



Full wwPDB EM Validation Report ⓘ

Nov 17, 2022 – 04:21 AM EST

PDB ID : 8EAQ
EMDB ID : EMD-27982
Title : Structure of the full-length IP3R1 channel determined at high Ca²⁺
Authors : Fan, G.; Baker, M.R.; Terry, L.E.; Arige, V.; Chen, M.; Seryshev, A.B.; Baker, M.L.; Ludtke, S.J.; Yule, D.I.; Serysheva, I.I.
Deposited on : 2022-08-29
Resolution : 3.26 Å(reported)
Based on initial model : 7LHE

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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

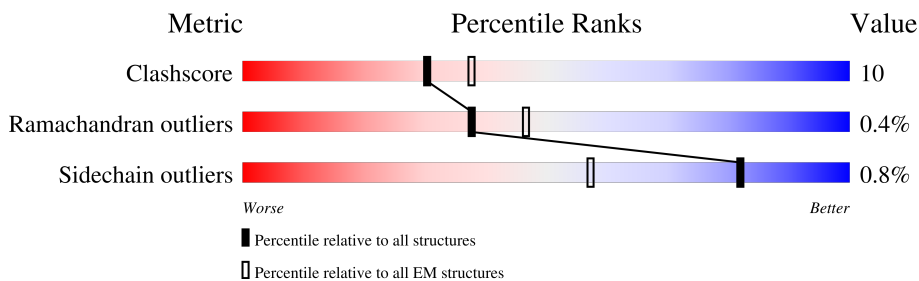
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.26 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	2750	
1	B	2750	
1	C	2750	
1	D	2750	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 77928 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 Inositol 1,4,5-trisphosphate receptor type 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2374	19195	12189	3321	3567	118	1	0
1	B	2374	19195	12189	3321	3567	118	1	0
1	C	2374	19195	12189	3321	3567	118	1	0
1	D	2374	19195	12189	3321	3567	118	1	0

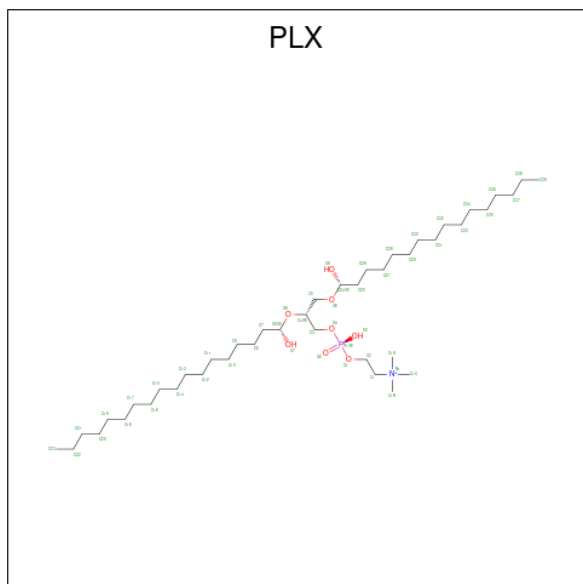
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
3	A	6	6	6	0
3	B	5	5	5	0
3	C	5	5	5	0
3	D	4	4	4	0

- Molecule 4 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (three-letter code: PLX) (formula: C₄₂H₈₉NO₈P).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
4	A	1	Total	C	N	O	P	0
			281	211	7	56	7	
4	A	1	Total	C	N	O	P	0
			281	211	7	56	7	
4	A	1	Total	C	N	O	P	0
			281	211	7	56	7	
4	A	1	Total	C	N	O	P	0
			281	211	7	56	7	
4	A	1	Total	C	N	O	P	0
			281	211	7	56	7	
4	A	1	Total	C	N	O	P	0
			281	211	7	56	7	
4	A	1	Total	C	N	O	P	0
			281	211	7	56	7	
4	B	1	Total	C	N	O	P	0
			281	211	7	56	7	
4	B	1	Total	C	N	O	P	0
			281	211	7	56	7	
4	B	1	Total	C	N	O	P	0
			281	211	7	56	7	
4	B	1	Total	C	N	O	P	0
			281	211	7	56	7	
4	B	1	Total	C	N	O	P	0
			281	211	7	56	7	

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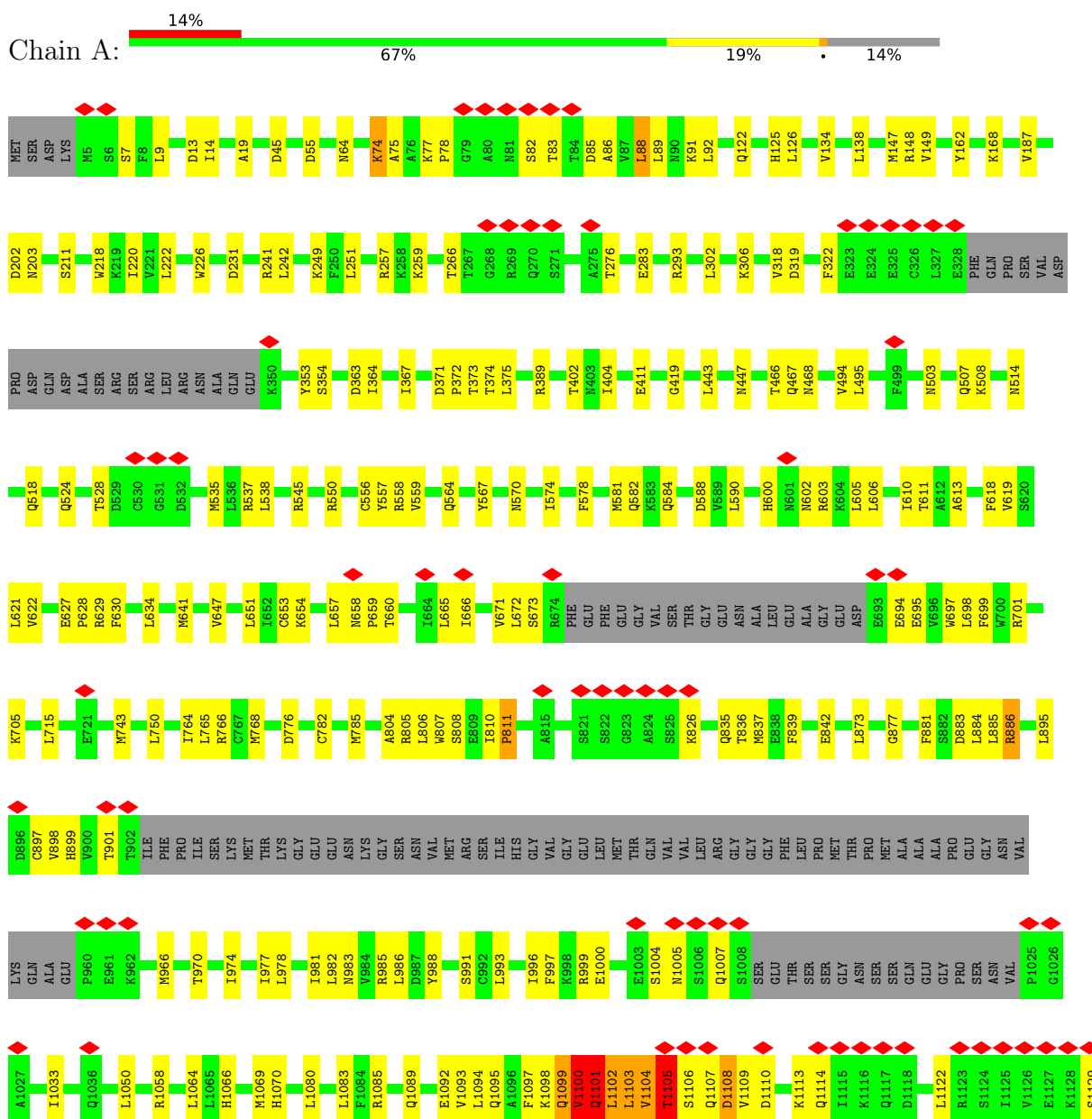
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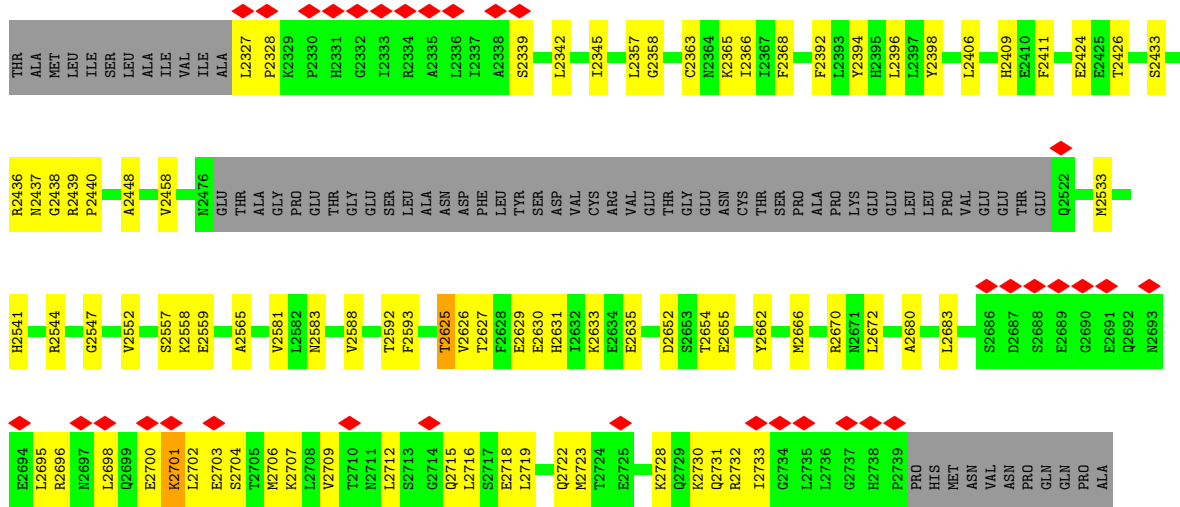
Mol	Chain	Residues	Atoms					AltConf
4	B	1	Total	C	N	O	P	0
			281	211	7	56	7	
4	B	1	Total	C	N	O	P	0
			281	211	7	56	7	
4	C	1	Total	C	N	O	P	0
			281	211	7	56	7	
4	C	1	Total	C	N	O	P	0
			281	211	7	56	7	
4	C	1	Total	C	N	O	P	0
			281	211	7	56	7	
4	C	1	Total	C	N	O	P	0
			281	211	7	56	7	
4	C	1	Total	C	N	O	P	0
			281	211	7	56	7	
4	C	1	Total	C	N	O	P	0
			281	211	7	56	7	
4	D	1	Total	C	N	O	P	0
			281	211	7	56	7	
4	D	1	Total	C	N	O	P	0
			281	211	7	56	7	
4	D	1	Total	C	N	O	P	0
			281	211	7	56	7	
4	D	1	Total	C	N	O	P	0
			281	211	7	56	7	
4	D	1	Total	C	N	O	P	0
			281	211	7	56	7	

