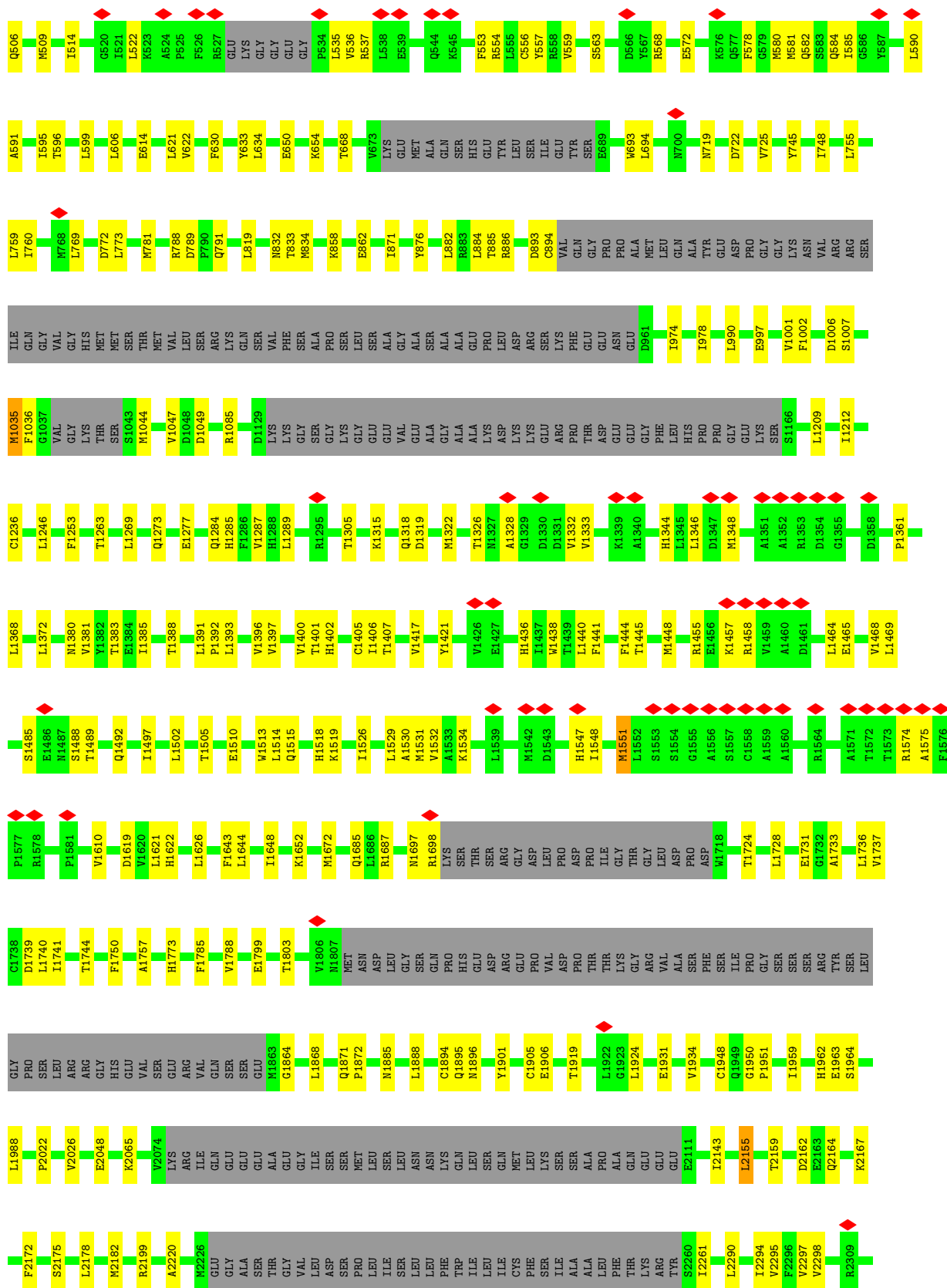




- Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3









4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	88082	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 ($e^-/\text{\AA}^2$)	66	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	4300	Depositor
Magnification	29000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.869	Depositor
Minimum map value	-0.421	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.15	Depositor
Map size ($\text{\AA}$)	422.912, 422.912, 422.912	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.826, 0.826, 0.826	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: CA, ATP, ZN, I3P

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	0.12	0/16403	0.30	0/22156
1	B	0.12	0/16384	0.29	0/22131
1	C	0.12	0/16535	0.29	0/22337
1	D	0.11	0/16726	0.27	0/22603
All	All	0.12	0/66048	0.29	0/89227

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	16106	16244	16243	269	0
1	B	16087	16225	16224	268	0
1	C	16234	16353	16362	235	0
1	D	16421	16536	16535	223	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	24	9	9	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	24	9	9	1	0
3	C	24	9	9	0	0
3	D	24	9	9	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	31	12	12	0	0
5	B	31	12	12	0	0
5	C	31	12	12	0	0
5	D	31	12	12	0	0
All	All	65076	65442	65448	990	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 8.

All (990) 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:1962:HIS:HD1	1:A:1964:SER:HG	0.98	0.95
1:B:1799:GLU:OE1	1:B:1866:SER:OG	1.91	0.89
1:C:354:LEU:HD12	1:C:417:LEU:HD12	1.55	0.87
1:D:1962:HIS:HD1	1:D:1964:SER:HG	1.24	0.85
1:D:1510:GLU:OE2	1:D:1547:HIS:NE2	2.08	0.84
1:A:1262:GLU:O	1:A:1266:HIS:ND1	2.11	0.83
1:C:2322:TYR:OH	1:C:2347:ASP:OD2	1.97	0.81
1:D:719:ASN:ND2	1:D:722:ASP:OD1	2.13	0.81
1:B:1448:MET:SD	1:B:1504:SER:OG	2.39	0.81
1:A:1298:GLN:N	1:A:1298:GLN:OE1	2.14	0.80
1:B:1895:GLN:O	1:B:1896:ASN:ND2	2.15	0.80
1:B:1302:PHE:O	1:B:1306:VAL:HG23	1.82	0.80
1:D:1322:MET:O	1:D:1326:THR:HG23	1.82	0.79
1:D:445:ALA:HB1	1:D:514:ILE:HD11	1.64	0.79
1:C:503:ARG:NH2	1:C:566:ASP:O	2.16	0.79
1:A:1115:ASP:OD1	1:A:1116:ARG:N	2.17	0.78
1:B:568:ARG:NH2	3:B:3002:I3P:O3	2.16	0.77
1:C:593:ASP:OD2	1:C:594:THR:N	2.18	0.77
1:A:733:LEU:HD22	1:A:780:LEU:HD22	1.66	0.77
1:D:451:MET:HE3	1:D:451:MET:O	1.85	0.77
1:B:881:LEU:O	1:B:885:THR:HG23	1.86	0.76
1:A:2191:MET:HE2	1:A:2194:ILE:HD12	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:585:ILE:HD13	1:B:595:ILE:HD12	1.67	0.76
1:B:1902:ASN:ND2	1:B:1905:CYS:SG	2.58	0.76
1:A:1747:GLU:N	1:A:1747:GLU:OE2	2.21	0.74
1:C:2011:GLU:N	1:C:2011:GLU:OE1	2.20	0.74
1:C:816:ASP:O	1:C:823:ARG:NH2	2.21	0.74
1:A:2571:PHE:O	1:A:2575:VAL:HG23	1.88	0.74
1:B:1188:GLN:N	1:B:1188:GLN:OE1	2.20	0.74
1:A:1302:PHE:O	1:A:1306:VAL:HG23	1.88	0.73
1:A:252:LEU:HD12	1:A:264:PHE:O	1.88	0.73
1:B:965:MET:HE1	1:B:1065:HIS:NE2	2.04	0.73
1:C:1097:LEU:HD12	1:C:1595:LEU:HD22	1.71	0.73
1:A:1914:MET:HE1	1:A:1936:LEU:HD23	1.71	0.72
1:D:1236:CYS:HB3	1:D:1246:LEU:HD12	1.71	0.72
1:C:479:LEU:O	1:C:483:VAL:HG23	1.89	0.72
1:A:800:ALA:N	1:A:1199:ASN:OD1	2.22	0.72
1:D:1737:VAL:HG11	1:D:1757:ALA:HB2	1.72	0.72
1:B:497:MET:HE2	1:B:497:MET:HA	1.69	0.72
1:B:1247:HIS:CD2	1:B:1250:LEU:HD12	2.25	0.72
1:D:886:ARG:NH1	1:D:1047:VAL:O	2.23	0.71
1:A:350:ILE:HD13	1:A:416:MET:HE2	1.71	0.71
1:A:1528:THR:HA	1:A:1531:MET:HE3	1.72	0.71
1:A:811:THR:OG1	1:A:814:ASP:OD2	2.09	0.71
1:C:1169:TYR:OH	1:C:1218:ASP:OD2	2.05	0.70
1:D:557:TYR:CE2	1:D:581:MET:HE1	2.26	0.70
1:C:673:VAL:HB	1:C:685:ILE:HG22	1.73	0.70
1:A:1127:TRP:CZ3	1:A:1172:VAL:HG21	2.26	0.70
1:D:1648:ILE:HG23	1:D:1736:LEU:HD22	1.72	0.70
1:A:1273:GLN:OE1	1:A:1273:GLN:N	2.24	0.70
1:B:300:TRP:CD2	1:B:381:VAL:HG22	2.27	0.69
1:D:451:MET:O	1:D:454:SER:OG	2.08	0.69
1:C:1183:CYS:O	1:C:1189:MET:HE1	1.93	0.69
1:A:733:LEU:CD2	1:A:780:LEU:HD22	2.21	0.69
1:A:1028:ILE:HG21	1:A:1598:ILE:HD11	1.74	0.69
1:A:707:SER:O	1:A:711:LEU:HD13	1.91	0.69
1:D:1485:SER:O	1:D:1488:SER:OG	2.10	0.69
1:A:743:ARG:NH1	1:A:787:ASP:OD1	2.24	0.68
1:B:1397:VAL:HG21	1:B:1436:HIS:HB3	1.75	0.68
1:C:1189:MET:SD	1:C:1190:ARG:N	2.66	0.68
1:D:1644:LEU:HD11	1:D:1672:MET:HE1	1.75	0.68
1:B:1919:THR:HG22	1:B:1924:LEU:HB2	1.74	0.68
1:C:673:VAL:HB	1:C:685:ILE:CG2	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:709:ARG:NH2	1:A:766:ASP:OD2	2.26	0.68
1:B:614:GLU:OE1	1:B:614:GLU:N	2.27	0.68
1:B:314:TYR:O	1:B:357:VAL:HG22	1.94	0.68
1:C:673:VAL:HG12	1:C:691:GLU:OE1	1.93	0.68
1:A:1687:ARG:NH1	1:A:1691:LEU:HD11	2.09	0.68
1:D:299:HIS:ND1	1:D:378:ASP:O	2.26	0.68
1:B:854:GLU:N	1:B:854:GLU:OE1	2.25	0.67
1:C:1456:GLU:O	1:C:1458:ARG:NH1	2.27	0.67
1:C:1919:THR:HG22	1:C:1924:LEU:HD23	1.76	0.67
1:B:631:LEU:HD11	1:B:728:TYR:CE1	2.30	0.67
1:D:1962:HIS:ND1	1:D:1964:SER:OG	2.23	0.67
1:C:673:VAL:HG13	1:C:690:GLU:N	2.10	0.67
1:A:1067:TYR:O	1:A:1071:VAL:HG23	1.95	0.66
1:B:1473:LEU:HD11	1:B:1522:VAL:HG22	1.77	0.66
1:C:1397:VAL:HG21	1:C:1436:HIS:HB3	1.76	0.66
1:B:1621:LEU:HD23	1:B:1643:PHE:CE2	2.29	0.66
1:D:1328:ALA:HB3	1:D:1332:VAL:HG21	1.78	0.66
1:A:250:LYS:CE	1:A:267:THR:HG22	2.26	0.66
1:C:1329:GLY:O	1:C:1333:VAL:HG22	1.96	0.66
1:C:974:ILE:O	1:C:978:ILE:HD12	1.95	0.66
1:A:252:LEU:HD13	1:A:417:LEU:HD11	1.76	0.65
1:C:1322:MET:SD	1:C:1322:MET:N	2.70	0.65
1:B:1338:ASP:OD1	1:B:1339:LYS:N	2.29	0.65
1:D:557:TYR:HE2	1:D:581:MET:HE1	1.62	0.65
1:A:252:LEU:HD11	1:A:263:VAL:HG12	1.76	0.64
1:B:496:ILE:HG23	1:B:562:HIS:NE2	2.12	0.64
1:B:1197:LEU:HD22	1:B:1202:ALA:HB3	1.79	0.64
1:B:1067:TYR:O	1:B:1071:VAL:HG23	1.98	0.64
1:B:1506:THR:HG23	1:B:1547:HIS:ND1	2.12	0.64
1:B:1428:MET:HE2	1:B:1428:MET:HA	1.78	0.64
1:C:621:LEU:HD12	1:C:622:VAL:N	2.12	0.64
1:C:673:VAL:HA	1:C:691:GLU:OE2	1.98	0.64
1:C:1469:LEU:HD11	1:C:1513:TRP:CZ3	2.32	0.64
1:D:1464:LEU:O	1:D:1468:VAL:HG23	1.98	0.64
1:B:480:VAL:CG2	1:B:496:ILE:HG21	2.28	0.63
1:B:503:ARG:NH2	1:B:566:ASP:O	2.31	0.63
1:C:885:THR:HG21	1:C:978:ILE:HG21	1.80	0.63
1:A:1097:LEU:HD11	1:A:1595:LEU:HD22	1.80	0.63
1:C:263:VAL:HG11	1:C:315:LEU:HD13	1.80	0.63
1:C:1441:PHE:O	1:C:1445:THR:HG23	1.98	0.63
1:A:1402:HIS:ND1	1:A:1404:ASP:O	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:451:MET:HE2	1:B:475:LEU:HD22	1.79	0.63
1:B:1473:LEU:HD11	1:B:1522:VAL:CG2	2.29	0.63
1:D:1396:VAL:O	1:D:1400:VAL:HG22	1.97	0.63
1:B:445:ALA:HB1	1:B:514:ILE:HD11	1.80	0.63
1:D:299:HIS:O	1:D:304:TYR:OH	2.12	0.63
1:B:840:TYR:O	1:B:844:VAL:HG23	1.99	0.63
1:A:267:THR:HG23	1:A:413:ILE:O	1.98	0.62
1:C:1325:LEU:HD21	1:C:1372:LEU:HD21	1.80	0.62
1:B:1506:THR:HG23	1:B:1547:HIS:CE1	2.34	0.62
1:B:746:LEU:HD21	1:B:1125:GLU:OE2	1.98	0.62
1:C:1541:PRO:O	1:C:1545:ASP:N	2.31	0.62
1:D:1531:MET:C	1:D:1531:MET:HE3	2.24	0.62
1:A:893:ASP:OD2	1:A:894:CYS:N	2.32	0.62
1:D:1441:PHE:O	1:D:1445:THR:HG23	2.00	0.62
1:A:2476:VAL:HG22	1:A:2480:LEU:HD13	1.82	0.62
1:B:757:VAL:HG22	1:B:785:HIS:CD2	2.34	0.62
1:D:1948:CYS:SG	1:D:1959:ILE:HD12	2.38	0.62
1:D:893:ASP:OD1	1:D:894:CYS:N	2.33	0.61
1:C:1594:LYS:HE3	1:C:1594:LYS:HA	1.80	0.61
1:A:410:GLU:N	1:A:410:GLU:OE2	2.32	0.61
1:D:2468:HIS:HB2	1:D:2479:ILE:HD13	1.83	0.61
1:B:568:ARG:NH1	1:B:572:GLU:OE1	2.34	0.61
1:C:2476:VAL:HG22	1:C:2480:LEU:HD13	1.83	0.61
1:C:315:LEU:HD11	1:C:354:LEU:HB3	1.83	0.61
1:D:1035:MET:HE2	1:D:1036:PHE:CE2	2.35	0.61
1:C:789:ASP:OD2	1:C:1123:LYS:NZ	2.28	0.61
1:A:506:GLN:NE2	1:A:563:SER:O	2.33	0.61
1:B:1396:VAL:HG21	1:B:1416:PHE:CE1	2.35	0.61
1:A:769:LEU:HB3	1:A:773:LEU:HD23	1.83	0.60
1:B:833:THR:CG2	1:B:866:LEU:HD21	2.31	0.60
1:B:972:LEU:HD11	1:B:1062:LEU:HD13	1.82	0.60
1:C:300:TRP:CD2	1:C:381:VAL:HG22	2.36	0.60
1:B:812:ILE:HD12	1:B:812:ILE:H	1.66	0.60
1:C:893:ASP:OD1	1:C:894:CYS:N	2.34	0.60
1:C:2546:ASP:OD1	1:C:2547:LYS:N	2.35	0.60
1:C:1445:THR:HG22	1:C:1501:LEU:CA	2.32	0.60
1:A:1127:TRP:CH2	1:A:1172:VAL:HG21	2.37	0.60
1:C:719:ASN:ND2	1:C:722:ASP:OD1	2.33	0.60
1:D:252:LEU:HD11	1:D:263:VAL:HG12	1.84	0.60
1:C:1203:HIS:NE2	1:C:1245:LEU:HD21	2.16	0.60
1:A:1247:HIS:CD2	1:A:1274:LEU:HD22	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:885:THR:HG22	1:B:978:ILE:HD13	1.84	0.60
1:C:673:VAL:HG13	1:C:689:GLU:C	2.27	0.60
1:B:2164:GLN:N	1:B:2164:GLN:OE1	2.35	0.59
1:D:2022:PRO:O	1:D:2026:VAL:HG23	2.01	0.59
1:A:1456:GLU:O	1:A:1458:ARG:NH1	2.34	0.59
1:B:1435:ASN:O	1:B:1439:THR:HG23	2.03	0.59
1:C:1445:THR:HG22	1:C:1501:LEU:HA	1.83	0.59
1:C:267:THR:HG23	1:C:413:ILE:O	2.02	0.59
1:D:568:ARG:NH1	1:D:572:GLU:OE1	2.35	0.59
1:C:439:ILE:H	1:C:439:ILE:HD12	1.68	0.59
1:B:1167:GLU:N	1:B:1167:GLU:OE1	2.34	0.59
1:C:363:ILE:HA	1:C:366:LEU:HD12	1.84	0.59
1:D:2143:ILE:H	1:D:2143:ILE:HD12	1.68	0.59
1:A:886:ARG:NH1	1:A:1047:VAL:O	2.36	0.59
1:D:1652:LYS:NZ	1:D:1739:ASP:OD1	2.35	0.59
1:B:782:LEU:HD13	1:B:866:LEU:HA	1.84	0.59
1:C:254:CYS:SG	1:C:308:HIS:ND1	2.74	0.59
1:A:1934:VAL:HG11	1:A:1988:LEU:HD13	1.85	0.58
1:C:466:GLN:OE1	1:C:469:ARG:NH2	2.36	0.58
1:D:1344:HIS:O	1:D:1348:MET:HG3	2.03	0.58
1:B:1050:GLU:OE1	1:B:1050:GLU:N	2.34	0.58
1:A:773:LEU:HD11	1:A:777:PHE:CE2	2.38	0.58
1:B:496:ILE:HG23	1:B:562:HIS:HE2	1.68	0.58
1:B:782:LEU:HD11	1:B:869:ASN:OD1	2.03	0.58
1:B:1033:GLU:OE2	1:B:1605:ARG:NH1	2.34	0.58
1:B:781:MET:HE2	1:B:781:MET:HA	1.84	0.58
1:B:1621:LEU:HD21	1:B:1647:LEU:HD22	1.84	0.58
1:C:1182:MET:HE3	1:C:1182:MET:O	2.03	0.58
1:D:1799:GLU:OE2	1:D:1803:THR:HG23	2.03	0.58
1:B:2359:ILE:O	1:B:2363:THR:HG23	2.03	0.58
1:C:1469:LEU:HD11	1:C:1513:TRP:HZ3	1.66	0.58
1:D:1736:LEU:O	1:D:1740:LEU:HD23	2.02	0.58
1:A:793:LEU:HD11	1:A:872:TYR:HD1	1.69	0.58
1:D:581:MET:HE2	1:D:595:ILE:HG13	1.85	0.58
1:A:1028:ILE:HD13	1:A:1598:ILE:HD11	1.84	0.58
1:B:1212:ILE:HG21	1:B:1221:MET:HE1	1.84	0.58
1:B:2225:TYR:OH	1:B:2338:GLU:OE2	2.13	0.58
1:D:1388:THR:HG22	1:D:1421:TYR:CE1	2.39	0.57
1:A:503:ARG:NH2	1:A:566:ASP:O	2.37	0.57
1:A:844:VAL:HG12	1:A:891:ILE:HD12	1.86	0.57
1:B:442:LEU:HD12	1:B:512:GLN:HE21	1.67	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1267:ILE:O	1:B:1271:ASN:ND2	2.36	0.57
1:B:1480:PHE:CD1	1:B:1532:VAL:HG21	2.39	0.57
1:B:1866:SER:O	1:B:1869:ILE:HG22	2.04	0.57
1:B:1961:THR:O	1:B:1961:THR:HG22	2.04	0.57
1:B:2130:ASP:OD1	1:B:2130:ASP:N	2.38	0.57
1:C:1626:LEU:HD12	1:C:1695:LEU:HD13	1.86	0.57
1:C:1934:VAL:HG11	1:C:1988:LEU:HD13	1.86	0.57
1:B:705:GLU:N	1:B:705:GLU:OE1	2.37	0.57
1:B:2546:ASP:OD1	1:B:2547:LYS:N	2.38	0.57
1:C:1469:LEU:HD22	1:C:1518:HIS:CG	2.39	0.57
1:C:1333:VAL:HG23	1:C:1333:VAL:O	2.05	0.57
1:C:2203:LEU:O	1:C:2207:ILE:HG13	2.04	0.57
1:B:1123:LYS:HD3	1:B:1126:LEU:HD13	1.85	0.57
1:D:479:LEU:O	1:D:483:VAL:HG23	2.04	0.57
1:A:1863:MET:HE2	1:A:1867:VAL:HG11	1.87	0.56
1:B:2022:PRO:O	1:B:2026:VAL:HG23	2.05	0.56
1:C:621:LEU:HD13	1:C:630:PHE:CD1	2.39	0.56
1:A:439:ILE:HD12	1:A:439:ILE:H	1.70	0.56
1:A:1773:HIS:HB2	1:A:1888:LEU:HD21	1.86	0.56
1:A:2025:LEU:O	1:A:2029:ILE:HG13	2.05	0.56
1:C:1654:LEU:O	1:C:1654:LEU:HD12	2.05	0.56
1:C:2359:ILE:O	1:C:2363:THR:HG23	2.05	0.56
1:A:1941:LEU:HD11	1:A:1973:LEU:CD1	2.35	0.56
1:D:1773:HIS:HB2	1:D:1888:LEU:HD21	1.87	0.56
1:C:2155:LEU:HD22	1:C:2178:LEU:HD21	1.88	0.56
1:D:451:MET:HG3	1:D:475:LEU:HD22	1.86	0.56
1:D:1622:HIS:HE1	1:D:1724:THR:HG23	1.70	0.56
1:A:614:GLU:N	1:A:614:GLU:OE1	2.34	0.56
1:D:480:VAL:HG11	1:D:493:VAL:HB	1.88	0.56
1:C:748:ILE:HG21	1:C:788:ARG:HD3	1.88	0.56
1:C:1092:PHE:O	1:C:1095:VAL:HG12	2.06	0.56
1:B:745:TYR:O	1:B:749:ASP:OD1	2.22	0.56
1:C:1120:MET:N	1:C:1120:MET:HE2	2.21	0.56
1:B:1373:ALA:C	1:B:1419:HIS:HD1	2.13	0.56
1:B:2143:ILE:HD13	1:B:2186:ARG:NH2	2.21	0.56
1:C:2468:HIS:HB2	1:C:2479:ILE:HD13	1.87	0.56
1:C:451:MET:HB3	1:C:475:LEU:HD22	1.88	0.56
1:C:2178:LEU:O	1:C:2182:MET:HG3	2.06	0.56
1:D:2172:PHE:HZ	1:D:2594:ILE:HG23	1.71	0.55
1:A:622:VAL:HG21	1:A:631:LEU:HD23	1.87	0.55
1:A:1092:PHE:O	1:A:1095:VAL:HG12	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1363:MET:HE3	1:A:1363:MET:O	2.06	0.55
1:A:1941:LEU:HD11	1:A:1973:LEU:HD13	1.88	0.55
1:B:1934:VAL:HG11	1:B:1988:LEU:HD13	1.88	0.55
1:C:871:ILE:HG23	1:C:881:LEU:HD21	1.88	0.55
1:D:2162:ASP:OD1	1:D:2164:GLN:N	2.39	0.55
1:B:1190:ARG:O	1:B:1194:GLN:HG3	2.06	0.55
1:A:480:VAL:HG13	1:A:496:ILE:HG21	1.87	0.55
1:A:1542:MET:HA	1:A:1542:MET:HE2	1.88	0.55
1:B:585:ILE:HD13	1:B:595:ILE:CD1	2.35	0.55
1:D:819:LEU:HD23	1:D:819:LEU:H	1.71	0.55
1:D:1962:HIS:CE1	1:D:1964:SER:HG	2.22	0.55
1:A:2468:HIS:HB2	1:A:2479:ILE:HD13	1.87	0.55
1:C:1603:GLU:OE1	1:C:1604:GLU:N	2.40	0.55
1:D:252:LEU:HD11	1:D:263:VAL:CG1	2.36	0.55
1:B:1320:MET:SD	1:B:1320:MET:N	2.80	0.55
1:A:1397:VAL:HG21	1:A:1436:HIS:HB3	1.89	0.55
1:A:1407:THR:O	1:A:1411:MET:HG3	2.07	0.55
1:B:997:GLU:O	1:B:1001:VAL:HG23	2.07	0.55
1:A:1048:ASP:C	1:A:1048:ASP:OD1	2.50	0.54
1:A:2009:ASP:C	1:A:2009:ASP:OD1	2.51	0.54
1:C:1622:HIS:HE1	1:C:1724:THR:HG23	1.72	0.54
1:A:303:LEU:HD22	1:A:392:LEU:HD22	1.89	0.54
1:B:252:LEU:HD12	1:B:264:PHE:O	2.06	0.54
1:C:743:ARG:NE	1:C:787:ASP:OD2	2.40	0.54
1:C:300:TRP:CE2	1:C:381:VAL:HG22	2.42	0.54
1:C:405:ILE:HG22	1:C:414:ARG:HB2	1.90	0.54
1:D:871:ILE:HD13	1:D:974:ILE:HG23	1.89	0.54
1:D:1514:LEU:HG	1:D:1519:LYS:HG3	1.89	0.54
1:A:772:ASP:OD1	1:A:773:LEU:N	2.41	0.54
1:A:2468:HIS:CB	1:A:2479:ILE:HD13	2.37	0.54
1:C:1937:VAL:HG12	1:C:1992:LEU:HD11	1.89	0.54
1:D:2155:LEU:CD2	1:D:2178:LEU:HD11	2.37	0.54
1:A:1492:GLN:CD	1:A:1493:THR:HG23	2.32	0.54
1:A:2164:GLN:N	1:A:2164:GLN:OE1	2.40	0.54
1:A:760:ILE:HG21	1:A:781:MET:HB2	1.89	0.54
1:C:391:HIS:ND1	1:C:394:THR:OG1	2.28	0.54
1:D:886:ARG:NE	1:D:1049:ASP:OD2	2.41	0.54
1:B:1514:LEU:HD23	1:B:1519:LYS:HG2	1.90	0.54
1:D:2553:VAL:HG11	1:D:2562:GLU:OE1	2.08	0.54
1:D:1322:MET:HE1	1:D:1372:LEU:HD23	1.90	0.53
1:B:593:ASP:OD1	1:B:594:THR:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1209:LEU:O	1:B:1212:ILE:HG22	2.07	0.53
1:B:1621:LEU:HD21	1:B:1647:LEU:CD2	2.38	0.53
1:C:1203:HIS:CD2	1:C:1245:LEU:HD21	2.43	0.53
1:A:611:THR:HB	1:A:614:GLU:OE1	2.09	0.53
1:A:1625:GLU:OE1	1:A:1625:GLU:N	2.41	0.53
1:A:2352:GLU:OE2	1:D:2367:ARG:NH2	2.42	0.53
1:A:1644:LEU:HD11	1:A:1672:MET:HE1	1.91	0.53
1:A:2054:TYR:CD1	1:A:2117:TYR:HB3	2.44	0.53
1:C:811:THR:OG1	1:C:814:ASP:OD2	2.22	0.53
1:D:1896:ASN:OD1	1:D:1896:ASN:O	2.26	0.53
1:B:589:ILE:O	1:B:589:ILE:HG22	2.07	0.53
1:B:1329:GLY:O	1:B:1333:VAL:HG22	2.08	0.53
1:C:2215:ILE:O	1:C:2219:ILE:HG13	2.09	0.53
1:D:1397:VAL:HG21	1:D:1436:HIS:HB3	1.91	0.53
1:D:1963:GLU:OE2	1:D:1963:GLU:N	2.38	0.53
1:C:1209:LEU:O	1:C:1212:ILE:HG22	2.09	0.53
1:D:506:GLN:NE2	1:D:563:SER:O	2.42	0.53
1:A:538:LEU:HD13	1:A:587:TYR:CE2	2.44	0.53
1:A:1338:ASP:OD2	1:A:1339:LYS:N	2.41	0.53
1:D:468:ASP:O	1:D:472:VAL:HG23	2.08	0.53
1:D:1644:LEU:O	1:D:1648:ILE:HG13	2.09	0.53
1:A:849:VAL:HB	1:A:852:ALA:HB2	1.91	0.53
1:B:695:THR:HG23	1:B:705:GLU:HG3	1.91	0.53
1:B:1120:MET:O	1:B:1127:TRP:NE1	2.35	0.53
1:B:1605:ARG:HG3	1:B:1606:LEU:HD23	1.90	0.53
1:D:1455:ARG:NH1	1:D:1465:GLU:OE2	2.35	0.53
1:A:239:ASP:O	1:A:285:VAL:HG12	2.09	0.53
1:B:1120:MET:SD	1:B:1127:TRP:NE1	2.81	0.53
1:B:1502:LEU:HD13	1:B:1529:LEU:HD22	1.91	0.53
1:A:622:VAL:HG23	1:A:630:PHE:HB2	1.90	0.53
1:C:405:ILE:HG22	1:C:414:ARG:CB	2.39	0.53
1:C:1089:MET:HE3	1:C:1089:MET:HA	1.91	0.53
1:C:656:VAL:HG11	1:C:739:MET:HE1	1.91	0.52
1:A:1209:LEU:O	1:A:1212:ILE:HG22	2.09	0.52
1:C:2476:VAL:HG23	1:C:2479:ILE:HD11	1.91	0.52
1:A:1328:ALA:HB3	1:A:1332:VAL:HG21	1.91	0.52
1:B:1915:CYS:HB3	1:B:1969:ILE:HD12	1.92	0.52
1:C:1796:ALA:CB	1:C:1870:MET:HE3	2.38	0.52
1:D:439:ILE:HD12	1:D:439:ILE:H	1.74	0.52
1:D:480:VAL:HG22	1:D:559:VAL:HG23	1.91	0.52
1:A:882:LEU:O	1:A:885:THR:OG1	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2536:THR:O	1:A:2536:THR:HG22	2.09	0.52
1:B:888:LEU:CD1	1:B:974:ILE:HG21	2.40	0.52
1:B:1651:THR:OG1	1:B:1665:VAL:HG11	2.10	0.52
1:B:1948:CYS:SG	1:B:1959:ILE:HD12	2.50	0.52
1:C:1089:MET:SD	1:C:1606:LEU:HD12	2.50	0.52
1:C:1502:LEU:HD13	1:C:1529:LEU:HD13	1.91	0.52
1:C:1689:MET:HA	1:C:1689:MET:HE2	1.91	0.52
1:C:871:ILE:HD11	1:C:884:LEU:CD2	2.40	0.51
1:C:1773:HIS:HB2	1:C:1888:LEU:HD21	1.91	0.51
1:D:1346:LEU:HD21	1:D:1402:HIS:NE2	2.26	0.51
1:A:1752:GLU:OE1	1:A:1752:GLU:HA	2.09	0.51
1:D:350:ILE:HD11	1:D:401:THR:HG21	1.91	0.51
1:D:1381:VAL:O	1:D:1385:ILE:HG13	2.11	0.51
1:D:1697:ASN:OD1	1:D:1697:ASN:N	2.44	0.51
1:A:1654:LEU:HD12	1:A:1654:LEU:O	2.09	0.51
1:D:497:MET:SD	1:D:497:MET:C	2.93	0.51
1:B:1032:ALA:O	1:B:1035:MET:HE2	2.10	0.51
1:B:1125:GLU:OE1	1:B:1126:LEU:N	2.44	0.51
1:C:745:TYR:O	1:C:749:ASP:OD2	2.29	0.51
1:D:1502:LEU:HG	1:D:1529:LEU:HD23	1.92	0.51