3 Residue-property plots

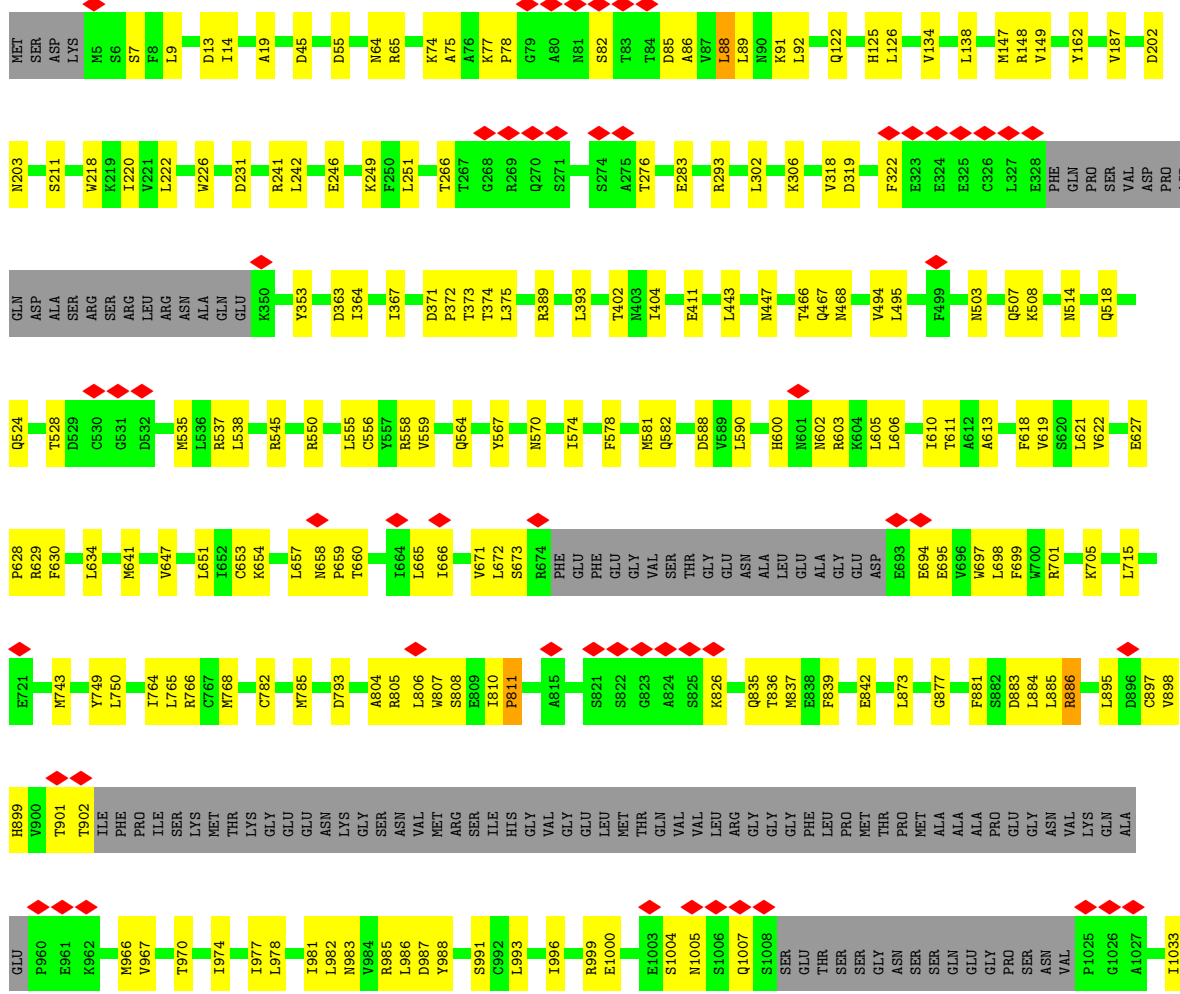
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

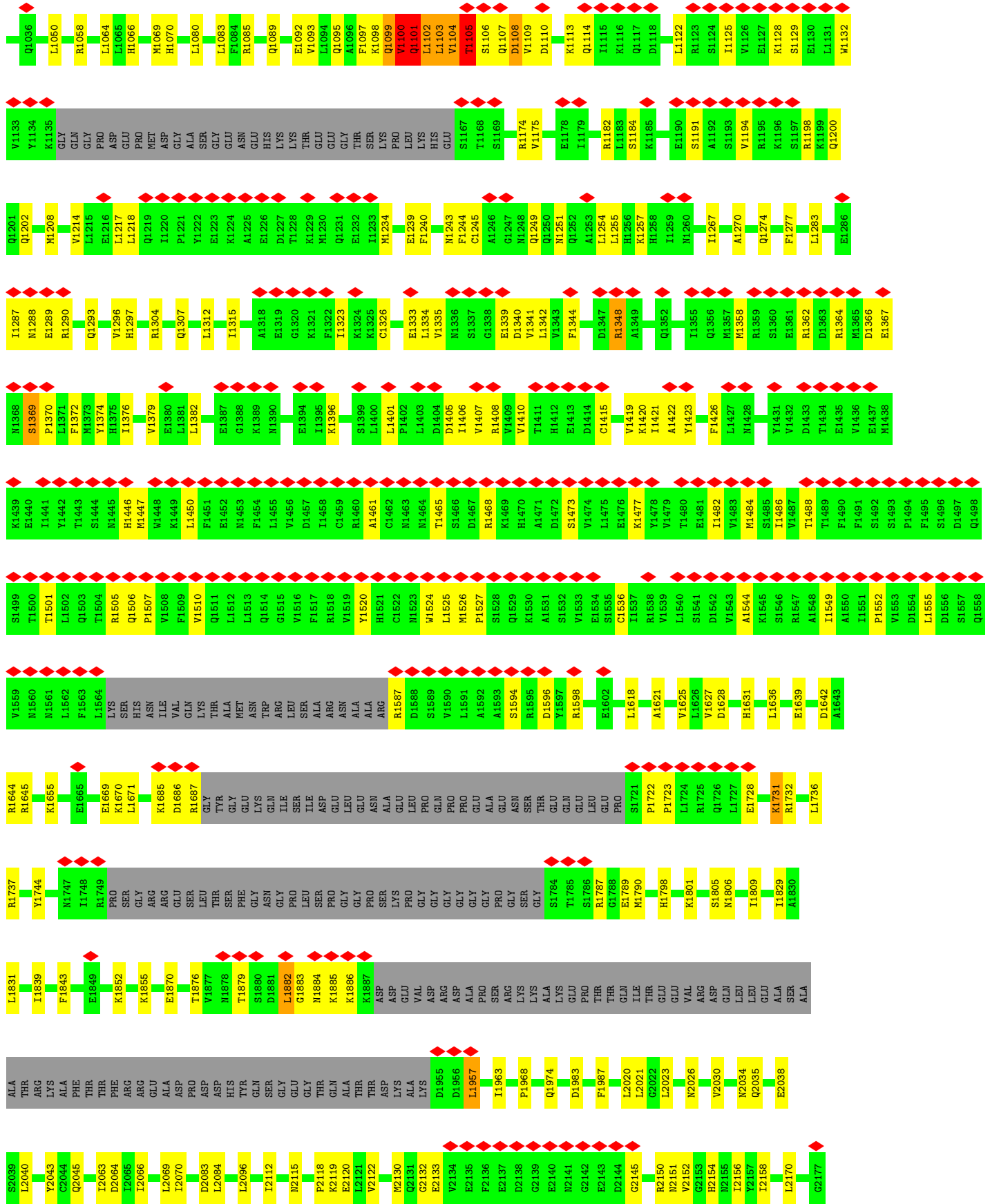
- Molecule 1: Inositol 1,4,5-trisphosphate receptor type 1