1:A:641:ASN:CG	1:A:641:ASN:O	2.53	0.51
1:A:1428:MET:HB2	1:A:1431:ILE:HD12	1.91	0.51
1:C:1799:GLU:C	1:C:1799:GLU:OE1	2.54	0.51
1:A:763:CYS:HB3	1:A:777:PHE:CE2	2.46	0.51
1:A:1651:THR:OG1	1:A:1665:VAL:HG11	2.11	0.51
1:A:871:ILE:HD11	1:A:884:LEU:CD2	2.41	0.51
1:B:315:LEU:HD11	1:B:354:LEU:HD13	1.92	0.51
1:B:871:ILE:HD11	1:B:884:LEU:HD21	1.93	0.51
1:B:1097:LEU:CD1	1:B:1595:LEU:HD22	2.41	0.51
1:B:1114:LEU:HD11	1:B:1202:ALA:HB2	1.91	0.51
1:B:1469:LEU:HD22	1:B:1518:HIS:CG	2.46	0.51
1:C:1976:ASN:O	1:C:1993:LYS:NZ	2.44	0.51
1:B:1533:ALA:HA	1:B:1538:ILE:HD11	1.93	0.51
1:D:2543:LEU:CD1	1:D:2610:LEU:HD12	2.41	0.51
1:B:354:LEU:HD12	1:B:417:LEU:HD12	1.93	0.51
1:C:650:GLU:OE2	1:C:654:LYS:NZ	2.44	0.51
1:D:1006:ASP:OD2	1:D:1007:SER:N	2.44	0.51
1:A:599:LEU:HB3	1:A:606:LEU:HD13	1.92	0.50
1:B:398:ILE:HD13	1:B:419:THR:HG22	1.93	0.50
1:C:760:ILE:HG21	1:C:781:MET:HB2	1.92	0.50
1:C:1885:ASN:ND2	1:C:1888:LEU:HD23	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1659:GLU:OE2	1:A:1659:GLU:N	2.37	0.50
1:B:300:TRP:CE2	1:B:381:VAL:HG22	2.46	0.50
1:C:1184:GLY:O	1:C:1190:ARG:NH2	2.41	0.50
1:C:1428:MET:HA	1:C:1428:MET:HE2	1.91	0.50
1:C:1697:ASN:O	1:C:1698:ARG:C	2.54	0.50
1:D:1285:HIS:O	1:D:1289:LEU:HD23	2.10	0.50
1:A:1386:LYS:HD3	1:A:1386:LYS:N	2.26	0.50
1:A:2191:MET:CE	1:A:2194:ILE:HD12	2.38	0.50
1:C:240:VAL:HA	1:C:284:GLU:HA	1.94	0.50
1:C:1189:MET:SD	1:C:1189:MET:C	2.95	0.50
1:A:602:ASN:HD22	1:A:605:LEU:HD12	1.75	0.50
1:D:509:MET:HE2	1:D:514:ILE:HG21	1.93	0.50
1:D:760:ILE:HG21	1:D:781:MET:HB2	1.93	0.50
1:B:476:LEU:O	1:B:480:VAL:HG12	2.12	0.50
1:C:1866:SER:O	1:C:1869:ILE:HG22	2.12	0.50
1:A:282:LEU:HD22	1:A:434:VAL:HG21	1.94	0.50
1:A:647:VAL:O	1:A:651:LEU:HD23	2.11	0.50
1:B:459:LEU:HD13	1:B:525:PRO:HD3	1.93	0.50
1:B:606:LEU:HD12	1:B:610:ILE:HG12	1.94	0.50
1:B:2468:HIS:HB2	1:B:2479:ILE:HD13	1.93	0.50
1:A:1124:SER:HA	1:A:1127:TRP:CD1	2.47	0.50
1:C:1531:MET:HE3	1:C:1531:MET:O	2.12	0.50
1:D:755:LEU:HD13	1:D:759:LEU:HD23	1.94	0.50
1:B:2266:VAL:O	1:B:2270:LEU:HG	2.11	0.50
1:C:1506:THR:HG23	1:C:1547:HIS:ND1	2.27	0.50
1:A:1612:ALA:O	1:A:1616:VAL:HG23	2.11	0.50
1:B:1603:GLU:OE2	1:B:1604:GLU:N	2.44	0.50
1:A:984:ASP:C	1:A:984:ASP:OD1	2.55	0.49
1:B:1035:MET:HE3	1:B:1036:PHE:CZ	2.46	0.49
1:D:2065:LYS:HE2	1:D:2065:LYS:HA	1.92	0.49
1:A:789:ASP:C	1:A:789:ASP:OD1	2.55	0.49
1:D:2048:GLU:N	1:D:2048:GLU:OE1	2.44	0.49
1:A:1266:HIS:HD1	1:A:1266:HIS:H	1.59	0.49
1:B:451:MET:CE	1:B:475:LEU:HD22	2.41	0.49
1:C:2226:MET:HE2	1:C:2226:MET:HA	1.94	0.49
1:C:2546:ASP:OD1	1:C:2546:ASP:C	2.55	0.49
1:D:509:MET:HA	1:D:514:ILE:HD12	1.94	0.49
1:A:663:ASP:OD2	1:A:663:ASP:N	2.44	0.49
1:A:1652:LYS:O	1:A:1655:MET:HE2	2.13	0.49
1:B:1125:GLU:C	1:B:1125:GLU:CD	2.81	0.49
1:B:1500:GLN:OE1	1:B:1500:GLN:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:885:THR:HG23	1:A:978:ILE:HD13	1.93	0.49
1:A:1746:ASN:OD1	1:A:1748:LYS:N	2.45	0.49
1:A:1974:ILE:HD11	1:A:1997:SER:HA	1.95	0.49
1:B:1731:GLU:OE1	1:B:1731:GLU:HA	2.13	0.49
1:C:1780:LYS:HE2	1:C:1780:LYS:HA	1.95	0.49
1:A:585:ILE:HD13	1:A:595:ILE:HD12	1.95	0.49
1:B:1444:PHE:CG	1:B:1472:VAL:HG13	2.48	0.49
1:D:1444:PHE:O	1:D:1448:MET:HG3	2.13	0.49
1:A:1333:VAL:HA	1:A:1368:LEU:HD21	1.95	0.49
1:B:602:ASN:HD22	1:B:605:LEU:HD12	1.78	0.49
1:C:1001:VAL:HG12	1:C:1002:PHE:CD1	2.48	0.49
1:A:871:ILE:HG23	1:A:881:LEU:HD21	1.95	0.49
1:B:833:THR:HG22	1:B:866:LEU:HD21	1.94	0.49
1:C:1970:ILE:HA	1:C:1973:LEU:HD12	1.94	0.49
1:D:522:LEU:HD22	1:D:557:TYR:HE1	1.77	0.49
1:D:1934:VAL:HG11	1:D:1988:LEU:HD13	1.95	0.49
1:D:2162:ASP:OD1	1:D:2162:ASP:C	2.56	0.49
1:A:1025:LEU:HD23	1:A:1601:ALA:CB	2.43	0.49
1:A:1053:ARG:O	1:A:1057:ARG:HG3	2.12	0.49
1:B:581:MET:HG3	1:B:595:ILE:HD11	1.94	0.49
1:B:969:LEU:HD23	1:B:969:LEU:C	2.38	0.49
1:C:305:ARG:NE	1:C:360:GLY:O	2.46	0.49
1:A:558:ARG:HD3	1:A:590:LEU:HD23	1.95	0.48
1:B:871:ILE:HD11	1:B:884:LEU:CD2	2.43	0.48
1:B:1260:GLU:O	1:B:1264:MET:HG3	2.13	0.48
1:D:267:THR:HG23	1:D:413:ILE:O	2.13	0.48
1:A:1033:GLU:OE2	1:A:1682:ARG:NH2	2.45	0.48
1:A:1115:ASP:OD1	1:A:1115:ASP:C	2.56	0.48
1:A:2048:GLU:OE1	1:A:2048:GLU:N	2.46	0.48
1:B:745:TYR:HA	1:B:748:ILE:HB	1.93	0.48
1:B:1407:THR:HG21	1:B:1464:LEU:HA	1.95	0.48
1:A:576:LYS:HD2	1:A:576:LYS:N	2.28	0.48
1:B:1960:VAL:HG23	1:B:2003:LEU:HD22	1.94	0.48
1:C:682:TYR:HB2	1:C:685:ILE:HD12	1.95	0.48
1:C:1881:CYS:SG	1:C:1892:LEU:HD12	2.53	0.48
1:D:1333:VAL:HG23	1:D:1333:VAL:O	2.13	0.48
1:D:1513:TRP:O	1:D:1514:LEU:CB	2.62	0.48
1:D:1905:CYS:SG	1:D:1962:HIS:NE2	2.83	0.48
1:A:1595:LEU:O	1:A:1598:ILE:HG22	2.13	0.48
1:A:2014:GLU:O	1:A:2018:ILE:HG13	2.13	0.48
1:D:252:LEU:HD13	1:D:417:LEU:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:451:MET:HG3	1:D:475:LEU:CD2	2.44	0.48
1:D:557:TYR:HH	1:D:584:GLN:CD	2.19	0.48
1:D:1397:VAL:O	1:D:1401:THR:HG23	2.12	0.48
1:A:580:MET:SD	1:A:580:MET:C	2.97	0.48
1:A:835:GLU:O	1:A:839:ASP:OD1	2.30	0.48
1:A:836:PHE:CD1	1:A:836:PHE:C	2.89	0.48
1:B:1894:CYS:O	1:B:1894:CYS:SG	2.72	0.48
1:B:2048:GLU:N	1:B:2048:GLU:OE1	2.47	0.48
1:C:252:LEU:HD11	1:C:417:LEU:HD11	1.95	0.48
1:D:1621:LEU:HD23	1:D:1643:PHE:HE2	1.79	0.48
1:A:1124:SER:HA	1:A:1127:TRP:NE1	2.28	0.48
1:C:1496:THR:O	1:C:1500:GLN:HG2	2.13	0.48
1:A:1428:MET:SD	1:A:1428:MET:N	2.87	0.48
1:B:541:LEU:HD13	1:B:550:GLN:HG3	1.94	0.48
1:A:1469:LEU:HD22	1:A:1518:HIS:CG	2.49	0.48
1:B:1437:ILE:N	1:B:1437:ILE:HD12	2.29	0.48
1:A:840:TYR:CD2	1:A:863:VAL:HG11	2.48	0.48
1:B:309:LEU:HD23	1:B:442:LEU:HD22	1.96	0.48
1:B:455:ALA:O	1:B:459:LEU:HG	2.13	0.48
1:C:1366:ILE:HD11	1:C:1409:VAL:HG23	1.94	0.48
1:D:781:MET:HE3	1:D:833:THR:HG22	1.95	0.48
1:D:1626:LEU:HD11	1:D:1698:ARG:HB2	1.95	0.48
1:A:250:LYS:HE2	1:A:267:THR:HG22	1.94	0.48
1:B:1097:LEU:HD11	1:B:1595:LEU:HD22	1.96	0.48
1:B:1197:LEU:CD2	1:B:1202:ALA:HB3	2.43	0.48
1:C:581:MET:HB3	1:C:595:ILE:HD11	1.95	0.48
1:D:451:MET:CG	1:D:475:LEU:HD22	2.44	0.48
1:D:2549:ASP:O	1:D:2550:ASN:OD1	2.32	0.48
1:B:1467:TYR:O	1:B:1471:VAL:HG22	2.14	0.47
1:B:1658:GLU:N	1:B:1658:GLU:OE1	2.46	0.47
1:C:1193:GLN:O	1:C:1197:LEU:HD23	2.14	0.47
1:D:882:LEU:O	1:D:885:THR:OG1	2.31	0.47
1:A:354:LEU:HD12	1:A:417:LEU:HD12	1.96	0.47
1:B:782:LEU:HD11	1:B:869:ASN:HB2	1.97	0.47
1:D:614:GLU:OE1	1:D:614:GLU:N	2.47	0.47
1:D:1574:ARG:O	1:D:1575:ALA:HB3	2.14	0.47
1:A:561:ARG:HE	1:A:597:ALA:HB2	1.79	0.47
1:B:667:ARG:NH1	1:B:754:GLN:OE1	2.48	0.47
1:B:1228:THR:O	1:B:1232:LEU:HG	2.14	0.47
1:C:802:LEU:HD11	1:C:1107:TYR:CE1	2.50	0.47
1:C:1203:HIS:O	1:C:1207:LEU:HG	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1950:GLY:N	1:C:1951:PRO:HA	2.29	0.47
1:A:1206:MET:HE2	1:A:1231:PHE:CD2	2.49	0.47
1:C:1924:LEU:HD22	1:C:1924:LEU:N	2.30	0.47
1:D:250:LYS:HE2	1:D:267:THR:HG22	1.96	0.47
1:D:1864:GLY:O	1:D:1868:LEU:HD23	2.14	0.47
1:A:1736:LEU:HD12	1:A:1740:LEU:HG	1.96	0.47
1:B:1124:SER:HB2	1:B:1212:ILE:HD11	1.96	0.47
1:C:1737:VAL:HG11	1:C:1757:ALA:HB2	1.95	0.47
1:D:668:THR:HG21	1:D:755:LEU:HD11	1.96	0.47
1:A:299:HIS:ND1	1:A:378:ASP:O	2.47	0.47
1:A:792:GLU:OE1	1:A:1118:ARG:NE	2.48	0.47
1:A:1626:LEU:HD22	1:A:1698:ARG:HB2	1.96	0.47
1:A:2065:LYS:N	1:A:2065:LYS:HD2	2.29	0.47
1:B:1063:THR:HG23	1:B:1075:LEU:HD21	1.95	0.47
1:B:1381:VAL:HG13	1:B:1382:TYR:N	2.30	0.47
1:B:1621:LEU:HD23	1:B:1643:PHE:HE2	1.74	0.47
1:C:599:LEU:HB3	1:C:606:LEU:HD13	1.96	0.47
1:D:1318:GLN:OE1	1:D:1380:ASN:ND2	2.47	0.47
1:A:1975:LEU:HD22	1:A:2024:GLU:HB3	1.97	0.47
1:A:2172:PHE:HZ	1:A:2594:ILE:HG23	1.78	0.47
1:B:315:LEU:HD12	1:B:316:ALA:N	2.29	0.47
1:B:654:LYS:HE3	1:B:746:LEU:HD13	1.96	0.47
1:B:845:VAL:CG2	1:B:887:THR:HG23	2.45	0.47
1:D:405:ILE:HD11	1:D:416:MET:HA	1.95	0.47
1:D:2159:THR:HG21	1:D:2167:LYS:HB3	1.97	0.47
1:A:1028:ILE:HD13	1:A:1598:ILE:CD1	2.45	0.47
1:B:1290:LEU:HD21	1:B:1299:TYR:HB2	1.97	0.47
1:B:1529:LEU:HD23	1:B:1529:LEU:C	2.40	0.47
1:B:2320:PHE:O	1:B:2324:VAL:HG23	2.15	0.47
1:C:1322:MET:HA	1:C:1322:MET:HE3	1.97	0.47
1:C:1502:LEU:HD21	1:C:1548:ILE:HD11	1.96	0.47
1:C:1509:LEU:HD12	1:C:1514:LEU:CD2	2.45	0.47
1:D:1621:LEU:HD23	1:D:1643:PHE:CE2	2.50	0.47
1:A:297:ALA:HB3	1:A:380:PHE:CE1	2.50	0.47
1:C:2010:SER:O	1:C:2014:GLU:HG2	2.15	0.47
1:D:435:PRO:O	1:D:439:ILE:HD12	2.14	0.47
1:A:622:VAL:HG23	1:A:630:PHE:CB	2.45	0.46
1:A:893:ASP:OD1	1:A:1057:ARG:NH2	2.48	0.46
1:C:1495:GLN:HA	1:C:1498:VAL:HG22	1.97	0.46
1:C:2155:LEU:CD2	1:C:2178:LEU:HD21	2.45	0.46
1:D:990:LEU:HG	1:D:1035:MET:HE1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1388:THR:HG22	1:D:1421:TYR:CD1	2.50	0.46
1:D:1489:THR:O	1:D:1492:GLN:NE2	2.47	0.46
1:A:1866:SER:O	1:A:1869:ILE:HG22	2.15	0.46
1:B:1969:ILE:O	1:B:1973:LEU:HD13	2.15	0.46
1:C:813:LYS:O	1:C:816:ASP:OD1	2.33	0.46
1:D:997:GLU:N	1:D:997:GLU:OE1	2.48	0.46
1:D:1740:LEU:O	1:D:1744:THR:HG22	2.15	0.46
1:D:2476:VAL:O	1:D:2479:ILE:HG13	2.15	0.46
1:A:2382:LEU:HD11	1:B:2346:PHE:HE1	1.79	0.46
1:B:585:ILE:HD12	1:B:591:ALA:HB3	1.96	0.46
1:B:1444:PHE:CE1	1:B:1472:VAL:HG22	2.50	0.46
1:C:480:VAL:HG13	1:C:496:ILE:HG21	1.97	0.46
1:A:1469:LEU:HD21	1:A:1513:TRP:HZ3	1.80	0.46
1:B:1621:LEU:HD13	1:B:1672:MET:SD	2.56	0.46
1:D:581:MET:HE3	1:D:581:MET:HA	1.95	0.46
1:D:1333:VAL:HA	1:D:1368:LEU:HD21	1.97	0.46
1:A:1066:ASP:OD1	1:A:1067:TYR:N	2.48	0.46
1:B:997:GLU:HG2	1:B:1028:ILE:HD11	1.97	0.46
1:B:1373:ALA:O	1:B:1419:HIS:ND1	2.38	0.46
1:C:477:GLU:HA	1:C:493:VAL:HG11	1.98	0.46
1:C:745:TYR:CZ	1:C:789:ASP:OD1	2.68	0.46
1:C:1914:MET:HE1	1:C:1936:LEU:HD23	1.97	0.46
1:B:301:ASN:OD1	1:B:302:GLY:N	2.49	0.46
1:C:1125:GLU:HA	1:C:1128:VAL:HG12	1.97	0.46
1:D:451:MET:HE1	1:D:472:VAL:HG22	1.96	0.46
1:D:871:ILE:HD11	1:D:884:LEU:CD2	2.46	0.46
1:A:252:LEU:HD11	1:A:263:VAL:CG1	2.45	0.46
1:A:2369:ILE:HG23	1:A:2512:ILE:HG23	1.98	0.46
1:A:2536:THR:O	1:A:2536:THR:CG2	2.64	0.46
1:B:391:HIS:HB2	1:B:398:ILE:HD11	1.97	0.46
1:B:442:LEU:HD12	1:B:512:GLN:NE2	2.31	0.46
1:B:702:GLU:OE1	1:B:702:GLU:N	2.49	0.46
1:D:769:LEU:HB3	1:D:773:LEU:HD23	1.97	0.46
1:A:800:ALA:HB2	1:A:1199:ASN:OD1	2.15	0.46
1:A:1878:GLN:OE1	1:A:1939:GLN:NE2	2.44	0.46
1:B:780:LEU:O	1:B:784:VAL:HG23	2.15	0.46
1:C:242:ARG:HB2	1:C:432:VAL:HB	1.97	0.46
1:C:2381:TYR:CZ	1:C:2385:ILE:HD11	2.50	0.46
1:A:641:ASN:O	1:A:641:ASN:OD1	2.34	0.46
1:A:1979:SER:HA	1:A:1982:CYS:SG	2.55	0.46
1:A:2049:VAL:O	1:A:2053:ILE:HD12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1214:TYR:HB3	1:B:1221:MET:HE3	1.97	0.46
1:C:612:LYS:HD2	1:C:613:THR:N	2.30	0.46
1:C:754:GLN:HB3	1:C:755:LEU:HD12	1.98	0.46
1:D:772:ASP:OD1	1:D:773:LEU:N	2.47	0.46
1:D:1400:VAL:HG21	1:D:1440:LEU:CD1	2.46	0.46
1:D:1505:THR:HG22	1:D:1526:ILE:HD13	1.97	0.46
1:D:2261:ILE:O	1:D:2261:ILE:HG22	2.15	0.46
1:B:239:ASP:O	1:B:285:VAL:HG12	2.16	0.46
1:B:282:LEU:CB	1:B:309:LEU:HD22	2.45	0.46
1:D:885:THR:CG2	1:D:978:ILE:HD13	2.46	0.46
1:D:1209:LEU:O	1:D:1212:ILE:HG22	2.16	0.46
1:D:1919:THR:HG22	1:D:1924:LEU:HD23	1.98	0.46
1:A:1783:GLU:OE2	1:A:1899:THR:N	2.46	0.45
1:B:1089:MET:HE2	1:B:1606:LEU:HD12	1.98	0.45
1:B:1469:LEU:HD21	1:B:1514:LEU:CD1	2.46	0.45
1:B:1961:THR:O	1:B:1961:THR:CG2	2.65	0.45
1:B:599:LEU:HB3	1:B:606:LEU:HD13	1.98	0.45
1:D:280:ASN:O	1:D:308:HIS:NE2	2.48	0.45
1:D:1741:ILE:HG21	1:D:1785:PHE:CE1	2.51	0.45
1:D:1672:MET:HE2	1:D:1728:LEU:HD11	1.98	0.45
1:A:803:TRP:HA	1:A:806:ILE:HD12	1.98	0.45
1:A:1527:ARG:O	1:A:1531:MET:HG3	2.16	0.45
1:A:1948:CYS:SG	1:A:1959:ILE:HD12	2.56	0.45
1:C:1525:CYS:O	1:C:1528:THR:OG1	2.29	0.45
1:D:536:VAL:HG12	1:D:537:ARG:N	2.32	0.45
1:D:599:LEU:HB3	1:D:606:LEU:HD13	1.99	0.45
1:D:1514:LEU:HD11	1:D:1518:HIS:HB2	1.97	0.45
1:D:1950:GLY:N	1:D:1951:PRO:HA	2.30	0.45
1:B:585:ILE:HD11	1:B:592:GLU:HG3	1.98	0.45
1:B:1396:VAL:HG22	1:B:1413:TYR:CE1	2.52	0.45
1:C:582:GLN:O	1:C:585:ILE:HG22	2.16	0.45
1:C:1606:LEU:HD22	1:C:1609:LEU:HD12	1.98	0.45
1:D:581:MET:HE3	1:D:581:MET:CA	2.47	0.45
1:A:580:MET:SD	1:A:581:MET:N	2.89	0.45
1:A:803:TRP:HB2	1:A:1099:ILE:HG12	1.97	0.45
1:A:1285:HIS:HD2	1:A:1289:LEU:HD23	1.81	0.45
1:A:1374:ALA:HA	1:A:1377:GLU:OE1	2.16	0.45
1:A:1950:GLY:N	1:A:1951:PRO:HA	2.32	0.45
1:A:2546:ASP:OD1	1:A:2547:LYS:N	2.49	0.45
1:B:781:MET:HE1	1:B:785:HIS:HB2	1.99	0.45
1:B:1381:VAL:HG13	1:B:1382:TYR:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:745:TYR:HA	1:A:748:ILE:HB	1.99	0.45
1:B:582:GLN:O	1:B:585:ILE:HG22	2.16	0.45
1:B:1225:LEU:O	1:B:1229:HIS:ND1	2.49	0.45
1:B:2476:VAL:O	1:B:2479:ILE:HG13	2.16	0.45
1:C:263:VAL:HG13	1:C:283:TRP:CZ2	2.52	0.45
1:A:473:ILE:HG23	1:A:555:LEU:HD11	1.99	0.45
1:A:2553:VAL:HG21	1:A:2609:SER:CB	2.47	0.45
1:B:1673:LEU:HD21	1:B:1728:LEU:HD22	1.97	0.45
1:C:1111:LYS:HG3	1:C:1200:MET:HE3	1.99	0.45
1:C:1503:GLN:HG2	1:C:1544:LEU:HD13	1.99	0.45
1:D:630:PHE:O	1:D:634:LEU:HG	2.16	0.45
1:D:1885:ASN:OD1	1:D:1888:LEU:HD23	2.16	0.45
1:A:842:ASN:O	1:A:845:VAL:HG12	2.17	0.45
1:A:1544:LEU:HA	1:A:1547:HIS:ND1	2.32	0.45
1:A:1902:ASN:ND2	1:A:1905:CYS:SG	2.90	0.45
1:B:350:ILE:HG21	1:B:416:MET:HE2	1.98	0.45
1:B:1124:SER:HA	1:B:1127:TRP:CE2	2.50	0.45
1:B:1528:THR:HA	1:B:1531:MET:HE3	1.98	0.45
1:B:1877:LEU:HD13	1:B:1947:TYR:OH	2.17	0.45
1:B:1950:GLY:N	1:B:1951:PRO:HA	2.31	0.45
1:C:252:LEU:CD1	1:C:417:LEU:HD11	2.47	0.45
1:C:263:VAL:HG13	1:C:283:TRP:HZ2	1.82	0.45
1:D:781:MET:HE3	1:D:833:THR:CG2	2.46	0.45
1:D:1513:TRP:O	1:D:1513:TRP:CD2	2.70	0.45
1:D:1799:GLU:OE2	1:D:1799:GLU:O	2.34	0.45
1:D:2155:LEU:HD21	1:D:2178:LEU:HD11	1.99	0.45
1:A:240:VAL:HA	1:A:284:GLU:HA	1.98	0.45
1:A:1097:LEU:CD1	1:A:1595:LEU:HD22	2.45	0.45
1:A:1488:SER:O	1:A:1536:ARG:NH1	2.50	0.45
1:A:1518:HIS:O	1:A:1522:VAL:HG23	2.17	0.45
1:A:1648:ILE:HG23	1:A:1736:LEU:HD22	1.99	0.45
1:B:749:ASP:O	1:B:753:GLN:HG2	2.17	0.45
1:B:1206:MET:HB3	1:B:1232:LEU:HD21	1.99	0.45
1:C:250:LYS:HD3	1:C:267:THR:HG22	1.98	0.45
1:D:1894:CYS:O	1:D:1894:CYS:SG	2.74	0.45
1:A:300:TRP:CZ2	1:A:381:VAL:HG13	2.53	0.44
1:A:1974:ILE:HD11	1:A:1997:SER:CA	2.47	0.44
1:B:647:VAL:O	1:B:651:LEU:HD23	2.16	0.44
1:B:2468:HIS:CB	1:B:2479:ILE:HD13	2.47	0.44
1:C:1542:MET:C	1:C:1542:MET:SD	3.00	0.44
1:D:1405:CYS:SG	1:D:1406:ILE:N	2.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1548:ILE:HA	1:D:1551:MET:HE2	1.99	0.44
1:A:2261:ILE:HG22	1:A:2261:ILE:O	2.18	0.44
1:D:693:TRP:O	1:D:694:LEU:HD12	2.17	0.44
1:A:396:THR:HG21	1:A:419:THR:HB	1.99	0.44
1:A:871:ILE:HD11	1:A:884:LEU:HD21	1.98	0.44
1:C:1785:PHE:O	1:C:1788:VAL:HG22	2.17	0.44
1:C:2009:ASP:C	1:C:2009:ASP:OD1	2.60	0.44
1:D:406:ASP:OD1	1:D:406:ASP:N	2.50	0.44
1:D:1269:LEU:HD12	1:D:1305:THR:HG23	1.99	0.44
1:D:1895:GLN:NE2	1:D:1901:TYR:O	2.50	0.44
1:B:653:CYS:SG	1:B:747:ALA:HB2	2.57	0.44
1:C:1396:VAL:HG22	1:C:1413:TYR:CE1	2.53	0.44
1:C:1697:ASN:OD1	1:C:1697:ASN:N	2.48	0.44
1:C:2261:ILE:HG22	1:C:2261:ILE:O	2.18	0.44
1:D:1085:ARG:HB2	1:D:1610:VAL:HG22	1.98	0.44
1:A:719:ASN:ND2	1:A:722:ASP:OD1	2.50	0.44
1:A:1246:LEU:HD13	1:A:1267:ILE:HG12	1.98	0.44
1:A:1514:LEU:HD11	1:A:1518:HIS:HB3	1.99	0.44
1:A:1885:ASN:OD1	1:A:1888:LEU:HD23	2.18	0.44
1:B:1192:LYS:N	1:B:1192:LYS:HD3	2.33	0.44
1:D:252:LEU:HD13	1:D:417:LEU:CD1	2.47	0.44
1:D:308:HIS:ND1	1:D:311:THR:OG1	2.31	0.44
1:D:596:THR:HG21	1:D:633:TYR:HB3	1.99	0.44
1:D:1380:ASN:HB2	1:D:1383:THR:HG22	1.99	0.44
1:D:1457:LYS:O	1:D:1458:ARG:HB2	2.18	0.44
1:A:1525:CYS:O	1:A:1529:LEU:HG	2.17	0.44
1:A:1644:LEU:HD22	1:A:1731:GLU:HG3	2.00	0.44
1:B:536:VAL:HG12	1:B:537:ARG:N	2.33	0.44
1:B:2546:ASP:OD1	1:B:2546:ASP:C	2.61	0.44
1:C:1223:GLU:OE2	1:C:1227:TYR:CE2	2.71	0.44
1:C:1386:LYS:O	1:C:1390:LEU:HD13	2.16	0.44
1:C:2172:PHE:HZ	1:C:2594:ILE:HG23	1.83	0.44
1:D:621:LEU:HD12	1:D:622:VAL:N	2.32	0.44
1:D:1531:MET:HE3	1:D:1532:VAL:N	2.32	0.44
1:A:477:GLU:HG3	1:A:493:VAL:HG11	1.99	0.44
1:A:1319:ASP:O	1:A:1323:THR:HG23	2.17	0.44
1:B:631:LEU:HD11	1:B:728:TYR:CD1	2.52	0.44
1:C:464:ILE:HG22	1:C:535:LEU:HD21	2.00	0.44
1:C:1345:LEU:O	1:C:1349:MET:HG3	2.17	0.44
1:C:1422:VAL:CG1	1:C:1478:ALA:HB1	2.48	0.44
1:A:1106:ASN:ND2	1:A:1182:MET:HE1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:464:ILE:HG22	1:B:535:LEU:HD21	2.00	0.44
1:C:577:GLN:O	1:C:580:MET:N	2.47	0.44
1:C:1397:VAL:O	1:C:1401:THR:HG23	2.18	0.44
1:C:1418:ASN:O	1:C:1422:VAL:HB	2.18	0.44
1:D:1514:LEU:HD12	1:D:1515:GLN:N	2.33	0.44
1:A:840:TYR:HD2	1:A:863:VAL:HG11	1.83	0.44
1:A:1740:LEU:O	1:A:1744:THR:HG22	2.18	0.44
1:B:240:VAL:HA	1:B:284:GLU:HA	1.99	0.44
1:B:893:ASP:O	1:B:894:CYS:C	2.59	0.44
1:B:990:LEU:HD23	1:B:1092:PHE:CD1	2.53	0.44
1:B:1229:HIS:HA	1:B:1232:LEU:HD12	2.00	0.44
1:B:2324:VAL:HA	1:B:2327:ILE:HD12	2.00	0.44
1:C:772:ASP:OD1	1:C:773:LEU:N	2.51	0.44
1:C:1372:LEU:HA	1:C:1375:CYS:SG	2.57	0.44
1:D:1284:GLN:HA	1:D:1287:VAL:HG22	2.00	0.44
1:D:1315:LYS:O	1:D:1319:ASP:OD2	2.36	0.44
1:D:2369:ILE:HG23	1:D:2512:ILE:HG23	2.00	0.44
1:A:1182:MET:O	1:A:1182:MET:SD	2.76	0.43
1:C:315:LEU:HD11	1:C:354:LEU:HD13	2.00	0.43
1:A:621:LEU:HD12	1:A:622:VAL:N	2.33	0.43
1:A:660:LYS:C	1:A:660:LYS:HD3	2.43	0.43
1:A:1696:GLN:O	1:A:1697:ASN:CB	2.66	0.43
1:A:2476:VAL:HG22	1:A:2480:LEU:CD1	2.47	0.43
1:B:308:HIS:CE1	1:B:311:THR:HG23	2.53	0.43
1:B:1411:MET:HA	1:B:1471:VAL:HG21	2.00	0.43
1:C:1621:LEU:HD12	1:C:1672:MET:HE2	2.01	0.43
1:C:1912:ASP:OD1	1:C:1912:ASP:C	2.60	0.43
1:D:2294:ILE:O	1:D:2297:VAL:HG12	2.17	0.43
1:A:1117:LEU:HD11	1:A:1172:VAL:HG13	1.99	0.43
1:A:1284:GLN:HA	1:A:1287:VAL:HG22	2.00	0.43
1:A:1331:ASP:OD2	1:A:1331:ASP:N	2.50	0.43
1:A:1501:LEU:O	1:A:1501:LEU:HD23	2.17	0.43
1:C:596:THR:HG21	1:C:633:TYR:HD1	1.82	0.43
1:D:789:ASP:C	1:D:789:ASP:OD1	2.60	0.43
1:A:2339:LEU:CD1	1:D:2389:LEU:HD11	2.47	0.43
1:B:482:PHE:O	1:B:505:ARG:NH1	2.51	0.43
1:B:1123:LYS:CD	1:B:1126:LEU:HD13	2.48	0.43
1:B:1456:GLU:O	1:B:1458:ARG:NH1	2.51	0.43
1:B:2261:ILE:O	1:B:2261:ILE:HG22	2.19	0.43
1:C:1328:ALA:HB3	1:C:1332:VAL:HG21	1.98	0.43
1:C:1871:GLN:HB3	1:C:1872:PRO:HD3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2125:GLU:OE1	1:C:2563:HIS:NE2	2.51	0.43
1:D:578:PHE:O	1:D:581:MET:HB2	2.18	0.43
1:A:308:HIS:CE1	1:A:311:THR:HG23	2.53	0.43
1:A:828:ASN:OD1	1:A:829:LYS:N	2.52	0.43
1:A:1253:PHE:CE2	1:A:1267:ILE:HD11	2.53	0.43
1:A:1393:LEU:O	1:A:1397:VAL:HG23	2.18	0.43
1:A:1524:ALA:O	1:A:1528:THR:HG23	2.19	0.43
1:B:608:LYS:N	1:B:608:LYS:HD2	2.32	0.43
1:B:826:LYS:HD3	1:B:875:PHE:CD2	2.53	0.43
1:B:1123:LYS:HD2	1:B:1126:LEU:HD22	2.01	0.43
1:C:1246:LEU:HD22	1:C:1253:PHE:CE2	2.53	0.43
1:C:1316:LYS:HD3	1:C:1316:LYS:N	2.34	0.43
1:D:1328:ALA:HB3	1:D:1332:VAL:CG2	2.47	0.43
1:D:1393:LEU:O	1:D:1397:VAL:HG23	2.18	0.43
1:D:2558:HIS:CE1	1:D:2563:HIS:ND1	2.87	0.43
1:A:722:ASP:HA	1:A:725:VAL:HG12	2.01	0.43
1:A:1120:MET:O	1:A:1127:TRP:NE1	2.52	0.43
1:A:1696:GLN:O	1:A:1697:ASN:HB3	2.18	0.43
1:C:1040:LYS:O	1:C:1041:THR:HG23	2.18	0.43
1:C:1530:ALA:O	1:C:1534:LYS:HG2	2.18	0.43
1:C:2215:ILE:HG21	1:C:2341:TYR:CD1	2.54	0.43
1:D:1648:ILE:CG2	1:D:1736:LEU:HD22	2.45	0.43
1:D:1871:GLN:HB3	1:D:1872:PRO:HD3	2.01	0.43
1:A:729:TYR:HE2	1:A:773:LEU:HD13	1.83	0.43
1:A:1616:VAL:HG21	1:A:1690:LEU:HD13	2.00	0.43
1:A:2187:LYS:O	1:A:2191:MET:HG3	2.18	0.43
1:A:2476:VAL:O	1:A:2479:ILE:HG13	2.18	0.43
1:B:240:VAL:CG2	1:B:439:ILE:HD11	2.49	0.43
1:B:405:ILE:HG22	1:B:414:ARG:HB2	2.00	0.43
1:B:867:ALA:O	1:B:871:ILE:HD12	2.19	0.43
1:B:2010:SER:O	1:B:2014:GLU:HG2	2.18	0.43
1:C:466:GLN:O	1:C:466:GLN:NE2	2.52	0.43
1:A:300:TRP:CD2	1:A:381:VAL:HG22	2.54	0.43
1:A:314:TYR:O	1:A:357:VAL:HG22	2.19	0.43
1:A:505:ARG:O	1:A:509:MET:HE2	2.18	0.43
1:A:819:LEU:HD23	1:A:819:LEU:H	1.84	0.43
1:B:781:MET:HE1	1:B:785:HIS:CD2	2.53	0.43
1:C:1349:MET:HE2	1:C:1406:ILE:H	1.83	0.43
1:C:1421:TYR:HA	1:C:1424:THR:HG23	2.01	0.43
1:C:1654:LEU:HD12	1:C:1654:LEU:C	2.43	0.43
1:D:557:TYR:CE2	1:D:591:ALA:HA	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:PHE:HE2	1:A:509:MET:SD	2.42	0.43
1:A:1219:ALA:O	1:A:1222:MET:HG2	2.18	0.43
1:B:309:LEU:HD23	1:B:442:LEU:CD2	2.49	0.43
1:B:1346:LEU:C	1:B:1346:LEU:HD23	2.44	0.43
1:B:1975:LEU:HD11	1:B:2020:LEU:HD12	2.01	0.43
1:C:1536:ARG:O	1:C:1537:ALA:HB3	2.19	0.43
1:C:1741:ILE:HG21	1:C:1785:PHE:CE1	2.54	0.43
1:D:858:LYS:O	1:D:862:GLU:HG2	2.18	0.43
1:D:1348:MET:HE3	1:D:1361:PRO:HG2	2.01	0.43
1:D:1626:LEU:HD11	1:D:1698:ARG:CB	2.49	0.43
1:B:1895:GLN:N	1:B:1900:ASN:OD1	2.50	0.43
1:C:2476:VAL:O	1:C:2479:ILE:HG13	2.19	0.43
1:D:493:VAL:O	1:D:496:ILE:HG22	2.19	0.43
1:D:582:GLN:O	1:D:585:ILE:HG22	2.19	0.43
1:D:769:LEU:HD13	1:D:773:LEU:CD2	2.49	0.43
1:D:791:GLN:N	1:D:791:GLN:CD	2.77	0.43
1:D:1465:GLU:O	1:D:1469:LEU:HG	2.19	0.43
1:A:398:ILE:HD13	1:A:419:THR:HG22	2.01	0.42
1:A:497:MET:HE3	1:A:497:MET:O	2.19	0.42
1:A:1062:LEU:HD22	1:A:1070:LEU:HD21	2.01	0.42
1:C:1284:GLN:HA	1:C:1287:VAL:HG22	2.00	0.42
1:D:1530:ALA:O	1:D:1534:LYS:HG2	2.18	0.42
1:D:2491:PRO:O	1:D:2495:VAL:HG23	2.18	0.42
1:A:1971:THR:HG22	1:A:2000:LEU:HD11	2.01	0.42
1:B:760:ILE:HG21	1:B:781:MET:HB2	2.01	0.42
1:B:1979:SER:HA	1:B:1982:CYS:SG	2.58	0.42
1:C:622:VAL:HG23	1:C:630:PHE:HB2	2.01	0.42
1:A:1381:VAL:HA	1:A:1384:GLU:HB3	2.01	0.42
1:B:263:VAL:HG21	1:B:315:LEU:HD13	2.01	0.42
1:B:451:MET:HE1	1:B:472:VAL:HA	2.02	0.42
1:B:1129:ASP:OD1	1:B:1129:ASP:C	2.61	0.42
1:C:581:MET:H	1:C:581:MET:HE2	1.85	0.42
1:C:2155:LEU:CD2	1:C:2178:LEU:HD11	2.50	0.42
1:C:2458:LEU:HD23	1:D:2220:ALA:HA	2.01	0.42
1:A:241:VAL:HA	1:A:434:VAL:HG23	2.01	0.42
1:A:482:PHE:O	1:A:505:ARG:NH1	2.52	0.42
1:B:2155:LEU:CD2	1:B:2178:LEU:HD21	2.49	0.42
1:C:572:GLU:OE2	1:C:573:HIS:N	2.53	0.42
1:C:745:TYR:OH	1:C:789:ASP:OD1	2.28	0.42
1:C:1469:LEU:HD21	1:C:1513:TRP:CZ3	2.54	0.42
1:D:1407:THR:HG21	1:D:1464:LEU:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1785:PHE:O	1:D:1788:VAL:HG22	2.19	0.42
1:A:606:LEU:HD23	1:A:645:ILE:CD1	2.49	0.42
1:A:2156:PHE:CD1	1:A:2565:MET:HE1	2.55	0.42
1:A:2320:PHE:O	1:A:2324:VAL:HG23	2.19	0.42
1:A:2390:PHE:HB2	1:A:2391:LEU:HD12	2.01	0.42
1:B:469:ARG:HD2	1:B:548:PRO:HB2	2.01	0.42
1:B:1344:HIS:C	1:B:1348:MET:HE3	2.43	0.42
1:B:1502:LEU:HD13	1:B:1529:LEU:CD2	2.49	0.42
1:B:2020:LEU:HD21	1:B:2025:LEU:HD22	2.02	0.42
1:D:745:TYR:HA	1:D:748:ILE:HB	2.02	0.42
1:D:1001:VAL:HG12	1:D:1002:PHE:CD1	2.54	0.42
1:D:1273:GLN:NE2	1:D:1277:GLU:OE2	2.53	0.42
1:D:1396:VAL:HG11	1:D:1417:VAL:CG2	2.49	0.42
1:A:1469:LEU:HD21	1:A:1513:TRP:CZ3	2.53	0.42
1:B:518:VAL:HG13	1:B:556:CYS:HB3	2.01	0.42
1:B:753:GLN:HA	1:B:753:GLN:OE1	2.20	0.42
1:B:1044:MET:SD	1:B:1044:MET:N	2.76	0.42
1:C:1380:ASN:HB2	1:C:1383:THR:HG22	2.02	0.42
1:C:1919:THR:CG2	1:C:1924:LEU:HD23	2.46	0.42
1:D:1438:TRP:CE3	1:D:1497:ILE:HG21	2.54	0.42
1:A:871:ILE:HD13	1:A:974:ILE:HG23	2.02	0.42
1:A:1737:VAL:HG11	1:A:1757:ALA:HB2	2.01	0.42
1:B:508:LEU:HD23	1:B:509:MET:HE1	2.01	0.42
1:B:1924:LEU:N	1:B:1924:LEU:HD22	2.35	0.42
1:D:1253:PHE:CE1	1:D:1263:THR:HG21	2.55	0.42
1:A:1212:ILE:CG2	1:A:1221:MET:HE1	2.50	0.42
1:A:1280:GLU:H	1:A:1280:GLU:CD	2.28	0.42
1:D:1513:TRP:O	1:D:1513:TRP:CG	2.73	0.42
1:D:1733:ALA:O	1:D:1737:VAL:HG23	2.20	0.42
1:D:2175:SER:HA	1:D:2178:LEU:HD12	2.02	0.42
1:A:1126:LEU:HD12	1:A:1126:LEU:N	2.35	0.42
1:B:519:PHE:HA	1:B:522:LEU:HD12	2.02	0.42
1:C:1929:ILE:HD12	1:C:1978:ILE:HD12	2.01	0.42
1:C:2226:MET:HE2	1:C:2226:MET:H	1.85	0.42
1:D:622:VAL:HG23	1:D:630:PHE:HB2	2.02	0.42
1:D:885:THR:HG23	1:D:978:ILE:HD13	2.01	0.42
1:D:1741:ILE:HG23	1:D:1750:PHE:HE1	1.85	0.42
1:A:840:TYR:O	1:A:844:VAL:HG23	2.20	0.42
1:A:1169:TYR:N	1:A:1169:TYR:CD2	2.87	0.42
1:A:2485:LYS:HB2	1:B:2460:MET:CE	2.50	0.42
1:B:505:ARG:O	1:B:509:MET:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:518:VAL:HG13	1:B:556:CYS:SG	2.59	0.42
1:B:1981:LEU:HD12	1:B:1981:LEU:O	2.20	0.42
1:C:1201:ASP:HA	1:C:1203:HIS:CE1	2.54	0.42
1:D:483:VAL:HG22	1:D:509:MET:CE	2.50	0.42
1:D:522:LEU:HD21	1:D:556:CYS:HB2	2.01	0.42
1:D:769:LEU:HD13	1:D:773:LEU:HD21	2.02	0.42
1:D:2290:LEU:HD11	1:D:2331:VAL:HG23	2.01	0.42
1:A:702:GLU:OE2	1:A:702:GLU:N	2.53	0.41
1:B:522:LEU:HD22	1:B:557:TYR:CE1	2.54	0.41
1:C:1336:TYR:HB2	1:C:1345:LEU:HD22	2.02	0.41
1:C:2558:HIS:CE1	1:C:2563:HIS:ND1	2.88	0.41
1:D:494:LEU:HD21	1:D:554:ARG:HD2	2.01	0.41
1:D:1322:MET:HE1	1:D:1372:LEU:CD2	2.49	0.41
1:D:2199:ARG:HG3	1:D:2199:ARG:HH11	1.85	0.41
1:A:611:THR:HG22	1:A:613:THR:H	1.84	0.41
1:A:1323:THR:O	1:A:1327:ASN:OD1	2.38	0.41
1:B:1435:ASN:HA	1:B:1438:TRP:CD1	2.55	0.41
1:B:1863:MET:HE2	1:B:1867:VAL:HG11	2.02	0.41
1:B:2155:LEU:HD22	1:B:2178:LEU:HD21	2.02	0.41
1:C:593:ASP:OD2	1:C:593:ASP:C	2.62	0.41
1:C:619:VAL:O	1:C:622:VAL:HG12	2.19	0.41
1:C:1111:LYS:HG3	1:C:1200:MET:CE	2.50	0.41
1:C:1476:ILE:HG22	1:C:1480:PHE:CE2	2.55	0.41
1:D:1455:ARG:HG3	1:D:1513:TRP:NE1	2.34	0.41
1:D:1896:ASN:O	1:D:1896:ASN:CG	2.63	0.41
1:A:1492:GLN:OE1	1:A:1493:THR:HG23	2.19	0.41
1:B:405:ILE:HG22	1:B:414:ARG:CB	2.51	0.41
1:B:518:VAL:HG11	1:B:560:LEU:HG	2.02	0.41
1:C:998:PHE:HA	1:C:1023:MET:HE3	2.02	0.41
1:C:1316:LYS:O	1:C:1320:MET:HG2	2.21	0.41
1:C:1322:MET:CE	1:C:1375:CYS:SG	3.08	0.41
1:C:2226:MET:HE2	1:C:2226:MET:CA	2.51	0.41
1:A:266:ARG:NH1	1:A:267:THR:O	2.53	0.41
1:A:315:LEU:HD12	1:A:316:ALA:N	2.35	0.41
1:A:1258:LEU:HD12	1:A:1259:LEU:HD23	2.03	0.41
1:D:522:LEU:HB3	1:D:580:MET:HE1	2.01	0.41
1:A:1741:ILE:HG23	1:A:1750:PHE:HE1	1.86	0.41
1:A:2184:TRP:CZ3	1:A:2307:PHE:HZ	2.37	0.41
1:B:1212:ILE:CG2	1:B:1221:MET:HE1	2.49	0.41
1:B:1333:VAL:HA	1:B:1368:LEU:HD21	2.02	0.41
1:C:401:THR:HG22	1:C:403:VAL:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:871:ILE:HD13	1:C:974:ILE:HG23	2.03	0.41
1:C:1182:MET:HE2	1:C:1193:GLN:OE1	2.20	0.41
1:C:1937:VAL:CG1	1:C:1992:LEU:HD11	2.50	0.41
1:D:451:MET:CE	1:D:472:VAL:HG22	2.51	0.41
1:D:1731:GLU:OE1	1:D:1731:GLU:HA	2.20	0.41
1:D:2178:LEU:O	1:D:2182:MET:HG3	2.20	0.41
1:A:798:LYS:HA	1:A:798:LYS:HE2	2.03	0.41
1:A:1751:GLN:HG2	1:A:1869:ILE:HD13	2.02	0.41
1:B:240:VAL:HG11	1:B:309:LEU:HD11	2.03	0.41
1:B:267:THR:N	1:B:413:ILE:O	2.52	0.41
1:B:975:LEU:O	1:B:979:LEU:HD23	2.20	0.41
1:B:1307:ILE:HD12	1:B:1371:LEU:HD12	2.03	0.41
1:C:577:GLN:O	1:C:581:MET:HE2	2.21	0.41
1:C:723:GLU:CD	1:C:723:GLU:C	2.89	0.41
1:C:743:ARG:NH1	1:C:788:ARG:O	2.54	0.41
1:C:1206:MET:HE3	1:C:1231:PHE:CD1	2.54	0.41
1:C:1223:GLU:OE2	1:C:1227:TYR:CZ	2.74	0.41
1:D:462:GLY:O	1:D:535:LEU:HD13	2.21	0.41
1:D:522:LEU:HD23	1:D:553:PHE:HD1	1.85	0.41
1:D:557:TYR:HE2	1:D:591:ALA:HA	1.85	0.41
1:D:1931:GLU:O	1:D:1934:VAL:HG12	2.21	0.41
1:A:451:MET:SD	1:A:451:MET:N	2.94	0.41
1:A:1124:SER:HA	1:A:1127:TRP:HE1	1.84	0.41
1:A:1533:ALA:HA	1:A:1538:ILE:HD11	2.01	0.41
1:B:558:ARG:HD3	1:B:590:LEU:HD23	2.02	0.41
1:B:841:LEU:HB3	1:B:887:THR:HG21	2.01	0.41
1:B:1227:TYR:HA	1:B:1230:GLN:OE1	2.20	0.41
1:B:1741:ILE:HG21	1:B:1785:PHE:CE1	2.56	0.41
1:B:2267:ALA:HA	1:B:2270:LEU:HD12	2.02	0.41
1:B:2553:VAL:HG21	1:B:2609:SER:HB3	2.02	0.41
1:C:554:ARG:O	1:C:558:ARG:HG2	2.20	0.41
1:C:775:ALA:HB1	1:C:862:GLU:HG3	2.02	0.41
1:C:1127:TRP:CE3	1:C:1127:TRP:C	2.99	0.41
1:D:364:ALA:O	1:D:391:HIS:NE2	2.50	0.41
1:D:834:MET:CE	1:D:876:TYR:CZ	3.04	0.41
1:D:2295:VAL:O	1:D:2298:VAL:HG22	2.19	0.41
1:A:606:LEU:HD23	1:A:645:ILE:HD13	2.02	0.41
1:A:1746:ASN:HB3	1:A:1749:ILE:HD12	2.01	0.41
1:B:709:ARG:HB2	1:B:709:ARG:NH1	2.36	0.41
1:B:1272:TYR:CD1	1:B:1272:TYR:C	2.98	0.41
1:C:1221:MET:O	1:C:1221:MET:SD	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1250:LEU:O	1:C:1250:LEU:HD23	2.20	0.41
1:C:1502:LEU:CD2	1:C:1548:ILE:HD11	2.51	0.41
1:D:590:LEU:N	1:D:590:LEU:HD12	2.35	0.41
1:D:1332:VAL:HG23	1:D:1333:VAL:HG13	2.03	0.41
1:A:1491:LEU:HD22	1:A:1536:ARG:HG3	2.02	0.41
1:A:1587:ASP:HB2	1:A:1590:ASN:HB3	2.03	0.41
1:B:798:LYS:HD3	1:B:798:LYS:N	2.36	0.41
1:B:972:LEU:HD11	1:B:1062:LEU:CD1	2.50	0.41
1:B:1655:MET:HG3	1:B:1749:ILE:HD13	2.01	0.41
1:C:241:VAL:HA	1:C:434:VAL:HG23	2.02	0.41
1:C:1349:MET:HE1	1:C:1409:VAL:HG11	2.03	0.41
1:C:1422:VAL:HG11	1:C:1478:ALA:HB1	2.02	0.41
1:C:1462:PRO:O	1:C:1466:LYS:HG2	2.21	0.41
1:C:1469:LEU:O	1:C:1473:LEU:HB3	2.21	0.41
1:C:1915:CYS:HB3	1:C:1925:LEU:HD11	2.02	0.41
1:C:1957:THR:OG1	1:C:2007:ARG:NH2	2.54	0.41
1:D:1619:ASP:OD2	1:D:1687:ARG:NH2	2.54	0.41
1:A:585:ILE:HD11	1:A:592:GLU:HG3	2.01	0.41
1:B:1120:MET:SD	1:B:1127:TRP:CE2	3.14	0.41
1:B:1393:LEU:CD2	1:B:1417:VAL:HG22	2.50	0.41
1:C:554:ARG:HD3	1:C:590:LEU:HD13	2.03	0.41
1:C:791:GLN:CD	1:C:791:GLN:N	2.80	0.41
1:C:1247:HIS:CD2	1:C:1274:LEU:HD22	2.56	0.41
1:C:1771:SER:O	1:C:1775:LEU:HG	2.21	0.41
1:A:698:ASP:OD1	1:A:699:LYS:N	2.52	0.40
1:A:749:ASP:OD2	1:A:749:ASP:N	2.51	0.40
1:B:1258:LEU:O	1:B:1262:GLU:HG3	2.21	0.40
1:B:1960:VAL:HG11	1:B:2012:ASN:HD22	1.86	0.40
1:B:2571:PHE:O	1:B:2575:VAL:HG23	2.21	0.40
1:D:1044:MET:SD	1:D:1044:MET:N	2.88	0.40
1:D:1391:LEU:HD12	1:D:1392:PRO:HD2	2.04	0.40
1:B:242:ARG:HB2	1:B:432:VAL:HB	2.03	0.40
1:B:1092:PHE:HA	1:B:1095:VAL:HG23	2.02	0.40
1:B:1502:LEU:HD21	1:B:1548:ILE:HD11	2.04	0.40
1:B:1527:ARG:O	1:B:1531:MET:HG3	2.21	0.40
1:B:2279:GLY:O	1:B:2283:ASN:OD1	2.39	0.40
1:C:1588:TYR:O	1:C:1592:ILE:HD12	2.22	0.40
1:C:2131:ARG:HH11	1:C:2131:ARG:HG2	1.86	0.40
1:D:788:ARG:HG2	1:D:789:ASP:H	1.87	0.40
1:D:990:LEU:CD1	1:D:1035:MET:HE1	2.51	0.40
1:A:839:ASP:OD1	1:A:839:ASP:N	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1644:LEU:HD22	1:A:1731:GLU:CG	2.50	0.40
1:A:2068:GLN:O	1:A:2072:LYS:HG3	2.22	0.40
1:B:505:ARG:O	1:B:509:MET:CE	2.70	0.40
1:C:2468:HIS:HB3	1:C:2479:ILE:HG21	2.01	0.40
1:D:650:GLU:O	1:D:654:LYS:HG2	2.22	0.40
1:D:1906:GLU:HA	1:D:1906:GLU:OE1	2.21	0.40
1:A:735:LEU:O	1:A:739:MET:HG3	2.21	0.40
1:A:2294:ILE:O	1:A:2297:VAL:HG12	2.21	0.40
1:B:297:ALA:HB3	1:B:380:PHE:CE1	2.57	0.40
1:B:1428:MET:SD	1:B:1430:GLU:HB2	2.62	0.40
1:B:2475:GLY:N	1:B:2478:ASP:OD2	2.54	0.40
1:C:673:VAL:HA	1:C:691:GLU:CD	2.46	0.40
1:C:1001:VAL:C	1:C:1002:PHE:HD1	2.29	0.40
1:C:2478:ASP:OD1	1:C:2478:ASP:N	2.54	0.40
1:D:722:ASP:HA	1:D:725:VAL:HG12	2.03	0.40
1:D:1333:VAL:HA	1:D:1368:LEU:CD2	2.52	0.40
1:A:250:LYS:HE3	1:A:267:THR:HG22	2.00	0.40
1:A:600:HIS:ND1	1:A:600:HIS:C	2.80	0.40
1:A:1203:HIS:HD2	1:A:1204:LYS:N	2.20	0.40
1:A:1457:LYS:O	1:A:1458:ARG:HB2	2.22	0.40
1:A:1492:GLN:OE1	1:A:1493:THR:N	2.51	0.40
1:A:2264:LEU:C	1:A:2264:LEU:HD23	2.47	0.40
1:B:813:LYS:O	1:B:816:ASP:OD1	2.39	0.40
1:B:1595:LEU:O	1:B:1598:ILE:HG22	2.22	0.40
1:C:1310:GLU:O	1:C:1310:GLU:CG	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1961/2671 (73%)	1930 (98%)	30 (2%)	1 (0%)	48 75