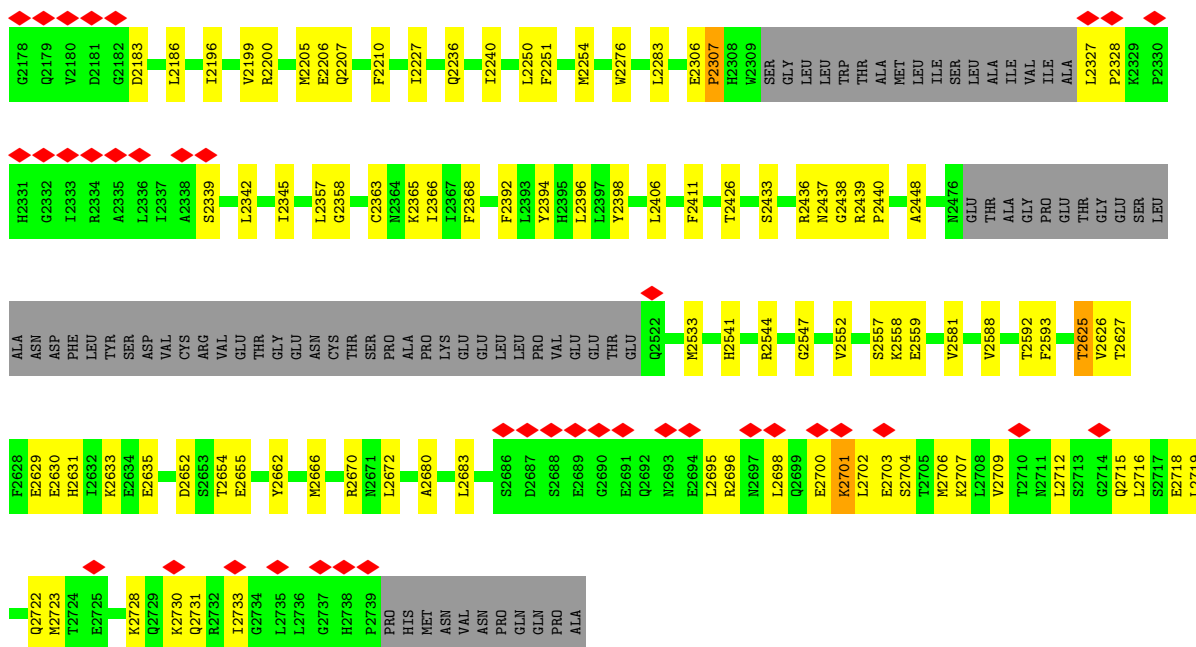




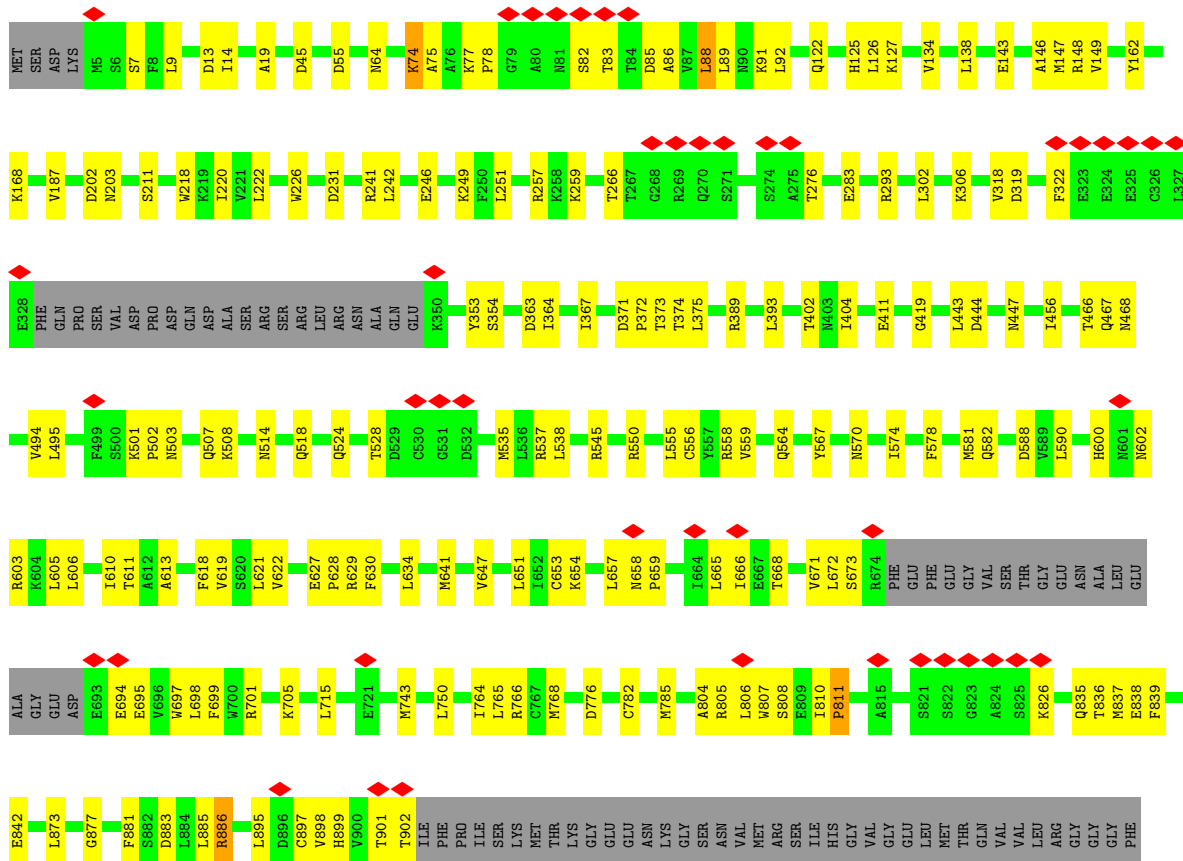
• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 1

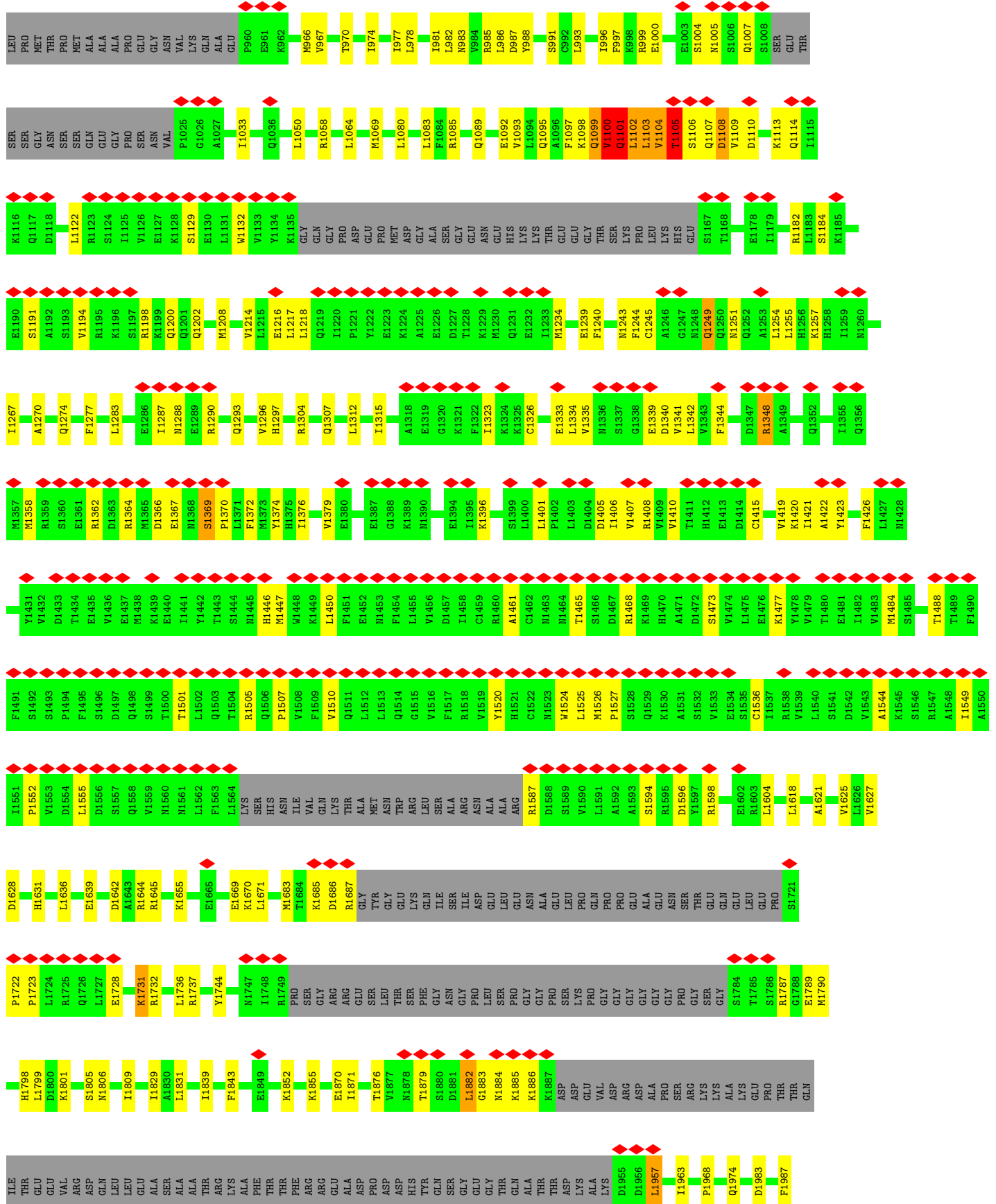


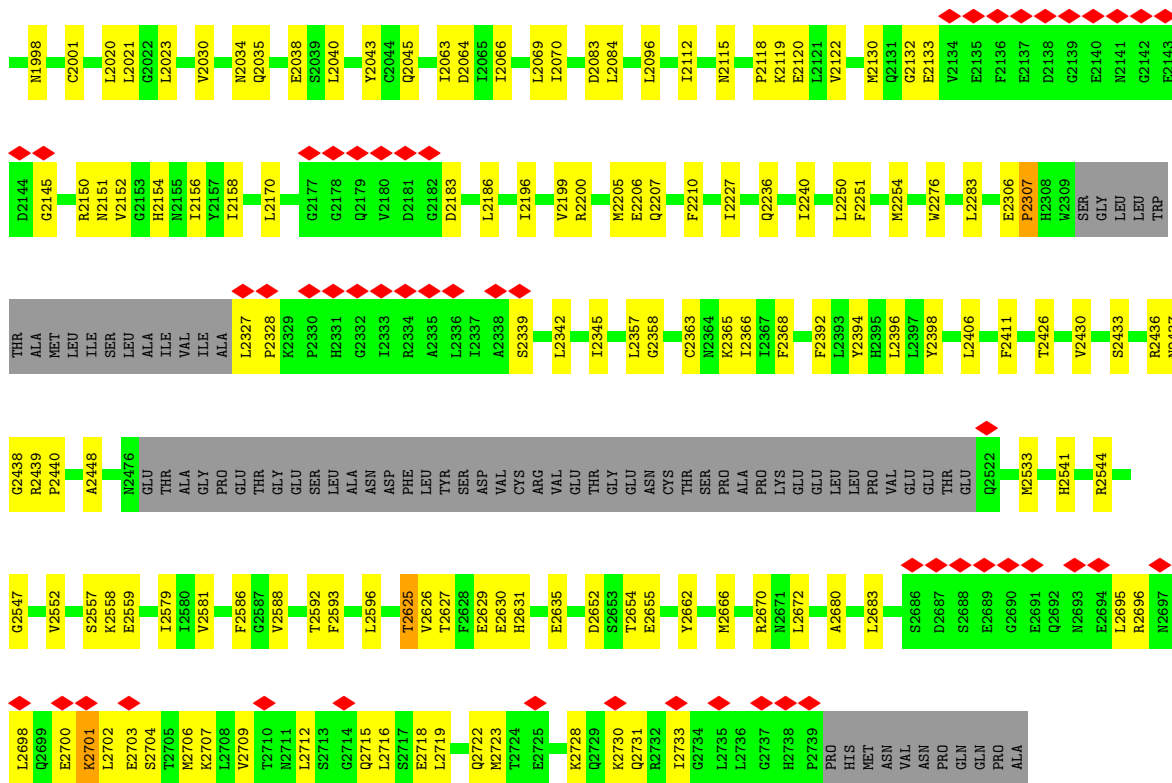




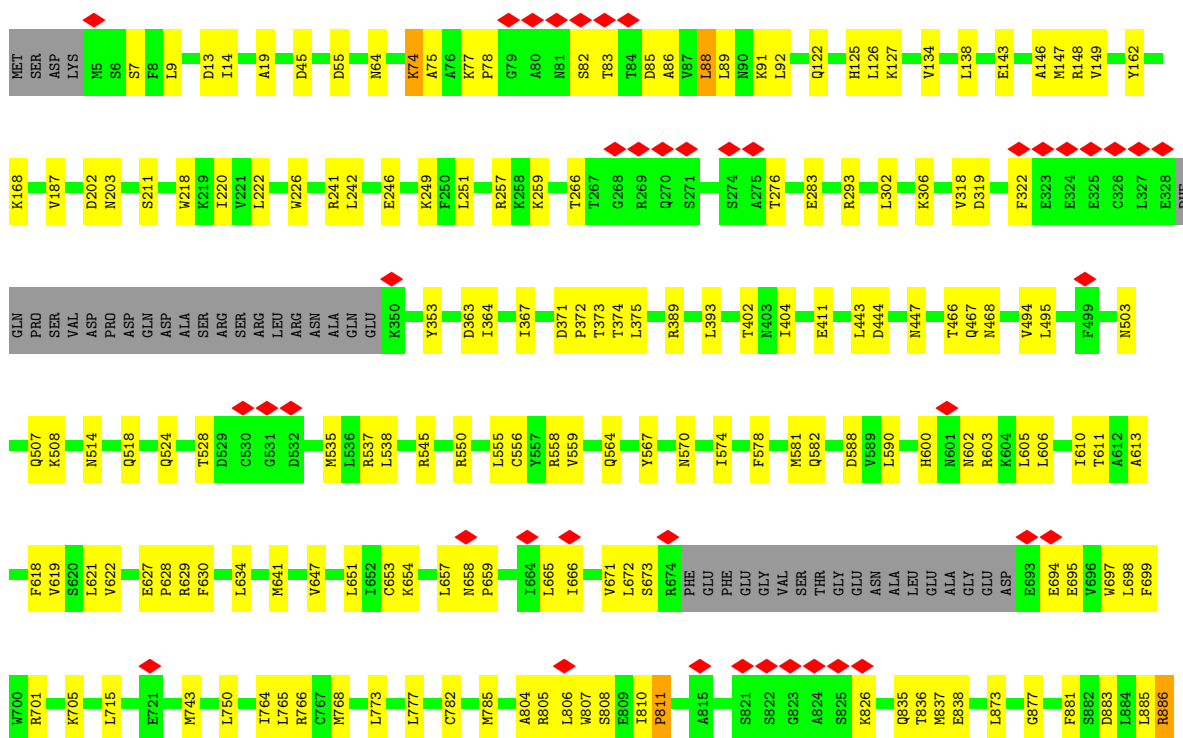
● Molecule 1: Inositol 1,4,5-trisphosphate receptor type 1