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1959/2671 (73%)	1937 (99%)	22 (1%)	0	100	100
1	C	1979/2671 (74%)	1948 (98%)	31 (2%)	0	100	100
1	D	2010/2671 (75%)	1975 (98%)	35 (2%)	0	100	100
All	All	7909/10684 (74%)	7790 (98%)	118 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1697	ASN

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	1807/2385 (76%)	1798 (100%)	9 (0%)	81	83
1	B	1805/2385 (76%)	1794 (99%)	11 (1%)	78	81
1	C	1821/2385 (76%)	1818 (100%)	3 (0%)	87	88
1	D	1838/2385 (77%)	1833 (100%)	5 (0%)	86	86
All	All	7271/9540 (76%)	7243 (100%)	28 (0%)	81	84

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	251	PHE
1	A	405	ILE
1	A	585	ILE
1	A	610	ILE
1	A	835	GLU
1	A	1203	HIS
1	A	1255	THR
1	A	1384	GLU
1	A	1655	MET
1	B	251	PHE

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Mol	Chain	Res	Type
1	B	606	LEU
1	B	711	LEU
1	B	761	PHE
1	B	972	LEU
1	B	1200	MET
1	B	1304	HIS
1	B	1625	GLU
1	B	1626	LEU
1	B	1658	GLU
1	B	2067	LEU
1	C	632	ASP
1	C	1250	LEU
1	C	1592	ILE
1	D	832	ASN
1	D	1035	MET
1	D	1551	MET
1	D	1685	GLN
1	D	2155	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	320	ASN
1	A	359	HIS
1	A	375	GLN
1	A	649	GLN
1	A	710	GLN
1	A	779	HIS
1	A	980	ASN
1	A	1084	GLN
1	A	1090	HIS
1	A	1102	GLN
1	A	1211	GLN
1	A	1247	HIS
1	A	1285	HIS
1	A	1359	HIS
1	A	1419	HIS
1	A	1884	HIS
1	A	1902	ASN
1	A	2063	HIS
1	A	2120	HIS
1	A	2179	HIS

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Mol	Chain	Res	Type
1	A	2185	GLN
1	A	2292	ASN
1	A	2468	HIS
1	B	359	HIS
1	B	512	GLN
1	B	600	HIS
1	B	601	ASN
1	B	625	ASN
1	B	649	GLN
1	B	704	HIS
1	B	783	HIS
1	B	791	GLN
1	B	1094	GLN
1	B	1170	GLN
1	B	1435	ASN
1	B	1477	ASN
1	B	1622	HIS
1	B	1790	HIS
1	B	1902	ASN
1	B	1965	ASN
1	B	1995	ASN
1	B	2069	HIS
1	B	2216	ASN
1	B	2292	ASN
1	B	2357	ASN
1	B	2467	ASN
1	B	2592	GLN
1	C	248	GLN
1	C	280	ASN
1	C	289	HIS
1	C	359	HIS
1	C	512	GLN
1	C	546	ASN
1	C	571	GLN
1	C	573	HIS
1	C	713	GLN
1	C	791	GLN
1	C	980	ASN
1	C	1065	HIS
1	C	1081	HIS
1	C	1285	HIS
1	C	1622	HIS

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Mol	Chain	Res	Type
1	C	1797	GLN
1	C	2292	ASN
1	C	2467	ASN
1	D	384	ASN
1	D	512	GLN
1	D	550	GLN
1	D	754	GLN
1	D	783	HIS
1	D	785	HIS
1	D	1031	GLN
1	D	1090	HIS
1	D	1094	GLN
1	D	1096	GLN
1	D	1168	ASN
1	D	1284	GLN
1	D	1285	HIS
1	D	1435	ASN
1	D	1477	ASN
1	D	1622	HIS
1	D	1885	ASN
1	D	2185	GLN
1	D	2216	ASN

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](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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
5	ATP	D	3004	-	32,33,33	0.26	0	48,52,52	0.66	0
5	ATP	A	3004	-	32,33,33	0.26	0	48,52,52	0.67	0
3	I3P	C	3002	-	24,24,24	2.19	3 (12%)	39,39,39	0.87	0
3	I3P	B	3002	-	24,24,24	2.19	3 (12%)	39,39,39	0.92	0
5	ATP	C	3004	-	32,33,33	0.26	0	48,52,52	0.67	0
5	ATP	B	3004	-	32,33,33	0.27	0	48,52,52	0.67	0
3	I3P	A	3002	-	24,24,24	2.19	3 (12%)	39,39,39	0.87	0
3	I3P	D	3002	-	24,24,24	2.19	3 (12%)	39,39,39	0.85	0

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
5	ATP	D	3004	-	-	2/22/38/38	0/3/3/3
5	ATP	A	3004	-	-	5/22/38/38	0/3/3/3
3	I3P	C	3002	-	-	1/15/39/39	0/1/1/1
3	I3P	B	3002	-	-	1/15/39/39	0/1/1/1
5	ATP	C	3004	-	-	2/22/38/38	0/3/3/3
5	ATP	B	3004	-	-	4/22/38/38	0/3/3/3
3	I3P	A	3002	-	-	0/15/39/39	0/1/1/1
3	I3P	D	3002	-	-	2/15/39/39	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3002	I3P	P4-O4	6.06	1.70	1.59
3	B	3002	I3P	P4-O4	6.06	1.70	1.59
3	C	3002	I3P	P4-O4	6.06	1.70	1.59
3	D	3002	I3P	P4-O4	6.05	1.70	1.59
3	C	3002	I3P	P5-O5	5.96	1.70	1.59
3	D	3002	I3P	P5-O5	5.94	1.69	1.59
3	B	3002	I3P	P5-O5	5.94	1.69	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3002	I3P	P5-O5	5.94	1.69	1.59
3	D	3002	I3P	P1-O1	5.78	1.69	1.59
3	C	3002	I3P	P1-O1	5.72	1.69	1.59
3	A	3002	I3P	P1-O1	5.71	1.69	1.59
3	B	3002	I3P	P1-O1	5.71	1.69	1.59

There are no bond angle outliers.

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	3004	ATP	C5'-O5'-PA-O2A
5	A	3004	ATP	C3'-C4'-C5'-O5'
5	A	3004	ATP	O4'-C4'-C5'-O5'
5	D	3004	ATP	O4'-C4'-C5'-O5'
5	D	3004	ATP	C3'-C4'-C5'-O5'
5	C	3004	ATP	C3'-C4'-C5'-O5'
3	D	3002	I3P	C6-C1-O1-P1
5	B	3004	ATP	PB-O3B-PG-O2G
5	A	3004	ATP	C5'-O5'-PA-O1A
5	A	3004	ATP	C5'-O5'-PA-O3A
3	B	3002	I3P	C6-C1-O1-P1
3	C	3002	I3P	C6-C1-O1-P1
5	C	3004	ATP	O4'-C4'-C5'-O5'
3	D	3002	I3P	C2-C1-O1-P1
5	B	3004	ATP	C3'-C4'-C5'-O5'
5	B	3004	ATP	PB-O3A-PA-O1A
5	B	3004	ATP	PB-O3A-PA-O2A

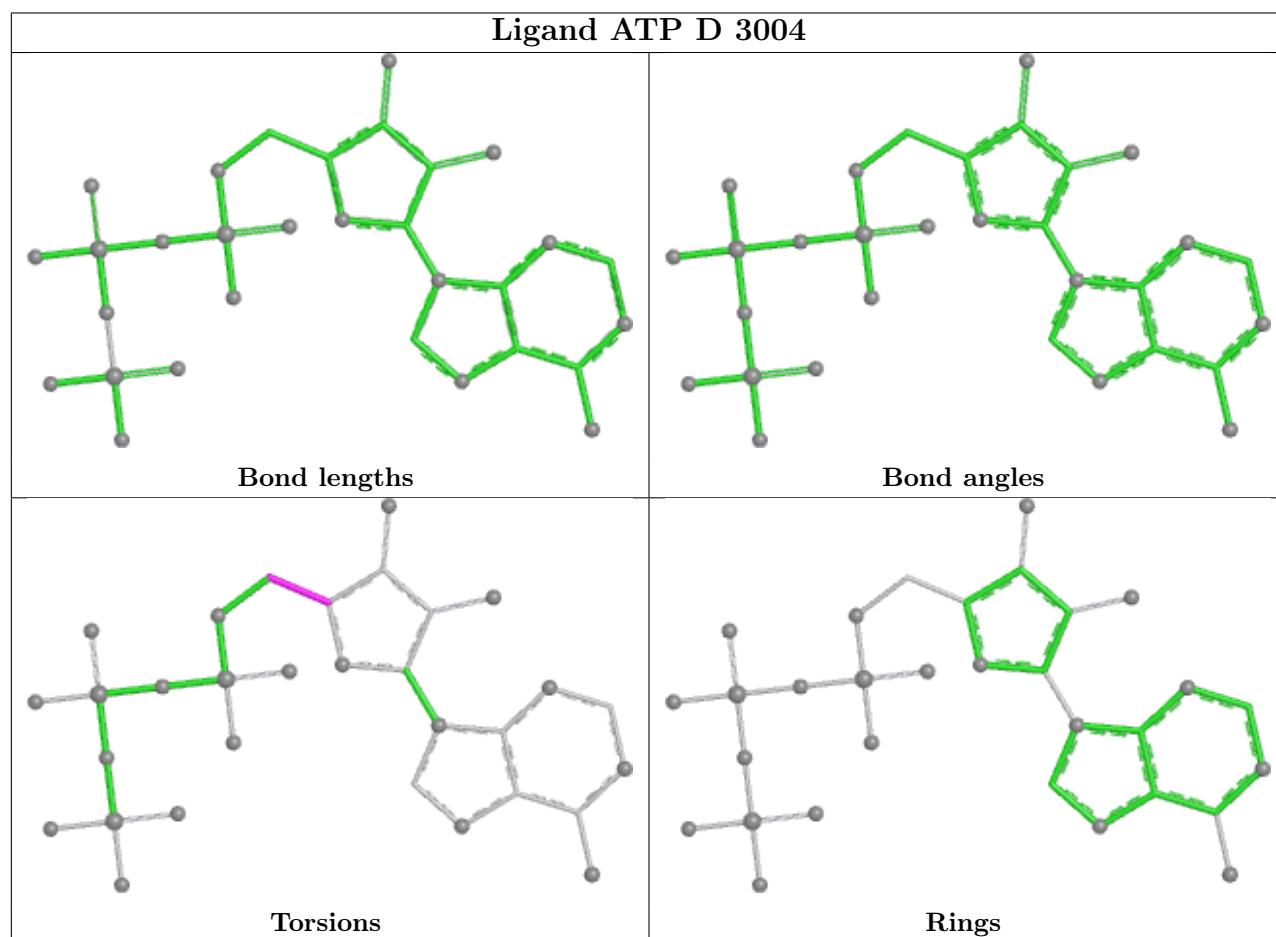
There are no ring outliers.

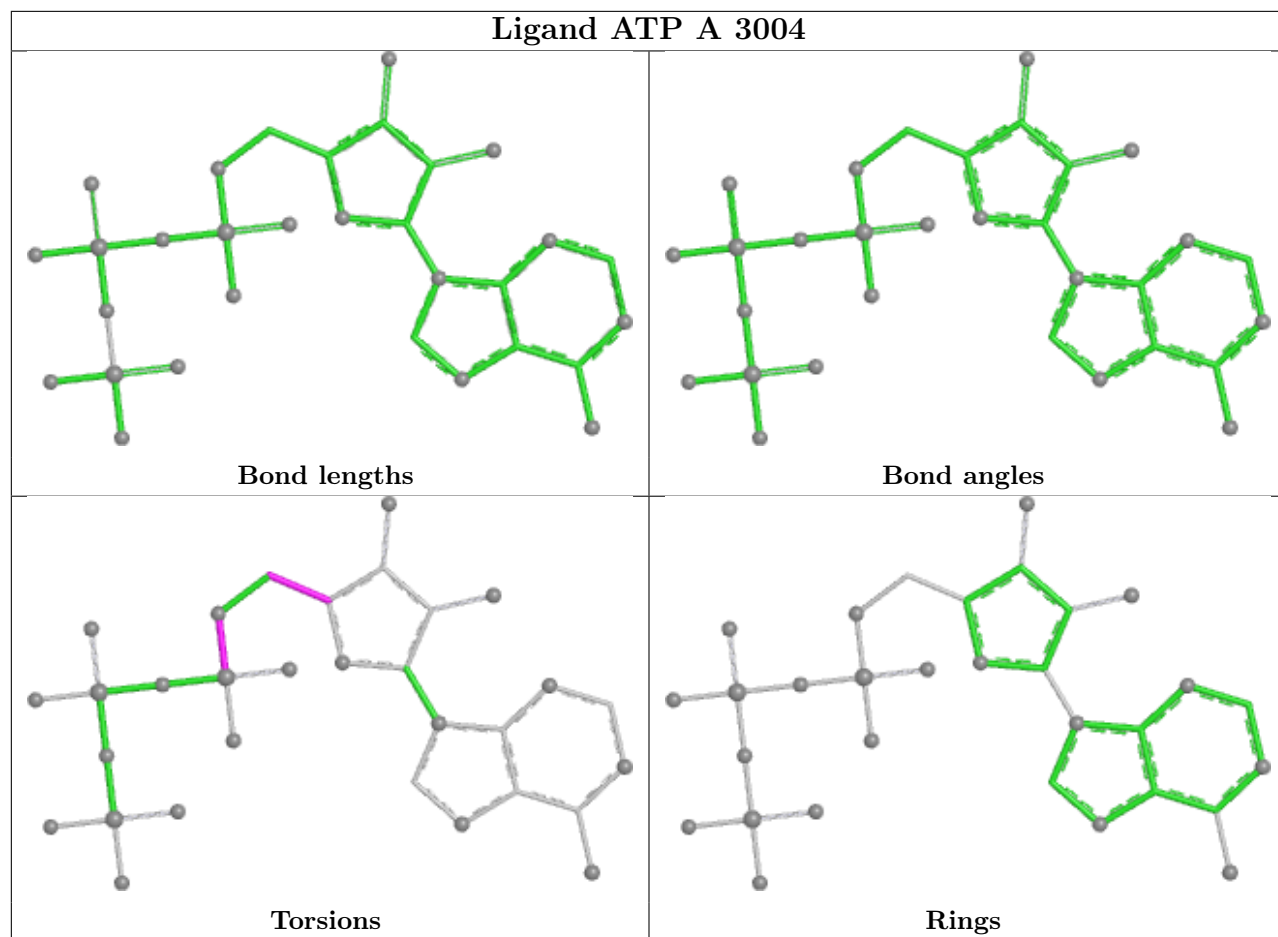
1 monomer is involved in 1 short contact:

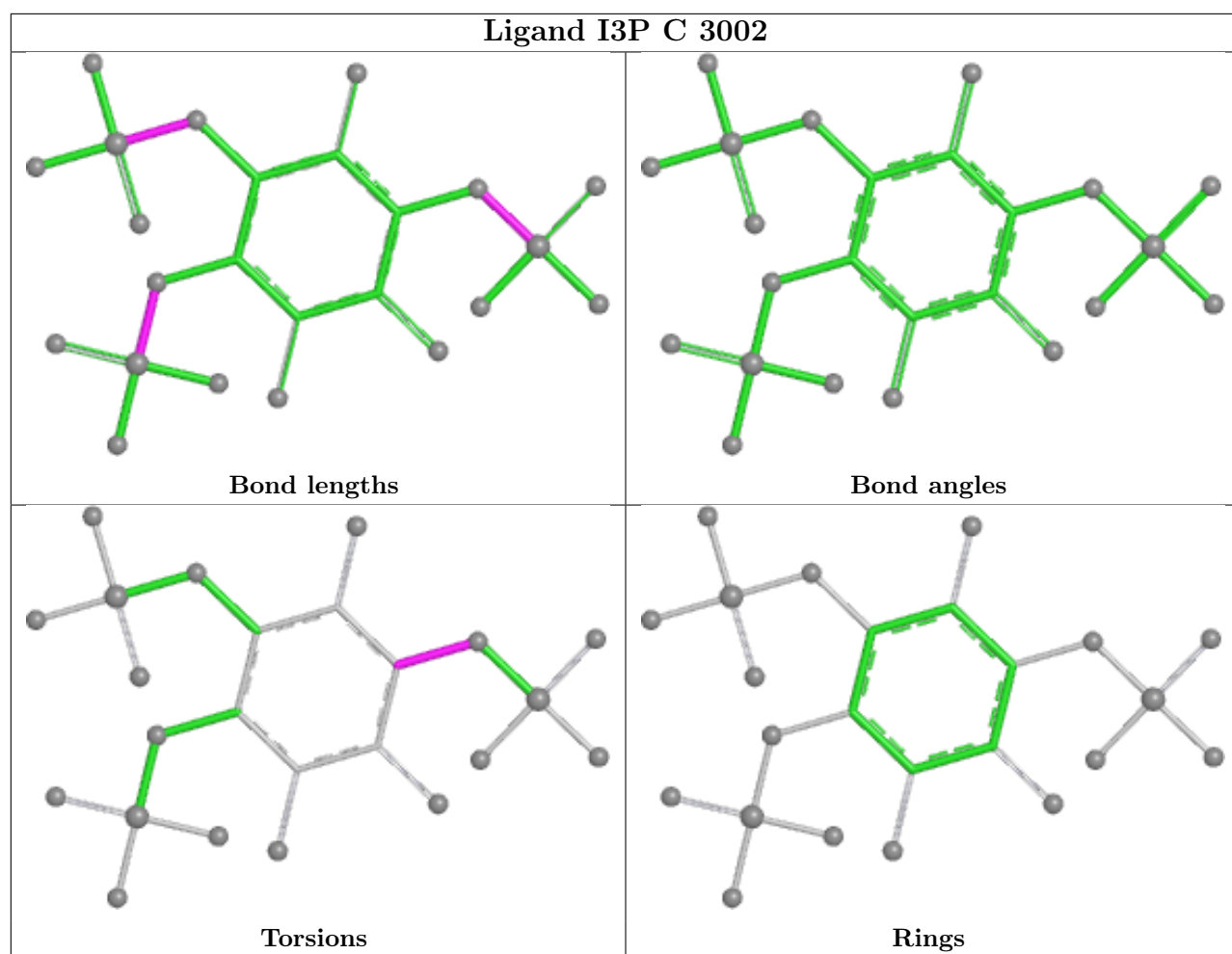
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	3002	I3P	1	0

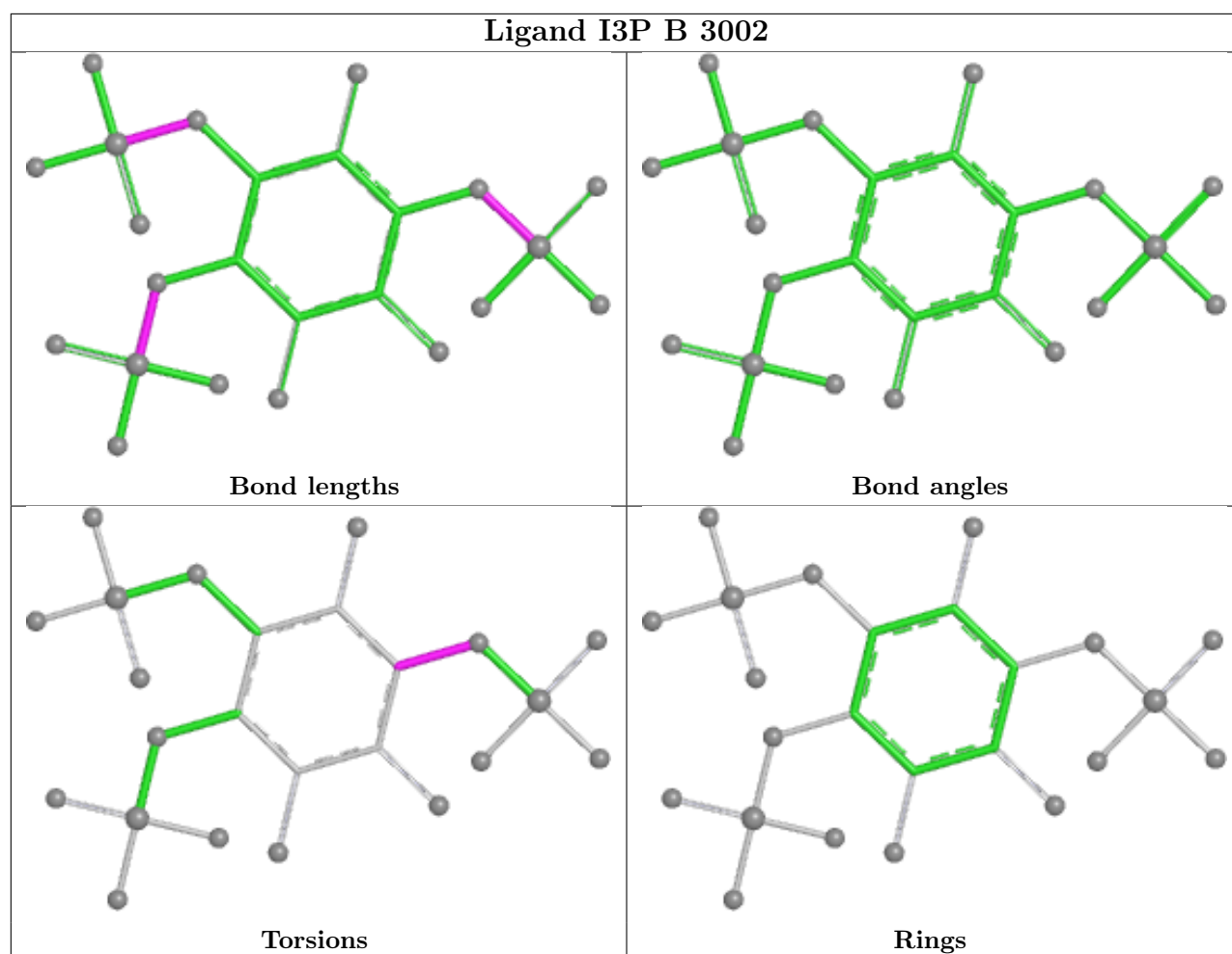
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

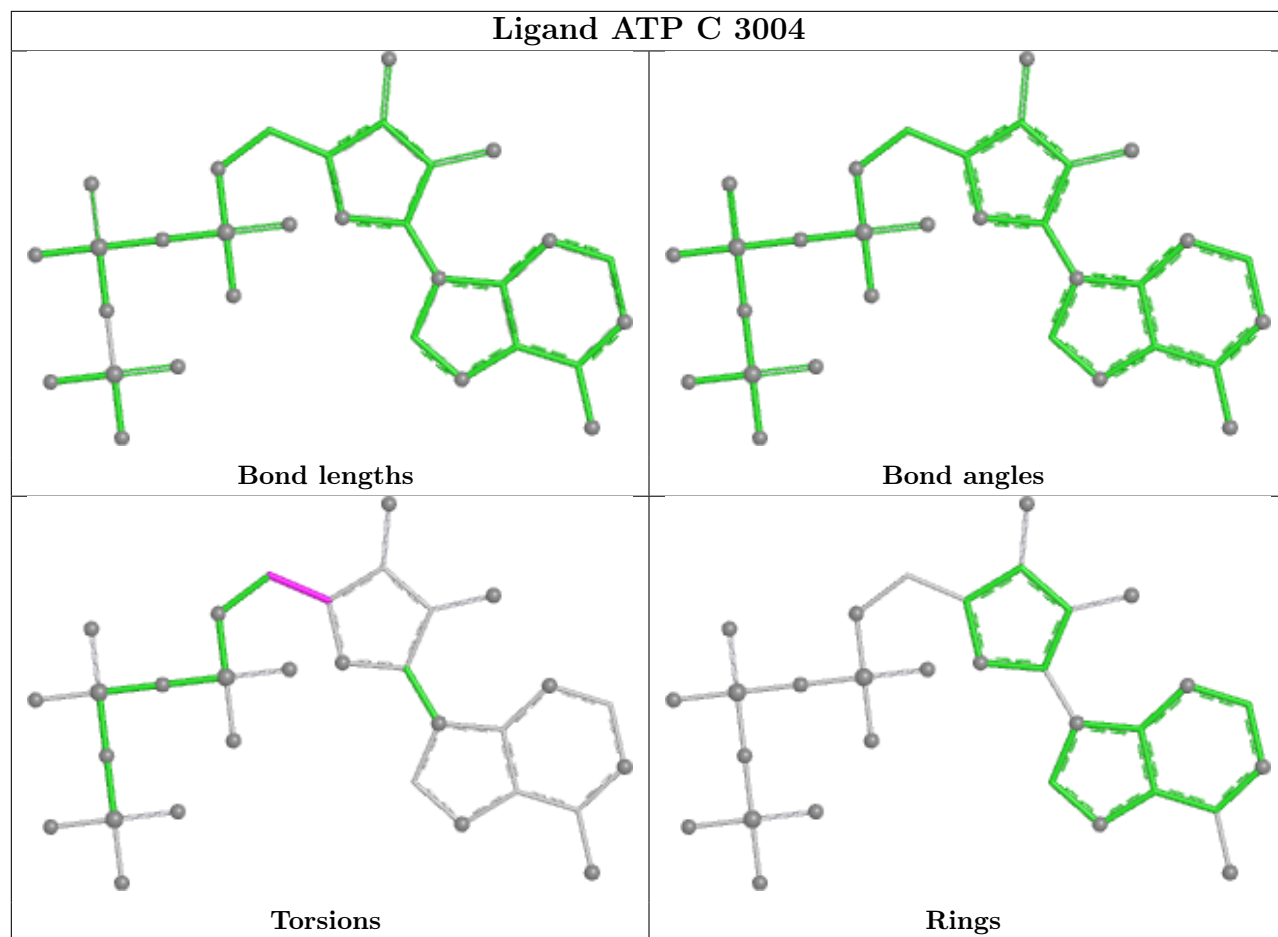
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

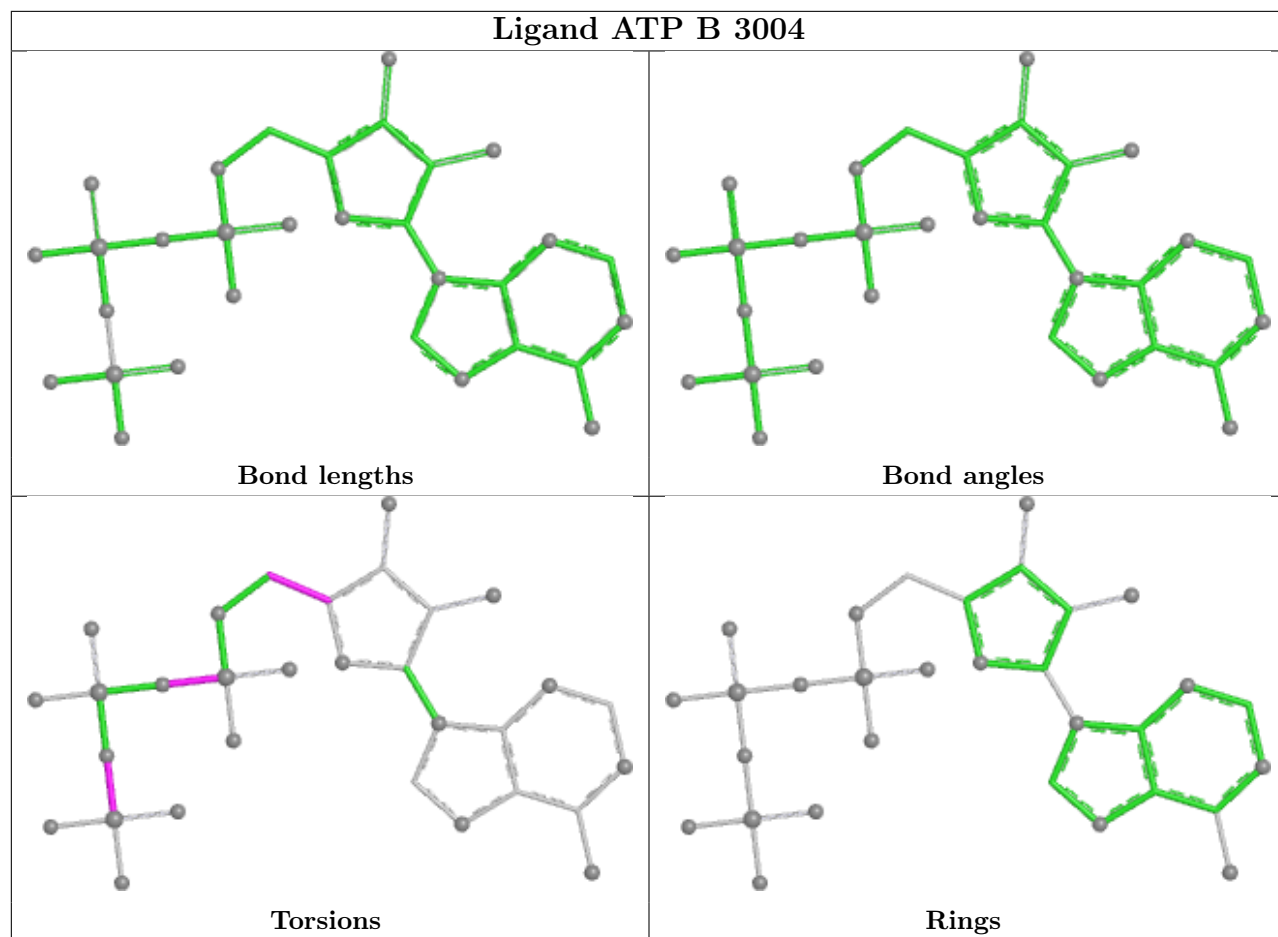


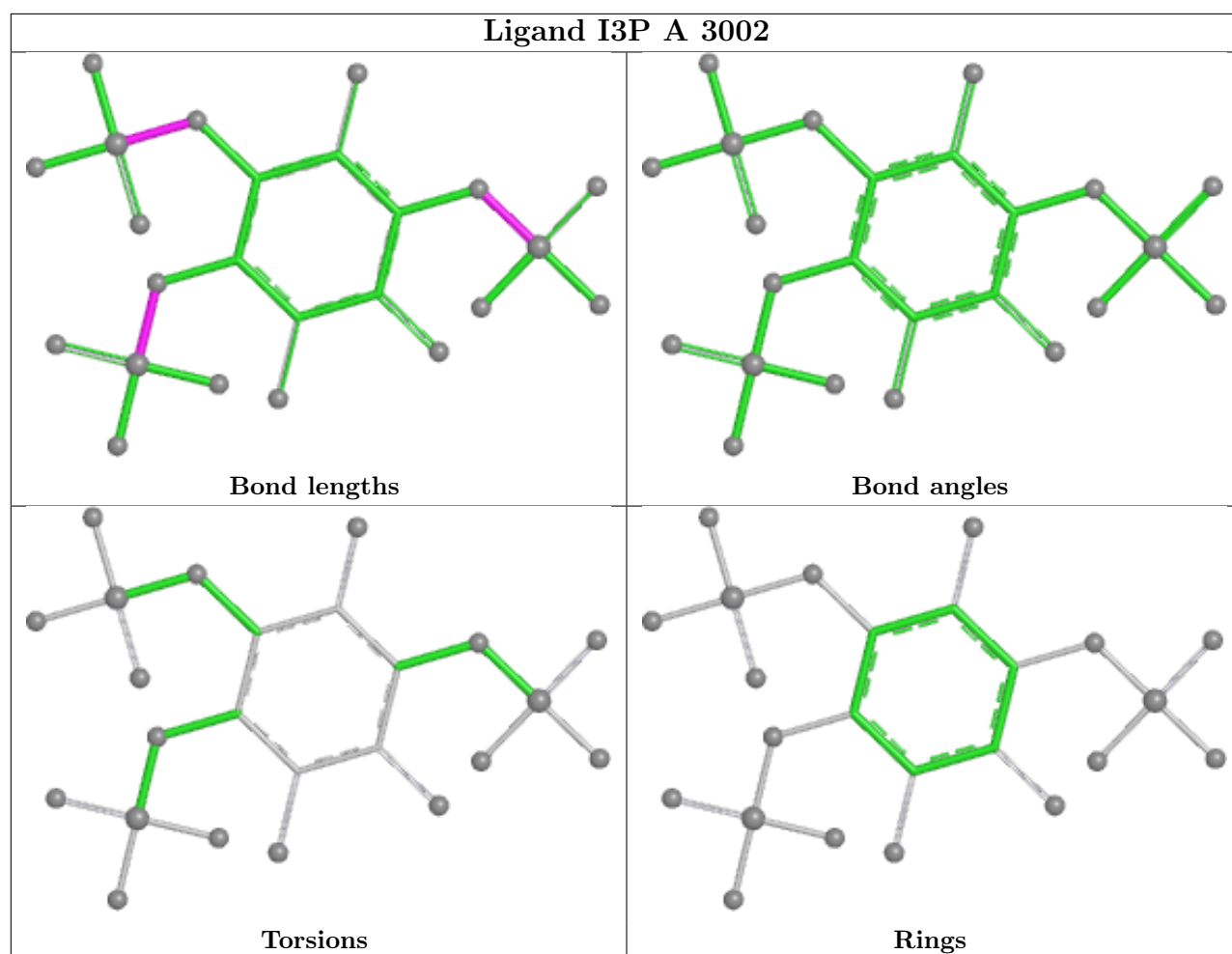


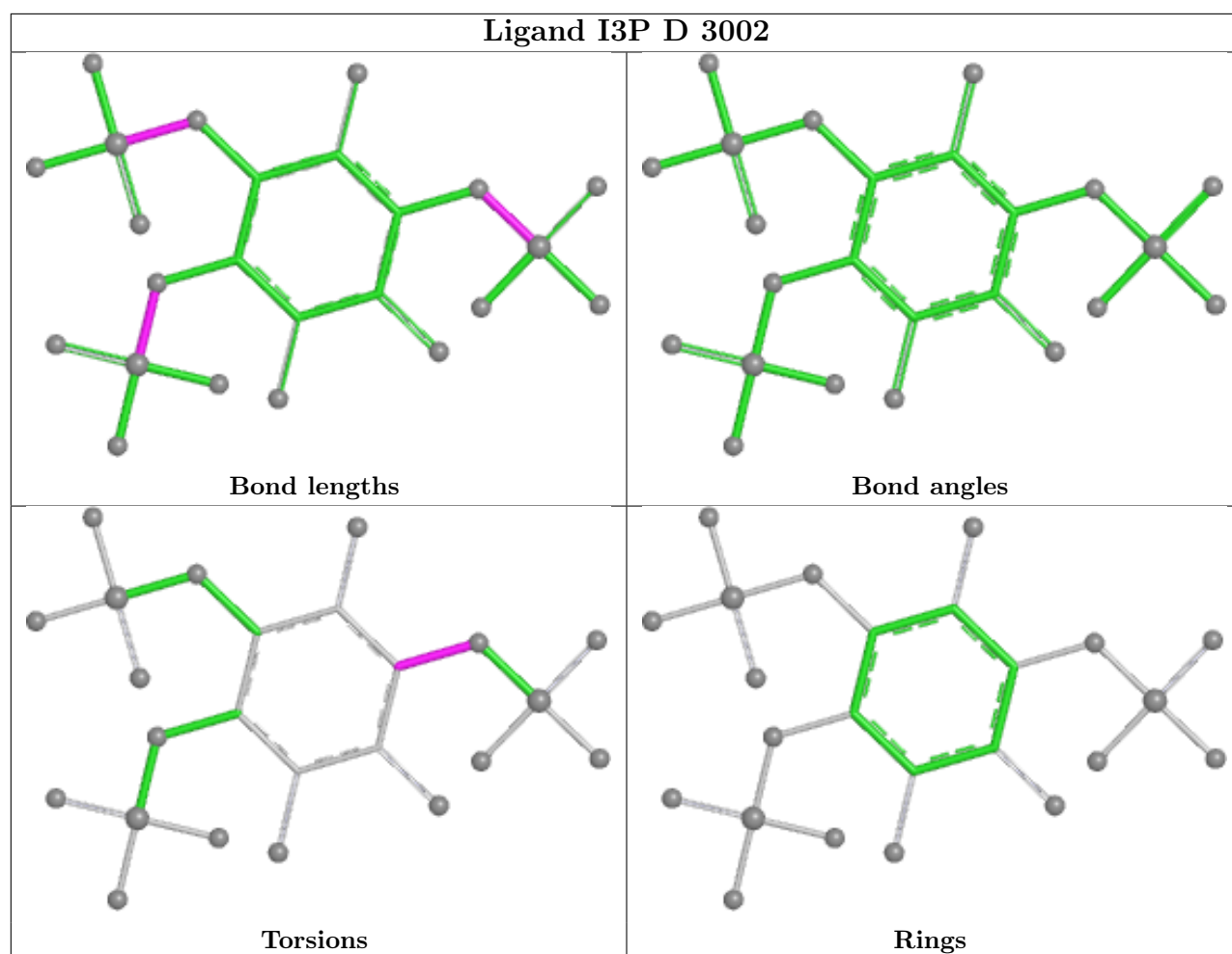












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

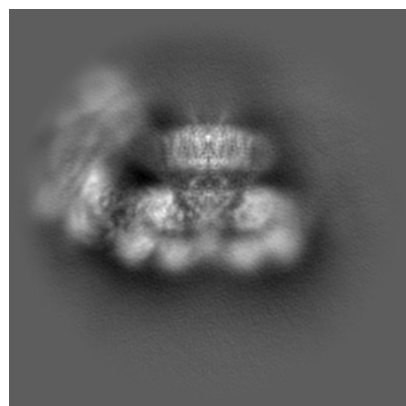
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41365. These allow visual inspection of the internal detail of the map and identification of artifacts.