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



L895	D896	C897	V898	H899	T901	T902	ILE	PHE	PRO	ILE	SER	MET	THR	LYS	GLY	GLU	GLU	ASN	ASN	GLY	SER	ASN	VAL	MET	ARG	SER	SER	ILE	HIS	GLY	VAL	GLY	GLU	LEU	MET	THR	GLN	VAL	VAL	LEU	ARG	GLY	GLY	PHE	LEU	PRO	MET	THR	PRO	ALA	ALA	ALA	PRO	GLU	GLY			
L896	D897	V898	H899	T901	T902	ASN	VAL	LYS	GLN	ALA	GLU	P960	E961	F962	N966	T970	Y974	Y977	L978	Y981	L982	N983	V984	F984	R985	L986	Y987	Y988	R991	C992	L993	Y996	F997	K998	R999	E1000	E1003	S1004	M1005	S1006	Q1007	S1008	SER	GLU	THR	SER	SER	GLY	ASN	VAL	L1122	R1123	S1124	I1125	V1126	E1127		
P1025	G1026	A1027	I1033	Q1036	L1050	R1058	L1064	H1065	H1066	M1069	H1070	L1080	L1083	F1084	R1085	Q1089	E1092	Y1093	L1094	Q1095	F1097	K1098	Y1099	Q1101	L1102	L1103	V1104	T1105	S1106	Q1107	D1108	V1109	D1110	K1113	Q1114	I1115	K1116	Q1117	D1118	L1122	R1123	S1124	I1125	V1126	E1127													
K1128	S1129	E1130	L1131	W1132	V1133	Y1134	K1135	GLY	GLN	GLY	PRO	ASP	ALA	GLY	SER	GLY	ALA	SER	GLY	GLU	ASN	HIS	LYS	LYS	E1092	Y1093	L1094	Q1095	F1097	K1098	Y1099	Q1101	L1102	L1103	V1104	T1105	S1106	Q1107	D1108	V1109	D1110	K1113	Q1114	I1115	K1116	Q1117	D1118	L1122	R1123	S1124	I1125	V1126	E1127					
S1197	R1198	L1199	Q1200	Q1201	Q1202	M1208	V1214	L1215	E1216	L1217	L1218	Q1219	I1220	P1221	Y1222	E1223	K1224	A1225	E1226	D1227	T1228	K1229	M1230	E1232	I1233	M1234	E1239	F1240	N1243	F1244	C1245	A1246	G1247	H1248	Q1249	M1251	Q1252	A1253	L1254	L1255	H1256	K1257	H1258	I1259	H1260	I1267	A1270	Q1274	F1277									
L1283	E1286	I1287	M1288	E1289	R1290	Q1293	V1296	H1297	R1304	Q1307	L1312	I1315	A1318	E1319	G1320	K1321	F1322	I1323	K1324	K1325	C1326	E1333	L1334	V1335	M1336	S1337	G1338	E1339	D1340	V1341	L1342	V1343	F1344	D1347	R1348	A1349	Q1352	I1355	Q1356	M1357	M1358	R1359	S1360	E1361	R1362	D1363												
R1364	M1365	D1366	W1368	S1369	P1370	L1371	Y1374	H1375	I1376	V1379	E1380	E1387	G1388	K1389	M1390	E1394	I1395	K1396	S1399	L1400	F1402	L1403	D1404	I1406	V1407	R1408	V1409	V1410	T1411	H1412	E1413	D1414	C1415	V1419	K1420	I1421	A1422	Y1423	F1426	L1427	H1428	V1431	V1432	D1433	T1434	E1435	V1436											
E1437	M1438	K1439	I1440	I1441	Y1442	T1443	S1444	H1446	M1447	K1449	L1450	F1451	N1452	N1453	F1454	L1455	V1456	D1457	I1458	C1459	R1460	A1461	C1462	N1463	M1464	T1465	S1466	D1467	R1468	K1469	H1470	A1471	D1472	S1473	V1474	L1475	E1476	K1477	Y1478	V1479	T1480	E1481	I1482	M1483	S1485	T1488	T1489	F1490	F1491	S1492	S1493	P1494	F1495	S1496	D1497			
Q1498	S1499	T1500	T1501	L1502	Q1503	T1504	R1505	Q1506	P1507	V1508	F1509	V1510	Q1511	L1512	L1513	Q1514	G1515	V1516	F1517	R1518	V1519	Y1520	H1521	C1522	W1524	L1525	M1526	P1527	S1528	Q1529	R1530	A1531	S1532	V1533	E1534	S1535	C1536	I1537	R1538	V1539	L1540	S1541	D1542	V1543	A1544	K1545	S1546	R1547	A1548	I1549	A1550	I1551	P1552	V1553	D1554	L1555	D1556	S1557
Q1558	V1559	M1560	M1561	L1562	F1563	L1564	LYS	SER	HIS	ILE	VAL	GLN	LYS	THR	ALA	MET	ASN	TRP	ARG	ARG	LEU	SER	ALA	ALA	ALA	ARG	R1587	D1588	S1589	V1590	L1591	A1592	A1593	S1594	R1595	D1596	Y1597	R1598	E1602	R1603	L1604	D1613	R1616	P1617	L1618	A1621	V1625	L1626	V1627	D1628	H1631							
L1636	E1639	D1642	A1643	R1644	R1645	K1655	E1665	E1669	K1670	L1671	M1683	T1684	K1685	D1686	R1687	TYR	GLY	THR	GLU	GLY	GLN	ILE	SER	ILE	ILE	ASP	S1588	S1589	V1590	L1591	A1592	A1593	S1594	R1595	D1596	Y1597	R1598	E1602	R1603	L1604	D1613	R1616	P1617	L1618	A1621	V1625	L1626	V1627	D1628	H1631								
R1725	Q1726	L1727	E1728	K1731	R1732	L1736	R1737	Y1744	M1747	I1748	R1749	PRO	SER	GLY	ARG	ARG	GLU	SER	LEU	THR	THR	PHE	GLY	ASN	GLY	PRO	LEU	GLU	ASN	ALA	ALA	LEU	PRO	LYS	PRO	GLY	GLY	PRO	GLY	GLY	GLY	ALA	ALA	ASN	SER	THR	GLY	S1784	T1785	S1786	R1787	G1788	E1789	M1790	H1798	L1799		
D1800	K1801	S1805	M1806	I1809	I1829	A1830	L1831	I1839	F1843	E1849	K1852	K1855	E1870	I1871	T1876	V1877	N1878	T1879	S1880	D1881	L1882	G1883	M1884	K1885	K1886	K1887	ASP	GLU	VAL	ASP	ARG	ASP	ALA	PRO	PRO	GLY	GLY	ALA	PRO	ARG	ARG	THR	LYS	LYS	ALA	LYS	GLU	THR	ILE	THR	GLU							

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	346731	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	46943	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.116	Depositor
Minimum map value	-0.062	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0118	Depositor
Map size (\AA)	359.52002, 359.52002, 359.52002	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.07, 1.07, 1.07	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: ZN, PLX, CA

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	0.27	0/19547	0.50	4/26382 (0.0%)
1	B	0.27	0/19547	0.50	4/26382 (0.0%)
1	C	0.27	0/19547	0.51	4/26382 (0.0%)
1	D	0.27	0/19547	0.50	4/26382 (0.0%)
All	All	0.27	0/78188	0.50	16/105528 (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	2
1	B	0	2
1	C	0	2
1	D	0	2
All	All	0	8

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1882	LEU	CA-CB-CG	5.99	129.08	115.30
1	C	1882	LEU	CA-CB-CG	5.99	129.08	115.30
1	D	1882	LEU	CA-CB-CG	5.98	129.06	115.30
1	A	1882	LEU	CA-CB-CG	5.98	129.05	115.30
1	B	1957	LEU	CA-CB-CG	5.47	127.88	115.30
1	A	1957	LEU	CA-CB-CG	5.46	127.86	115.30
1	C	1957	LEU	CA-CB-CG	5.44	127.82	115.30
1	D	1957	LEU	CA-CB-CG	5.44	127.81	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	88	LEU	CA-CB-CG	5.37	127.64	115.30
1	D	88	LEU	CA-CB-CG	5.37	127.64	115.30
1	A	88	LEU	CA-CB-CG	5.36	127.64	115.30
1	C	88	LEU	CA-CB-CG	5.35	127.61	115.30
1	A	634	LEU	CA-CB-CG	5.34	127.58	115.30
1	D	634	LEU	CA-CB-CG	5.34	127.57	115.30
1	B	634	LEU	CA-CB-CG	5.33	127.57	115.30
1	C	634	LEU	CA-CB-CG	5.33	127.57	115.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1098	LYS	Mainchain
1	A	665	LEU	Peptide
1	B	1098	LYS	Mainchain
1	B	665	LEU	Peptide
1	C	1098	LYS	Mainchain
1	C	665	LEU	Peptide
1	D	1098	LYS	Mainchain
1	D	665	LEU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	19195	0	19276	410	0
1	B	19195	0	19276	400	0
1	C	19195	0	19276	409	0
1	D	19195	0	19276	398	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	6	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	4	0	0	0	0
4	A	281	0	412	21	0
4	B	281	0	412	20	0
4	C	281	0	412	19	0
4	D	281	0	412	23	0
All	All	77928	0	78752	1551	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 10.

All (1551) 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:D:806:LEU:HD11	1:D:1104:VAL:N	1.84	0.93
1:A:806:LEU:HD11	1:A:1104:VAL:N	1.84	0.92
1:B:806:LEU:HD11	1:B:1104:VAL:N	1.84	0.92
1:C:806:LEU:HD11	1:C:1104:VAL:N	1.84	0.92
1:A:1101:GLN:O	1:A:1102:LEU:HB2	1.75	0.86
1:A:1101:GLN:HG3	1:A:1208:MET:HE3	1.58	0.85
1:C:1101:GLN:HG3	1:C:1208:MET:HE3	1.58	0.85
1:D:1101:GLN:O	1:D:1102:LEU:HB2	1.75	0.85
1:B:1101:GLN:HG3	1:B:1208:MET:HE3	1.58	0.85
1:C:1101:GLN:O	1:C:1102:LEU:HB2	1.75	0.84
1:D:1101:GLN:HG3	1:D:1208:MET:HE3	1.58	0.84
1:B:1101:GLN:O	1:B:1102:LEU:HB2	1.75	0.84
1:B:2541:HIS:HB3	1:B:2552:VAL:HG11	1.64	0.80
1:A:2541:HIS:HB3	1:A:2552:VAL:HG11	1.64	0.80
1:C:2541:HIS:HB3	1:C:2552:VAL:HG11	1.64	0.79
1:D:2541:HIS:HB3	1:D:2552:VAL:HG11	1.64	0.79
1:B:2625:THR:HG23	1:B:2626:VAL:H	1.48	0.78
1:D:2722:GLN:NE2	1:D:2723:MET:SD	2.57	0.78
1:C:1080:LEU:HD11	1:C:1671:LEU:HD21	1.65	0.78
1:B:2722:GLN:NE2	1:B:2723:MET:SD	2.57	0.78
1:C:806:LEU:HD21	1:C:1104:VAL:HB	1.66	0.78
1:C:2722:GLN:NE2	1:C:2723:MET:SD	2.57	0.78
1:A:85:ASP:H	1:C:1886:LYS:HB2	1.49	0.78
1:A:2625:THR:HG23	1:A:2626:VAL:H	1.48	0.78
1:D:1080:LEU:HD11	1:D:1671:LEU:HD21	1.65	0.78
1:A:806:LEU:HD21	1:A:1104:VAL:HB	1.66	0.78
1:A:1080:LEU:HD11	1:A:1671:LEU:HD21	1.65	0.77
1:A:895:LEU:O	1:A:899:HIS:ND1	2.18	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2722:GLN:NE2	1:A:2723:MET:SD	2.57	0.77
1:B:806:LEU:HD21	1:B:1104:VAL:HB	1.66	0.77
1:D:806:LEU:HD21	1:D:1104:VAL:HB	1.66	0.77
1:C:2625:THR:HG23	1:C:2626:VAL:H	1.48	0.77
1:D:2625:THR:HG23	1:D:2626:VAL:H	1.48	0.77
1:C:2533:MET:HE1	4:C:5108:PLX:H32	1.67	0.77
1:B:1080:LEU:HD11	1:B:1671:LEU:HD21	1.65	0.77
1:B:1886:LYS:HB2	1:D:85:ASP:H	1.50	0.77
1:C:85:ASP:H	1:D:1886:LYS:HB2	1.49	0.77
1:B:2533:MET:HE1	4:B:5107:PLX:H32	1.67	0.76
1:C:895:LEU:O	1:C:899:HIS:ND1	2.18	0.75
1:C:2436:ARG:HG3	4:C:5113:PLX:H22	1.67	0.75
1:B:2436:ARG:HG3	4:B:5112:PLX:H22	1.67	0.75
1:A:1882:LEU:HD21	1:B:92:LEU:HD21	1.70	0.73
1:A:92:LEU:HD21	1:C:1882:LEU:HD21	1.70	0.73
1:D:2064:ASP:OD1	1:D:2115:ASN:ND2	2.22	0.73
1:A:1100:VAL:O	1:A:1101:GLN:HB3	1.88	0.73
1:A:1886:LYS:HB2	1:B:85:ASP:H	1.53	0.73
1:C:1100:VAL:O	1:C:1101:GLN:HB3	1.88	0.73
1:C:2064:ASP:OD1	1:C:2115:ASN:ND2	2.22	0.73
1:C:564:GLN:HB3	1:C:574:ILE:HD12	1.69	0.73
1:B:600:HIS:O	1:B:603:ARG:NH1	2.22	0.73
1:D:600:HIS:O	1:D:603:ARG:NH1	2.22	0.73
1:D:564:GLN:HB3	1:D:574:ILE:HD12	1.69	0.73
1:D:895:LEU:O	1:D:899:HIS:ND1	2.18	0.73
1:B:564:GLN:HB3	1:B:574:ILE:HD12	1.69	0.72
1:B:2064:ASP:OD1	1:B:2115:ASN:ND2	2.22	0.72
1:A:600:HIS:O	1:A:603:ARG:NH1	2.22	0.72
1:B:1100:VAL:O	1:B:1101:GLN:HB3	1.88	0.72
1:A:564:GLN:HB3	1:A:574:ILE:HD12	1.69	0.72
1:C:92:LEU:HD21	1:D:1882:LEU:HD21	1.70	0.72
1:C:600:HIS:O	1:C:603:ARG:NH1	2.22	0.72
1:B:276:THR:O	1:B:508:LYS:NZ	2.20	0.71
1:B:558:ARG:HH21	1:B:590:LEU:HD13	1.55	0.71
1:A:2064:ASP:OD1	1:A:2115:ASN:ND2	2.22	0.71
1:A:558:ARG:HH21	1:A:590:LEU:HD13	1.55	0.71
1:B:1882:LEU:HD21	1:D:92:LEU:HD21	1.71	0.71
1:B:895:LEU:O	1:B:899:HIS:ND1	2.18	0.71
1:D:558:ARG:HH21	1:D:590:LEU:HD13	1.55	0.71
1:D:1100:VAL:O	1:D:1101:GLN:HB3	1.88	0.71
1:B:2306:GLU:HG2	1:B:2307:PRO:HD3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2306:GLU:HG2	1:C:2307:PRO:HD3	1.73	0.70
1:A:537:ARG:HE	1:A:538:LEU:H	1.38	0.70
1:C:558:ARG:HH21	1:C:590:LEU:HD13	1.55	0.70
1:C:1627:VAL:HG12	1:C:1631:HIS:CE1	2.27	0.70
1:A:1883:GLY:HA2	1:B:89:LEU:HD11	1.74	0.70
1:C:276:THR:O	1:C:508:LYS:NZ	2.20	0.70
1:D:537:ARG:HE	1:D:538:LEU:H	1.38	0.70
1:A:2670:ARG:HH21	1:A:2672:LEU:HD11	1.57	0.70
1:B:1627:VAL:HG12	1:B:1631:HIS:CE1	2.27	0.70
1:B:2670:ARG:HH21	1:B:2672:LEU:HD11	1.57	0.70
1:D:2306:GLU:HG2	1:D:2307:PRO:HD3	1.73	0.70
1:A:2306:GLU:HG2	1:A:2307:PRO:HD3	1.73	0.69
1:C:537:ARG:HE	1:C:538:LEU:H	1.38	0.69
1:C:2670:ARG:HH21	1:C:2672:LEU:HD11	1.57	0.69
1:D:2670:ARG:HH21	1:D:2672:LEU:HD11	1.57	0.69
1:B:537:ARG:HE	1:B:538:LEU:H	1.38	0.69
1:C:806:LEU:HD11	1:C:1104:VAL:CA	2.22	0.69
1:D:806:LEU:HD11	1:D:1104:VAL:CA	2.22	0.69
1:A:1627:VAL:HG12	1:A:1631:HIS:CE1	2.27	0.69
1:B:806:LEU:HD11	1:B:1104:VAL:CA	2.22	0.69
1:D:1627:VAL:HG12	1:D:1631:HIS:CE1	2.27	0.69
1:A:806:LEU:HD11	1:A:1104:VAL:CA	2.22	0.68
1:A:1798:HIS:HA	1:A:1801:LYS:NZ	2.08	0.68
1:B:1798:HIS:HA	1:B:1801:LYS:NZ	2.08	0.68
1:A:2236:GLN:NE2	1:C:2629:GLU:OE2	2.26	0.68
1:A:276:THR:O	1:A:508:LYS:NZ	2.20	0.68
1:D:1642:ASP:OD1	1:D:1645:ARG:NH2	2.27	0.68
1:C:2199:VAL:HG12	1:C:2205:MET:HG2	1.76	0.68
1:C:1642:ASP:OD1	1:C:1645:ARG:NH2	2.27	0.68
1:A:1488:THR:OG1	1:A:1536:CYS:SG	2.52	0.68
1:B:1488:THR:OG1	1:B:1536:CYS:SG	2.52	0.68
1:D:1296:VAL:HG21	1:D:1333:GLU:HB3	1.76	0.68
1:D:1798:HIS:HA	1:D:1801:LYS:NZ	2.08	0.68
1:B:1296:VAL:HG21	1:B:1333:GLU:HB3	1.76	0.68
1:D:2199:VAL:HG12	1:D:2205:MET:HG2	1.75	0.68
1:A:2680:ALA:HB3	1:A:2683:LEU:HD23	1.76	0.68
1:A:1296:VAL:HG21	1:A:1333:GLU:HB3	1.76	0.67
1:A:2436:ARG:HG3	4:A:5114:PLX:H22	1.74	0.67
1:D:1488:THR:OG1	1:D:1536:CYS:SG	2.52	0.67
1:B:2680:ALA:HB3	1:B:2683:LEU:HD23	1.76	0.67
1:C:1798:HIS:HA	1:C:1801:LYS:NZ	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1488:THR:OG1	1:C:1536:CYS:SG	2.52	0.67
1:B:1642:ASP:OD1	1:B:1645:ARG:NH2	2.27	0.67
1:C:1296:VAL:HG21	1:C:1333:GLU:HB3	1.76	0.67