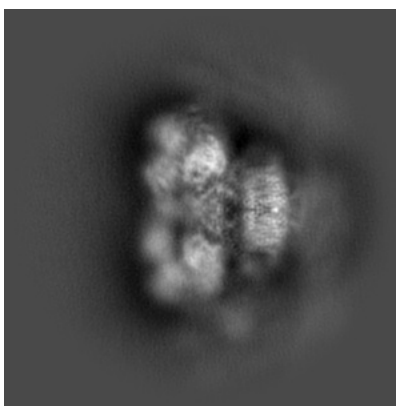
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

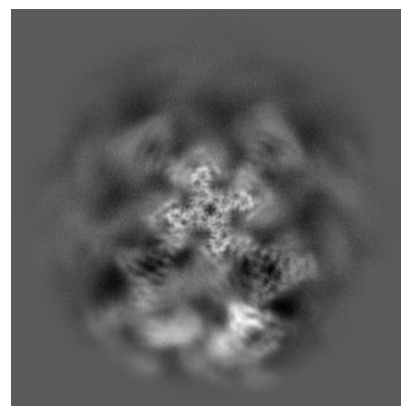
6.1.1 Primary map



X

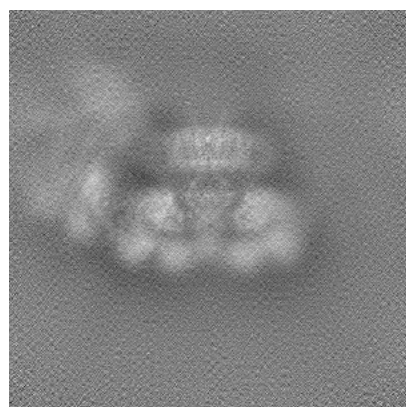


Y

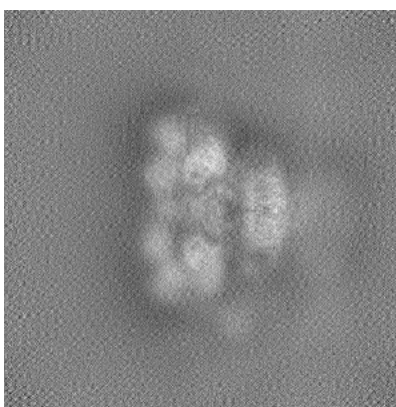


Z

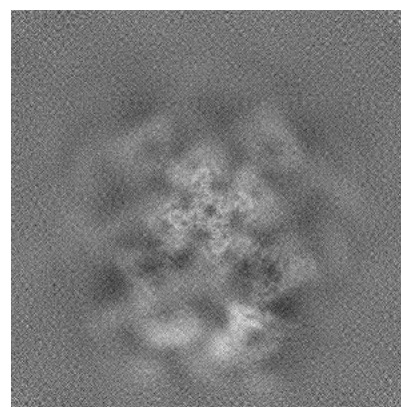
6.1.2 Raw map



X



Y

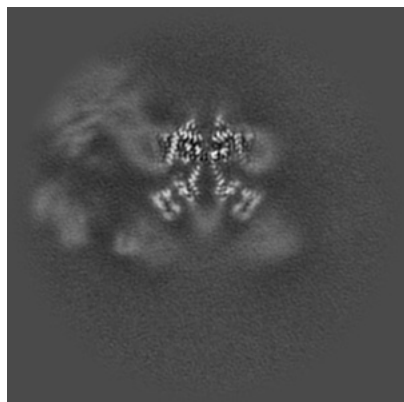


Z

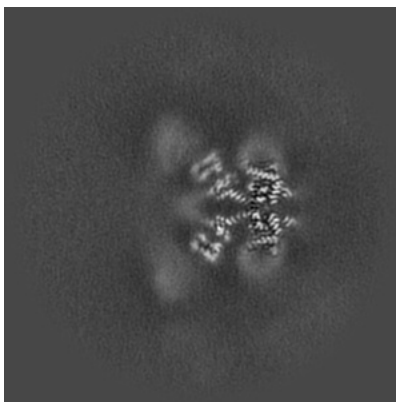
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

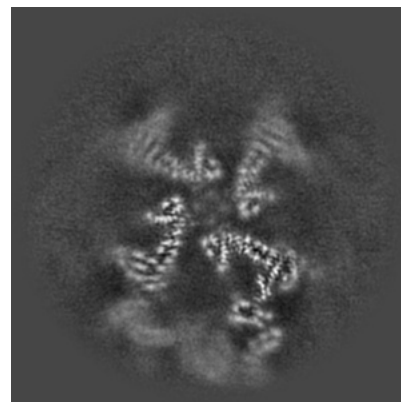
6.2.1 Primary map



X Index: 256

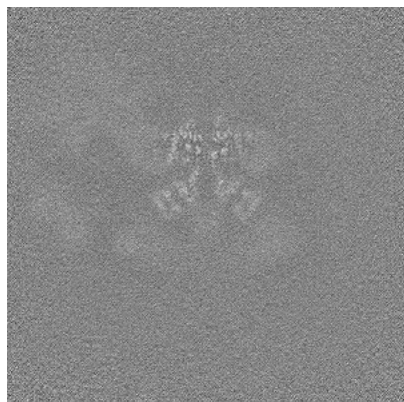


Y Index: 256



Z Index: 256

6.2.2 Raw map



X Index: 256



Y Index: 256

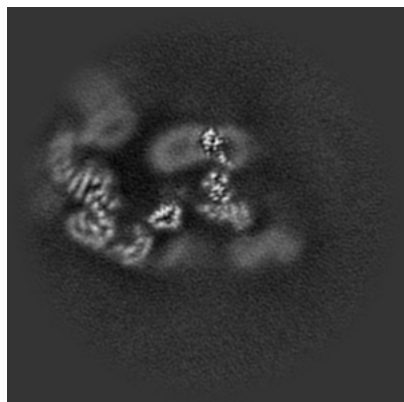


Z Index: 256

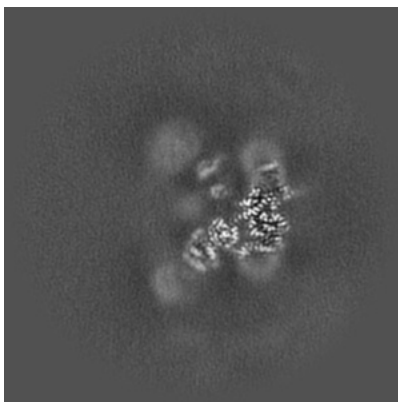
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

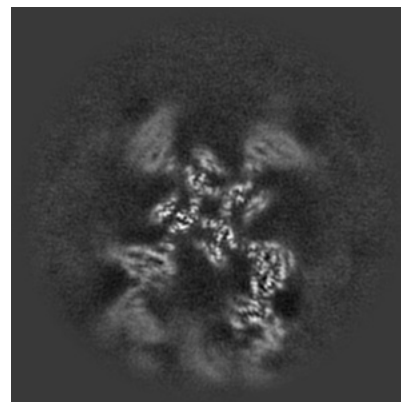
6.3.1 Primary map



X Index: 293

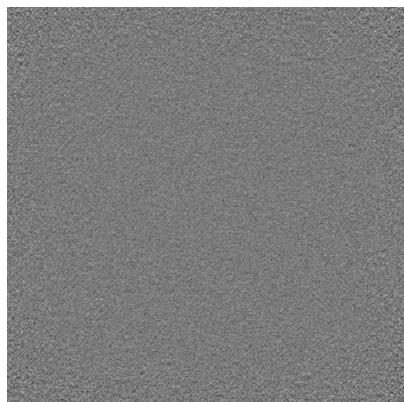


Y Index: 247

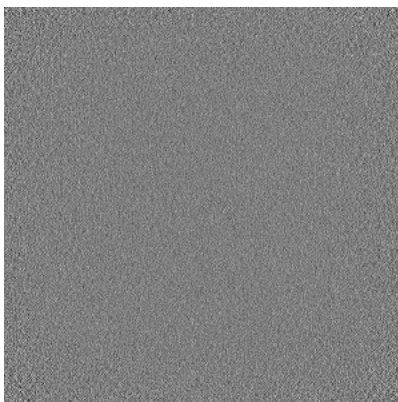


Z Index: 266

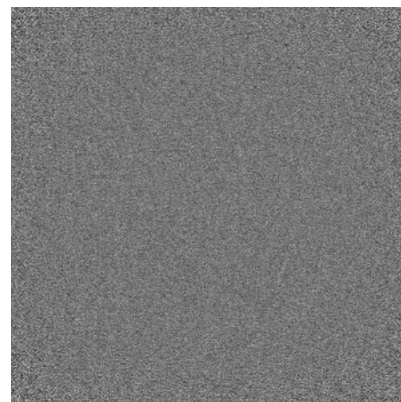
6.3.2 Raw map



X Index: 0



Y Index: 0

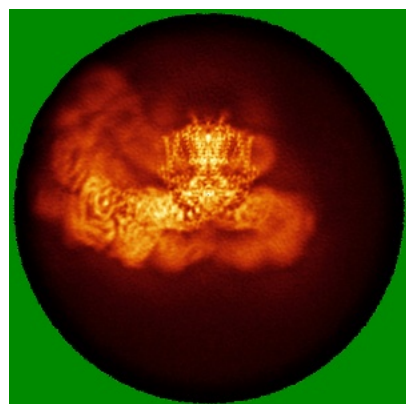


Z Index: 0

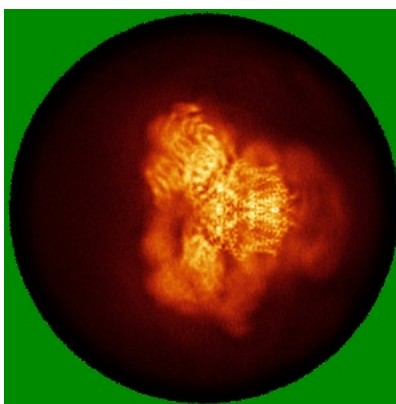
The images above show the largest variance slices of the map in three orthogonal directions.

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

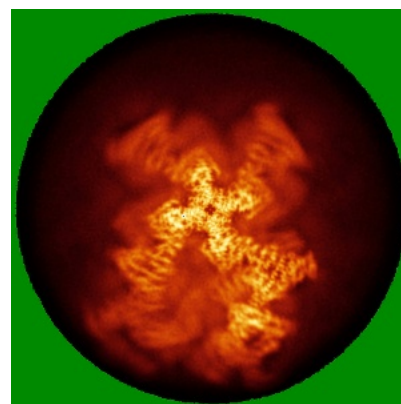
6.4.1 Primary map



X

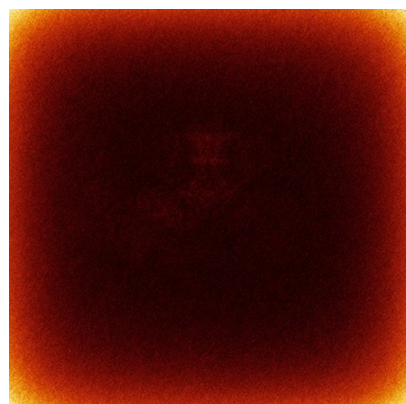


Y

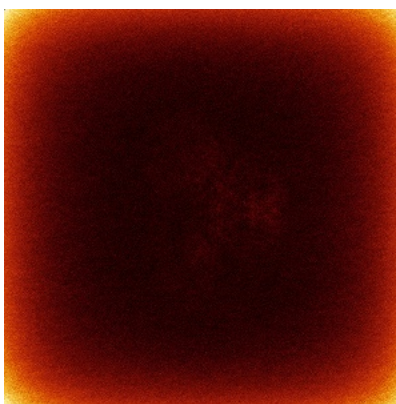


Z

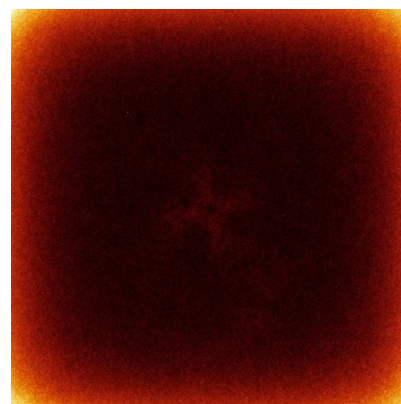
6.4.2 Raw map



X



Y

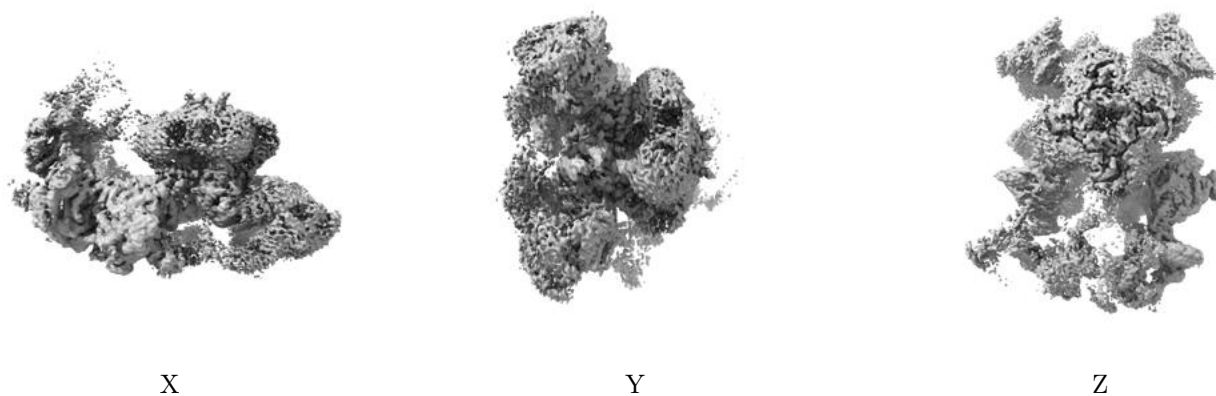


Z

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.

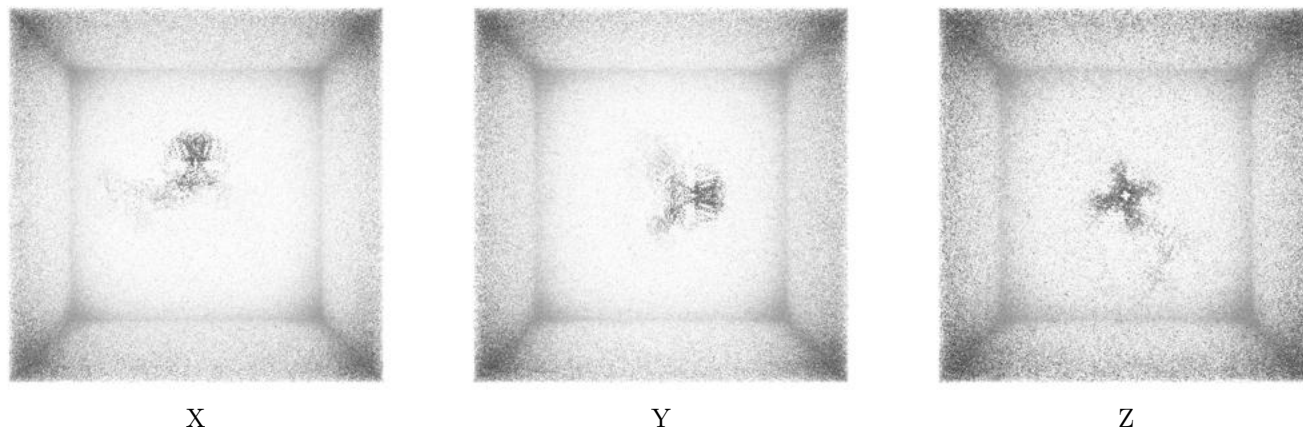
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. 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.

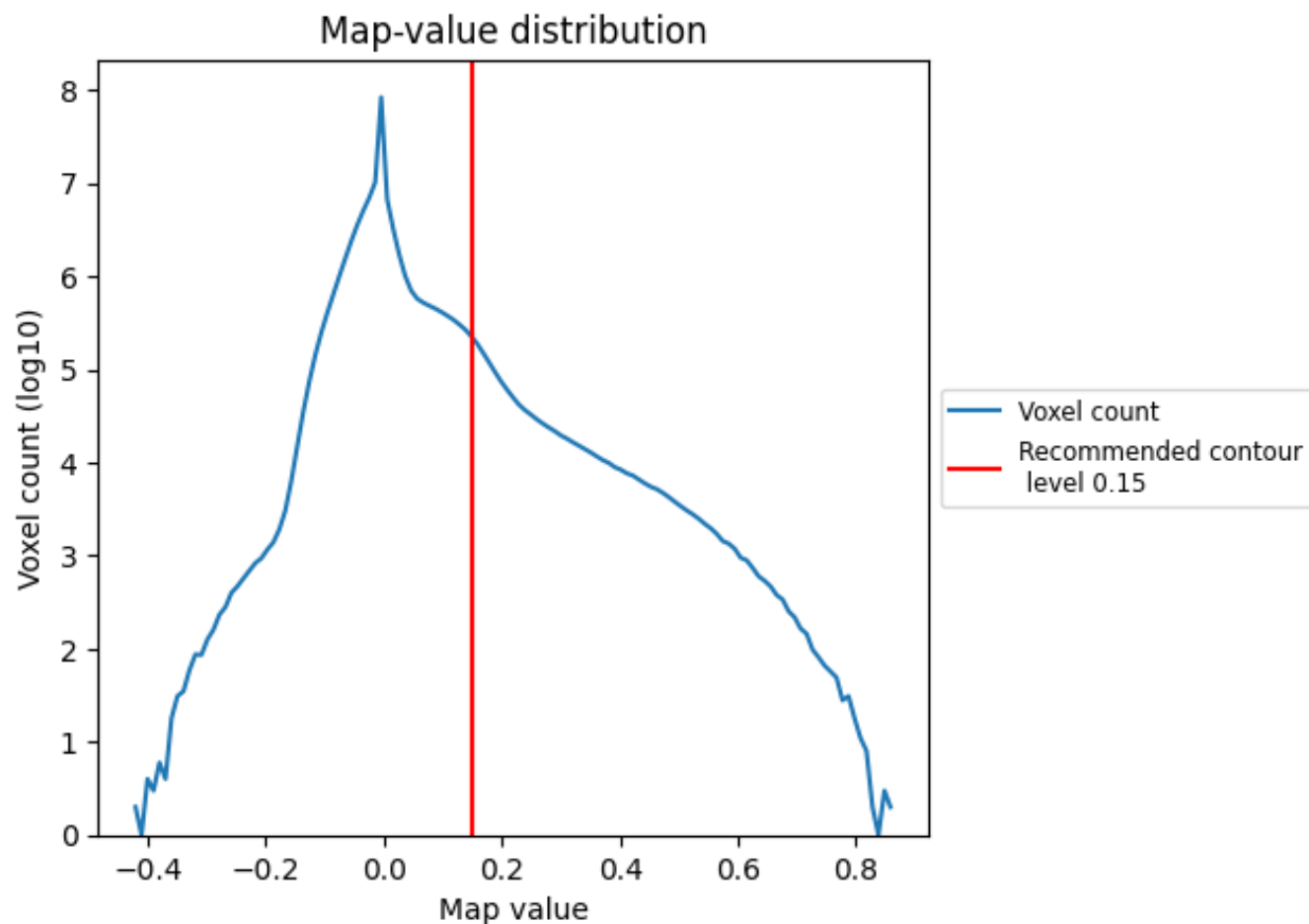
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