1:A:1642:ASP:OD1	1:A:1645:ARG:NH2	2.27	0.67
1:D:1107:GLN:O	1:D:1109:VAL:N	2.28	0.67
1:A:2132:GLY:HA3	1:A:2150:ARG:HG2	1.78	0.66
1:C:826:LYS:NZ	1:C:877:GLY:O	2.28	0.66
1:C:806:LEU:CD1	1:C:1104:VAL:N	2.58	0.66
1:D:276:THR:O	1:D:508:LYS:NZ	2.20	0.66
1:A:826:LYS:NZ	1:A:877:GLY:O	2.28	0.66
1:A:1107:GLN:O	1:A:1109:VAL:N	2.28	0.66
1:C:2132:GLY:HA3	1:C:2150:ARG:HG2	1.78	0.66
1:B:826:LYS:NZ	1:B:877:GLY:O	2.29	0.66
1:C:1107:GLN:O	1:C:1109:VAL:N	2.28	0.66
1:D:806:LEU:CD1	1:D:1104:VAL:N	2.58	0.66
1:D:2436:ARG:HG3	4:D:5111:PLX:H22	1.76	0.66
1:D:2680:ALA:HB3	1:D:2683:LEU:HD23	1.76	0.66
1:B:806:LEU:CD1	1:B:1104:VAL:N	2.58	0.66
1:C:2680:ALA:HB3	1:C:2683:LEU:HD23	1.76	0.66
1:A:2199:VAL:HG12	1:A:2205:MET:HG2	1.75	0.66
1:B:1107:GLN:O	1:B:1109:VAL:N	2.28	0.66
1:A:2240:ILE:HG22	1:A:2672:LEU:HD23	1.78	0.66
1:B:86:ALA:HA	1:B:89:LEU:HD23	1.78	0.66
1:C:883:ASP:OD1	1:C:886:ARG:NH2	2.29	0.66
1:D:826:LYS:NZ	1:D:877:GLY:O	2.29	0.66
1:D:2118:PRO:HB3	1:D:2170:LEU:HD13	1.78	0.66
1:B:2199:VAL:HG12	1:B:2205:MET:HG2	1.76	0.66
1:D:2240:ILE:HG22	1:D:2672:LEU:HD23	1.78	0.66
1:A:2533:MET:HE1	4:A:5109:PLX:H32	1.77	0.65
1:D:86:ALA:HA	1:D:89:LEU:HD23	1.78	0.65
1:D:2132:GLY:HA3	1:D:2150:ARG:HG2	1.78	0.65
1:C:2118:PRO:HB3	1:C:2170:LEU:HD13	1.78	0.65
1:A:2118:PRO:HB3	1:A:2170:LEU:HD13	1.78	0.65
1:B:2132:GLY:HA3	1:B:2150:ARG:HG2	1.78	0.65
1:D:619:VAL:HG11	1:D:659:PRO:HG2	1.79	0.65
1:C:2240:ILE:HG22	1:C:2672:LEU:HD23	1.78	0.65
1:B:2118:PRO:HB3	1:B:2170:LEU:HD13	1.78	0.65
1:A:883:ASP:OD1	1:A:886:ARG:NH2	2.29	0.65
1:B:694:GLU:OE1	1:B:766:ARG:NH2	2.30	0.65
1:B:2240:ILE:HG22	1:B:2672:LEU:HD23	1.78	0.65
1:A:694:GLU:OE1	1:A:766:ARG:NH2	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:806:LEU:CD1	1:A:1104:VAL:N	2.58	0.65
1:B:619:VAL:HG11	1:B:659:PRO:HG2	1.79	0.65
1:B:1526:MET:SD	1:B:1527:PRO:HD2	2.37	0.65
1:D:1526:MET:SD	1:D:1527:PRO:HD2	2.37	0.65
1:B:883:ASP:OD1	1:B:886:ARG:NH2	2.29	0.64
1:C:619:VAL:HG11	1:C:659:PRO:HG2	1.79	0.64
1:D:883:ASP:OD1	1:D:886:ARG:NH2	2.29	0.64
1:A:619:VAL:HG11	1:A:659:PRO:HG2	1.79	0.64
1:C:86:ALA:HA	1:C:89:LEU:HD23	1.78	0.64
1:D:1831:LEU:HG	1:D:1839:ILE:HD13	1.80	0.64
1:A:1526:MET:SD	1:A:1527:PRO:HD2	2.37	0.64
1:D:2631:HIS:ND1	1:D:2635:GLU:OE2	2.30	0.64
1:A:86:ALA:HA	1:A:89:LEU:HD23	1.78	0.64
1:C:1526:MET:SD	1:C:1527:PRO:HD2	2.37	0.64
1:A:402:THR:HG22	1:A:404:ILE:H	1.63	0.64
1:B:402:THR:HG22	1:B:404:ILE:H	1.63	0.64
1:C:807:TRP:HZ3	1:C:1102:LEU:N	1.96	0.64
1:C:1831:LEU:HG	1:C:1839:ILE:HD13	1.80	0.64
1:B:1831:LEU:HG	1:B:1839:ILE:HD13	1.80	0.63
1:D:807:TRP:HZ3	1:D:1102:LEU:N	1.96	0.63
1:D:2394:TYR:HB2	4:D:5110:PLX:H111	1.80	0.63
1:A:2629:GLU:OE2	1:B:2236:GLN:NE2	2.27	0.63
1:D:653:CYS:HA	1:D:743:MET:HE3	1.80	0.63
1:D:1687:ARG:NH2	1:D:1789:GLU:O	2.31	0.63
1:D:694:GLU:OE1	1:D:766:ARG:NH2	2.30	0.63
1:B:1267:ILE:HG23	1:B:1307:GLN:HG3	1.80	0.63
1:A:1831:LEU:HG	1:A:1839:ILE:HD13	1.80	0.62
1:A:1267:ILE:HG23	1:A:1307:GLN:HG3	1.80	0.62
1:B:2631:HIS:ND1	1:B:2635:GLU:OE2	2.30	0.62
1:C:694:GLU:OE1	1:C:766:ARG:NH2	2.30	0.62
1:D:1267:ILE:HG23	1:D:1307:GLN:HG3	1.80	0.62
1:A:443:LEU:O	1:A:447:ASN:ND2	2.31	0.62
1:A:807:TRP:HZ3	1:A:1102:LEU:N	1.96	0.62
1:B:807:TRP:HZ3	1:B:1102:LEU:N	1.96	0.62
1:B:1687:ARG:NH2	1:B:1789:GLU:O	2.31	0.62
1:C:402:THR:HG22	1:C:404:ILE:H	1.63	0.62
1:D:1367:GLU:HB3	1:D:1370:PRO:HD2	1.81	0.62
1:A:1687:ARG:NH2	1:A:1789:GLU:O	2.31	0.62
1:C:249:LYS:HZ3	1:C:266:THR:HG23	1.64	0.62
1:C:2236:GLN:NE2	1:D:2629:GLU:OE2	2.31	0.62
1:C:443:LEU:O	1:C:447:ASN:ND2	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1687:ARG:NH2	1:C:1789:GLU:O	2.31	0.62
4:B:5109:PLX:H251	4:B:5109:PLX:H122	1.82	0.62
1:D:402:THR:HG22	1:D:404:ILE:H	1.63	0.62
1:B:1005:ASN:ND2	1:B:1596:ASP:OD2	2.33	0.62
1:B:2070:ILE:HD12	1:B:2096:LEU:HD12	1.82	0.62
1:D:804:ALA:HB1	1:D:1102:LEU:CD2	2.30	0.62
4:A:5111:PLX:H251	4:A:5111:PLX:H122	1.82	0.61
1:D:2070:ILE:HD12	1:D:2096:LEU:HD12	1.82	0.61
1:B:653:CYS:HA	1:B:743:MET:HE3	1.82	0.61
1:C:1367:GLU:HB3	1:C:1370:PRO:HD2	1.81	0.61
1:D:1415:CYS:O	1:D:1420:LYS:NZ	2.34	0.61
1:A:1005:ASN:ND2	1:A:1596:ASP:OD2	2.33	0.61
1:A:1415:CYS:O	1:A:1420:LYS:NZ	2.34	0.61
1:C:1267:ILE:HG23	1:C:1307:GLN:HG3	1.80	0.61
1:D:1005:ASN:ND2	1:D:1596:ASP:OD2	2.33	0.61
4:D:5108:PLX:H122	4:D:5108:PLX:H251	1.82	0.61
1:B:804:ALA:HB1	1:B:1102:LEU:CD2	2.30	0.61
1:C:1005:ASN:ND2	1:C:1596:ASP:OD2	2.33	0.61
1:A:89:LEU:HD11	1:C:1883:GLY:HA2	1.81	0.61
1:A:804:ALA:HB1	1:A:1102:LEU:CD2	2.30	0.61
1:A:1501:THR:O	1:A:1505:ARG:NH1	2.34	0.61
1:B:363:ASP:OD1	1:B:364:ILE:N	2.34	0.61
1:C:804:ALA:HB1	1:C:1102:LEU:CD2	2.30	0.61
1:D:1501:THR:O	1:D:1505:ARG:NH1	2.34	0.61
1:D:1974:GLN:OE1	1:D:2035:GLN:NE2	2.34	0.61
1:A:202:ASP:OD1	1:A:203:ASN:N	2.33	0.61
1:A:1069:MET:HA	1:A:1655:LYS:HG2	1.83	0.61
1:B:1069:MET:HA	1:B:1655:LYS:HG2	1.83	0.61
1:B:1501:THR:O	1:B:1505:ARG:NH1	2.34	0.61
1:B:1883:GLY:HA2	1:D:89:LEU:HD11	1.82	0.61
1:C:1415:CYS:O	1:C:1420:LYS:NZ	2.34	0.61
1:C:1501:THR:O	1:C:1505:ARG:NH1	2.34	0.61
1:C:1974:GLN:OE1	1:C:2035:GLN:NE2	2.34	0.61
1:A:1244:PHE:O	1:A:1251:ASN:ND2	2.34	0.61
1:B:1415:CYS:O	1:B:1420:LYS:NZ	2.34	0.61
1:C:82:SER:H	1:D:1885:LYS:HG2	1.64	0.61
1:C:202:ASP:OD1	1:C:203:ASN:N	2.33	0.61