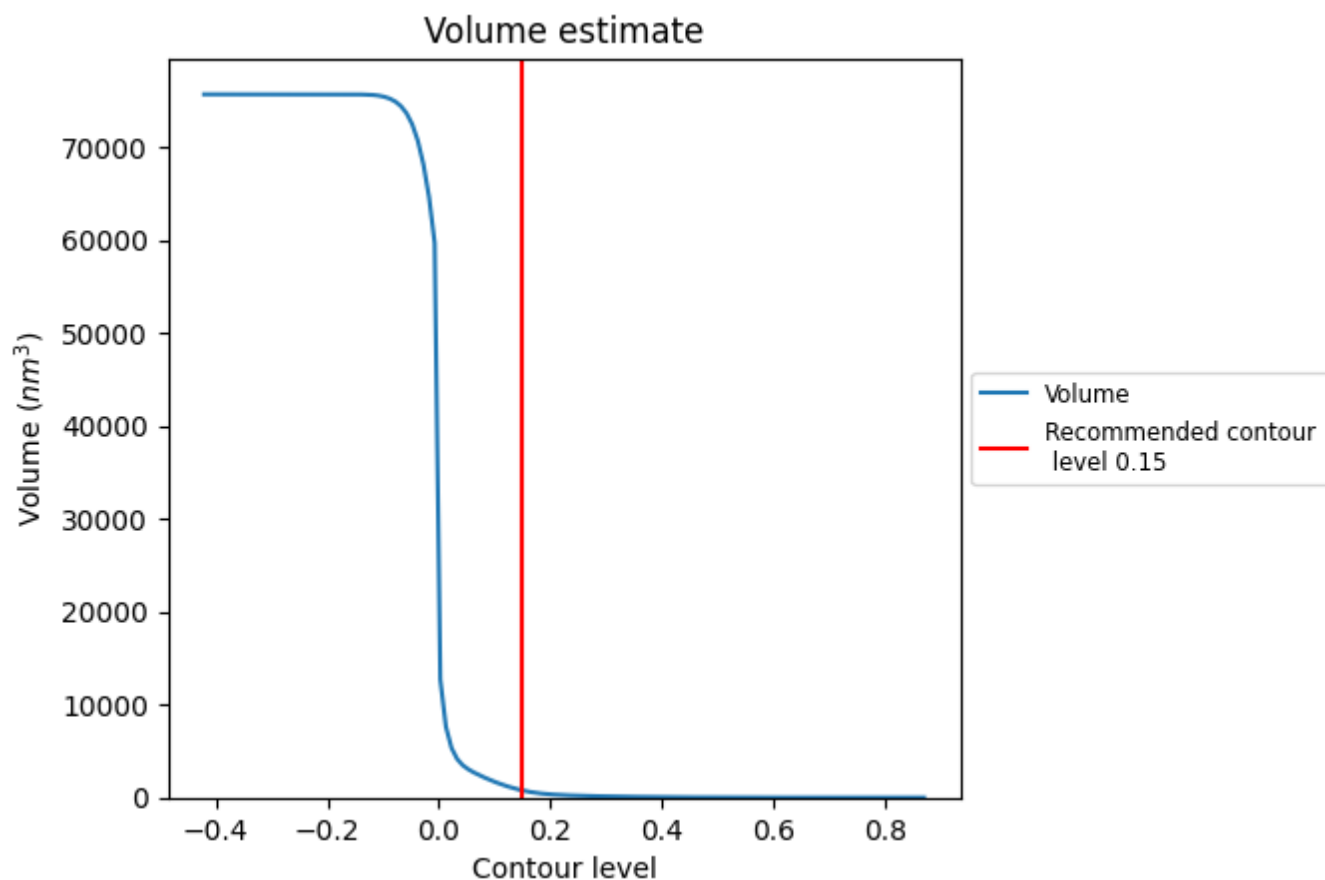
This section contains the results of statistical analysis of the map.

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.

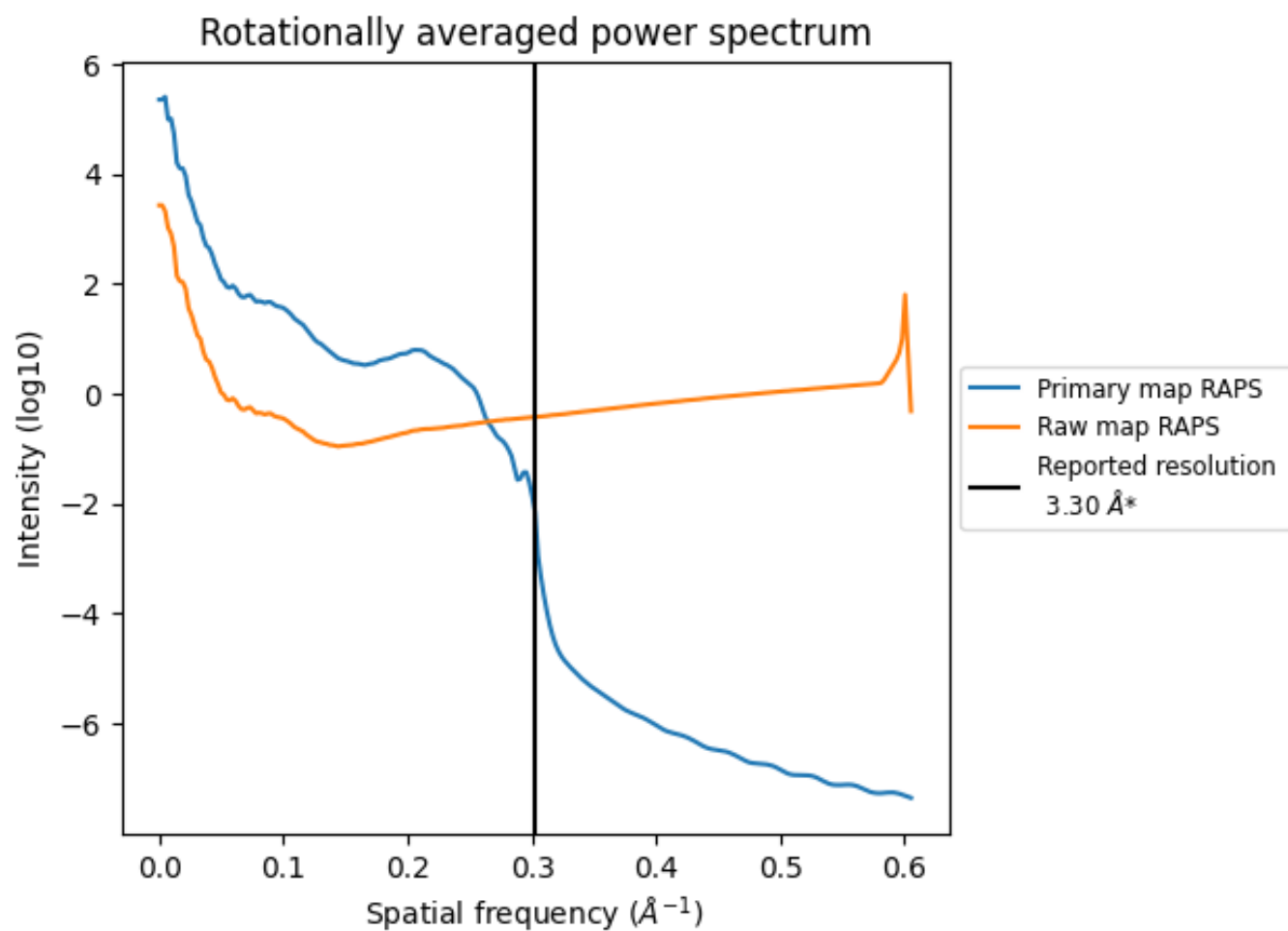
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 764 nm³; this corresponds to an approximate mass of 690 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 ⓘ

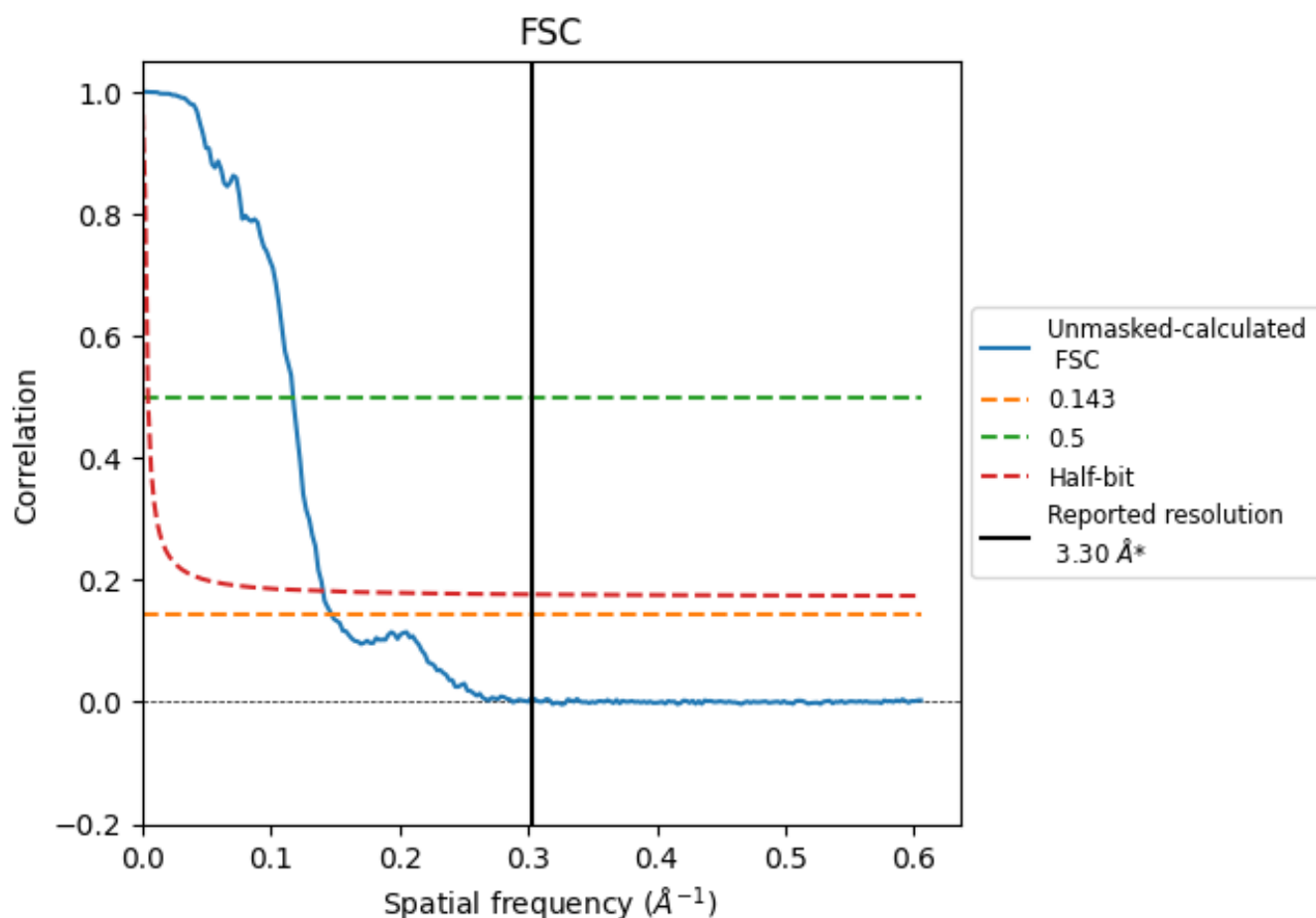


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 $0.303 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

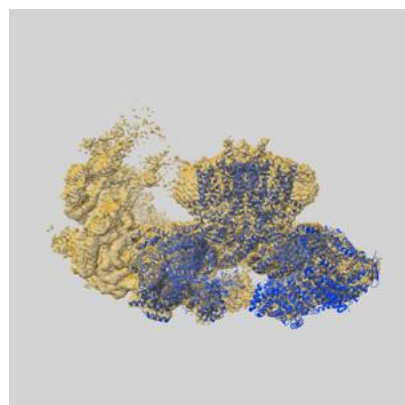
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.78	8.52	7.11

*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 6.78 differs from the reported value 3.3 by more than 10 %

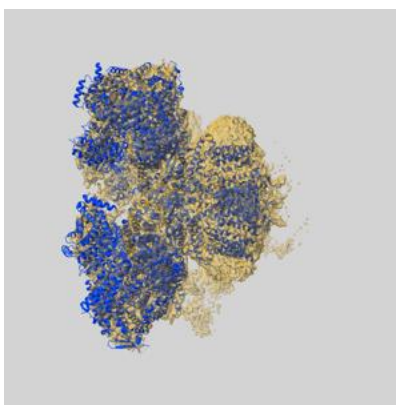
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-41365 and PDB model 8TL9. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

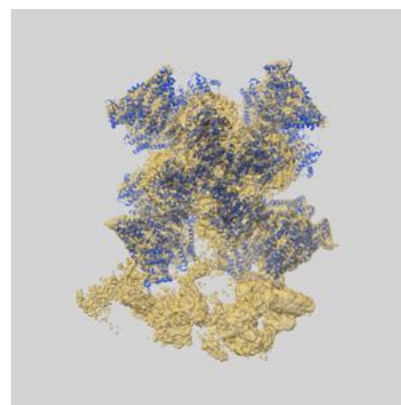
9.1 Map-model overlay [i](#)



X



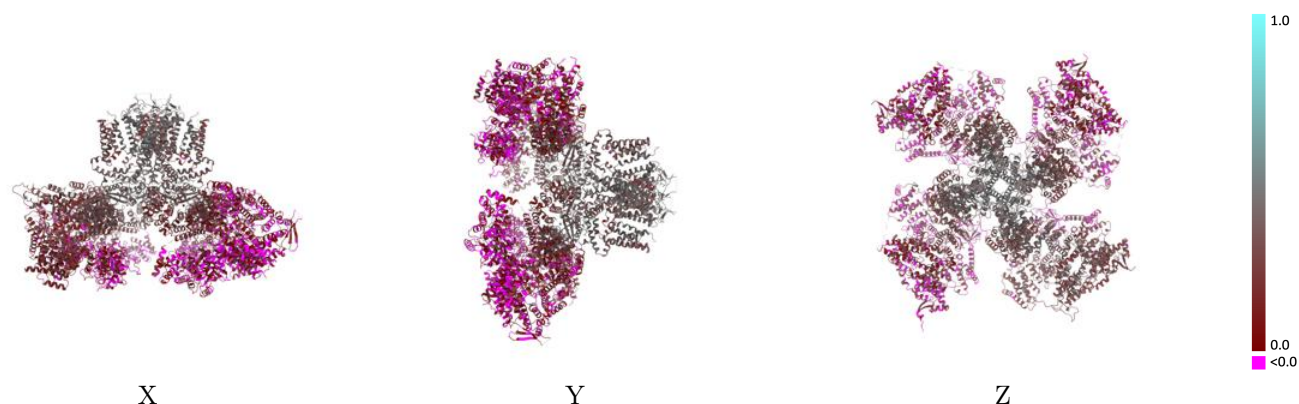
Y



Z

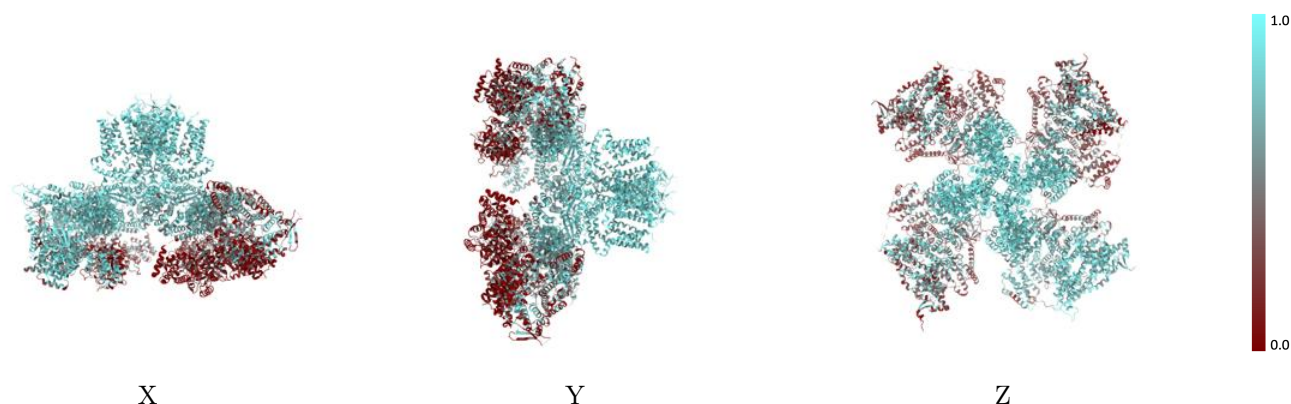
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



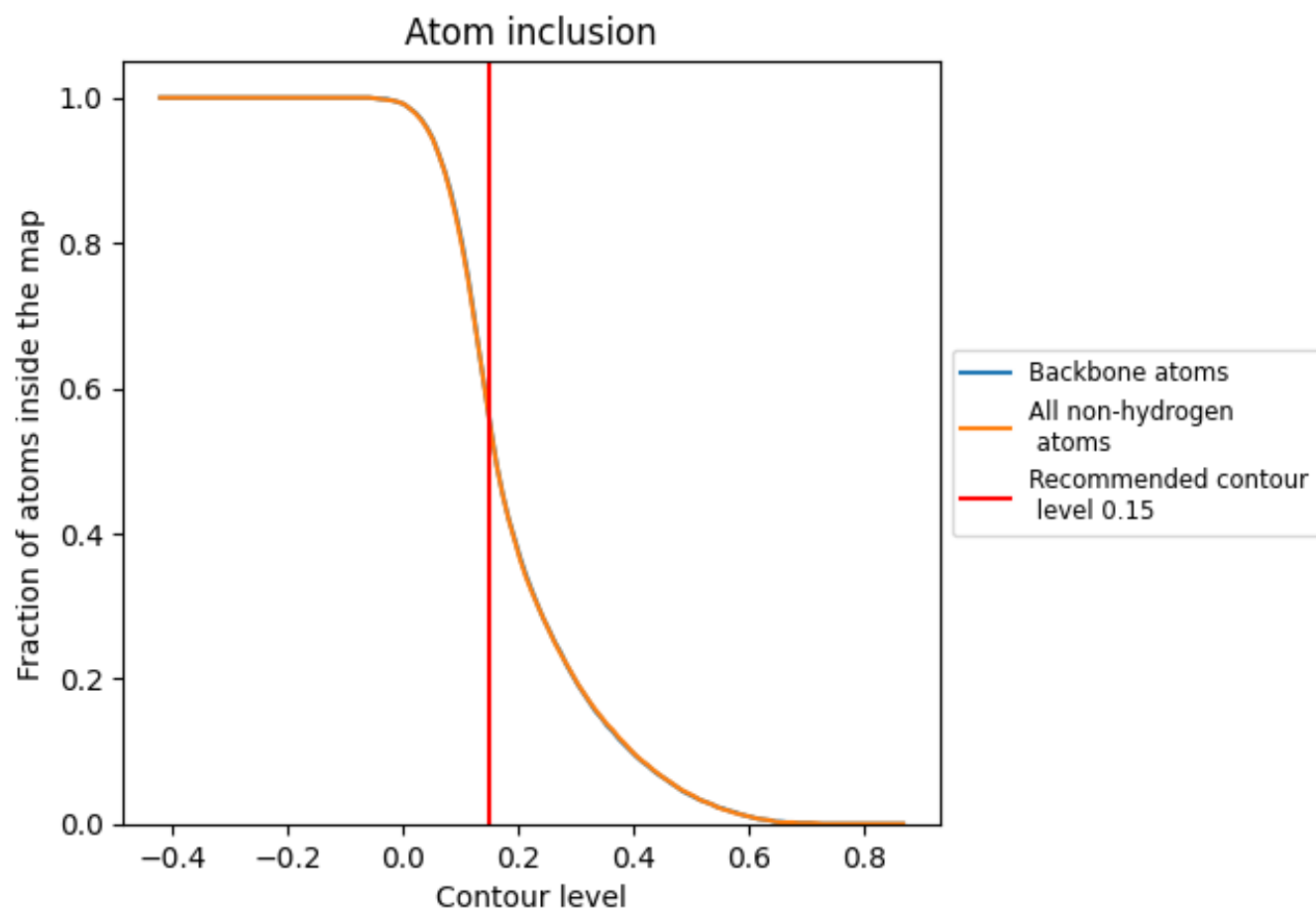
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 56% of all backbone atoms, 56% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5580	0.1960
A	0.4890	0.1590
B	0.4520	0.1630
C	0.5790	0.1900
D	0.7300	0.2700