1:C:302:LEU:HB3	1:C:367:ILE:HD11	1.82	0.61
1:A:653:CYS:HA	1:A:743:MET:HE3	1.83	0.61
1:A:1367:GLU:HB3	1:A:1370:PRO:HD2	1.81	0.61
1:A:1974:GLN:OE1	1:A:2035:GLN:NE2	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:ASP:OD1	1:B:203:ASN:N	2.33	0.61
1:D:2433:SER:HB2	1:D:2593:PHE:HD1	1.66	0.61
1:A:764:ILE:HG21	1:A:785:MET:HB2	1.83	0.61
1:B:764:ILE:HG21	1:B:785:MET:HB2	1.83	0.61
1:B:2433:SER:HB2	1:B:2593:PHE:HD1	1.66	0.61
1:C:2631:HIS:ND1	1:C:2635:GLU:OE2	2.30	0.61
4:C:5110:PLX:H251	4:C:5110:PLX:H122	1.82	0.61
1:D:202:ASP:OD1	1:D:203:ASN:N	2.33	0.61
1:B:1244:PHE:O	1:B:1251:ASN:ND2	2.34	0.60
1:B:1885:LYS:HG2	1:D:82:SER:H	1.64	0.60
1:C:653:CYS:HA	1:C:743:MET:HE3	1.83	0.60
1:D:1552:PRO:HD2	1:D:1555:LEU:HD23	1.82	0.60
1:A:363:ASP:OD1	1:A:364:ILE:N	2.34	0.60
1:B:249:LYS:HZ3	1:B:266:THR:HG23	1.66	0.60
1:B:2437:ASN:HB3	1:B:2440:PRO:HG2	1.83	0.60
1:C:2433:SER:HB2	1:C:2593:PHE:HD1	1.66	0.60
1:D:302:LEU:HB3	1:D:367:ILE:HD11	1.82	0.60
1:D:611:THR:HG23	1:D:613:ALA:H	1.66	0.60
1:D:764:ILE:HG21	1:D:785:MET:HB2	1.83	0.60
1:A:2070:ILE:HD12	1:A:2096:LEU:HD12	1.82	0.60
1:A:2433:SER:HB2	1:A:2593:PHE:HD1	1.66	0.60
1:A:2695:LEU:HD23	1:B:2696:ARG:HE	1.66	0.60
1:B:1367:GLU:HB3	1:B:1370:PRO:HD2	1.81	0.60
1:C:611:THR:HG23	1:C:613:ALA:H	1.66	0.60
1:A:82:SER:H	1:C:1885:LYS:HG2	1.66	0.60
1:B:302:LEU:HB3	1:B:367:ILE:HD11	1.82	0.60
1:C:2070:ILE:HD12	1:C:2096:LEU:HD12	1.82	0.60
1:D:2437:ASN:HB3	1:D:2440:PRO:HG2	1.83	0.60
1:B:1798:HIS:HA	1:B:1801:LYS:HZ3	1.64	0.60
1:A:249:LYS:HZ3	1:A:266:THR:HG23	1.66	0.60
1:C:89:LEU:HD11	1:D:1883:GLY:HA2	1.83	0.60
1:C:1552:PRO:HD2	1:C:1555:LEU:HD23	1.82	0.60
1:A:1552:PRO:HD2	1:A:1555:LEU:HD23	1.82	0.60
1:A:302:LEU:HB3	1:A:367:ILE:HD11	1.82	0.60
1:A:611:THR:HG23	1:A:613:ALA:H	1.66	0.60
1:A:2437:ASN:HB3	1:A:2440:PRO:HG2	1.83	0.60
1:B:1421:ILE:HG13	1:B:1422:ALA:H	1.66	0.60
1:B:1552:PRO:HD2	1:B:1555:LEU:HD23	1.82	0.60
1:B:1687:ARG:NH2	1:B:1790:MET:O	2.35	0.60
1:B:1974:GLN:OE1	1:B:2035:GLN:NE2	2.34	0.60
1:C:764:ILE:HG21	1:C:785:MET:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1687:ARG:NH2	1:C:1790:MET:O	2.35	0.60
1:A:1484:MET:HB3	1:A:1536:CYS:SG	2.42	0.60
1:A:1886:LYS:CB	1:B:86:ALA:H	2.15	0.60
1:B:1484:MET:HB3	1:B:1536:CYS:SG	2.42	0.60
1:C:1069:MET:HA	1:C:1655:LYS:HG2	1.83	0.60
1:C:1244:PHE:O	1:C:1251:ASN:ND2	2.34	0.60
1:D:1798:HIS:HA	1:D:1801:LYS:HZ3	1.65	0.60
1:B:1407:VAL:HG21	1:B:1446:HIS:HB3	1.84	0.59
1:C:1421:ILE:HG13	1:C:1422:ALA:H	1.66	0.59
1:D:363:ASP:OD1	1:D:364:ILE:N	2.34	0.59
1:A:2631:HIS:ND1	1:A:2635:GLU:OE2	2.30	0.59
1:B:2439:ARG:NH2	4:B:5108:PLX:O4	2.36	0.59
1:D:1069:MET:HA	1:D:1655:LYS:HG2	1.83	0.59
1:A:1339:GLU:OE1	1:B:467:GLN:NE2	2.30	0.59
1:A:1687:ARG:NH2	1:A:1790:MET:O	2.35	0.59
1:C:2437:ASN:HB3	1:C:2440:PRO:HG2	1.83	0.59
1:D:249:LYS:HZ3	1:D:266:THR:HG23	1.66	0.59
1:B:1339:GLU:OE1	1:D:467:GLN:NE2	2.31	0.59
1:A:1288:ASN:HB3	1:A:1290:ARG:HG2	1.85	0.59
1:B:1639:GLU:HA	1:B:1644:ARG:HD3	1.85	0.59
1:C:1484:MET:HB3	1:C:1536:CYS:SG	2.42	0.59
4:B:5108:PLX:H102	4:B:5108:PLX:H262	1.85	0.59
1:C:85:ASP:OD2	1:D:1884:ASN:N	2.36	0.59
1:D:1407:VAL:HG21	1:D:1446:HIS:HB3	1.85	0.59
1:D:1421:ILE:HG13	1:D:1422:ALA:H	1.66	0.59
1:D:1484:MET:HB3	1:D:1536:CYS:SG	2.42	0.59
1:B:611:THR:HG23	1:B:613:ALA:H	1.66	0.59
1:B:2629:GLU:OE2	1:D:2236:GLN:NE2	2.30	0.59
1:C:363:ASP:OD1	1:C:364:ILE:N	2.34	0.59
1:D:1244:PHE:O	1:D:1251:ASN:ND2	2.34	0.59
1:A:1421:ILE:HG13	1:A:1422:ALA:H	1.66	0.59
4:A:5110:PLX:H102	4:A:5110:PLX:H262	1.85	0.59
1:A:1000:GLU:HG3	1:A:1033:ILE:HG12	1.85	0.59
1:A:1341:VAL:O	1:A:1374:TYR:OH	2.21	0.59
1:A:1639:GLU:HA	1:A:1644:ARG:HD3	1.85	0.59
1:C:1407:VAL:HG21	1:C:1446:HIS:HB3	1.84	0.59
1:A:222:LEU:HD23	1:A:293:ARG:HH12	1.68	0.58
1:A:2394:TYR:HB2	4:A:5113:PLX:H111	1.85	0.58
1:B:2438:GLY:HA3	4:B:5110:PLX:H32	1.85	0.58
1:A:1407:VAL:HG21	1:A:1446:HIS:HB3	1.85	0.58
1:B:1885:LYS:HD3	1:D:82:SER:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:222:LEU:HD23	1:D:293:ARG:HH12	1.68	0.58
1:B:1341:VAL:O	1:B:1374:TYR:OH	2.21	0.58
1:D:1687:ARG:NH2	1:D:1790:MET:O	2.35	0.58
1:A:567:TYR:HD2	1:A:570:ASN:HB2	1.69	0.58
1:C:2438:GLY:HA3	4:C:5111:PLX:H32	1.85	0.58
1:D:1000:GLU:HG3	1:D:1033:ILE:HG12	1.85	0.58
1:D:2533:MET:HE1	4:D:5106:PLX:H32	1.86	0.58
1:B:1000:GLU:HG3	1:B:1033:ILE:HG12	1.85	0.58
1:B:1288:ASN:HB3	1:B:1290:ARG:HG2	1.85	0.58
1:C:2439:ARG:NH2	4:C:5109:PLX:O4	2.36	0.58
1:D:1639:GLU:HA	1:D:1644:ARG:HD3	1.85	0.58
1:B:147:MET:HB2	1:B:211:SER:HB3	1.85	0.58
1:B:567:TYR:HD2	1:B:570:ASN:HB2	1.69	0.58
1:C:82:SER:HB2	1:D:1885:LYS:HD3	1.85	0.58
4:C:5109:PLX:H102	4:C:5109:PLX:H262	1.84	0.58
1:A:147:MET:HB2	1:A:211:SER:HB3	1.85	0.58
1:B:1884:ASN:N	1:D:85:ASP:OD2	2.37	0.58
1:C:1000:GLU:HG3	1:C:1033:ILE:HG12	1.85	0.58
1:D:1288:ASN:HB3	1:D:1290:ARG:HG2	1.85	0.58
1:A:85:ASP:N	1:C:1886:LYS:HB2	2.18	0.58
1:C:222:LEU:HD23	1:C:293:ARG:HH12	1.68	0.58
1:D:567:TYR:HD2	1:D:570:ASN:HB2	1.69	0.58
1:D:1341:VAL:O	1:D:1374:TYR:OH	2.21	0.58
1:C:1639:GLU:HA	1:C:1644:ARG:HD3	1.85	0.58
1:D:371:ASP:OD2	1:D:389:ARG:NH1	2.36	0.58
1:B:1101:GLN:O	1:B:1101:GLN:HG2	2.04	0.57
1:C:1288:ASN:HB3	1:C:1290:ARG:HG2	1.85	0.57
1:C:1341:VAL:O	1:C:1374:TYR:OH	2.21	0.57
1:C:147:MET:HB2	1:C:211:SER:HB3	1.85	0.57
1:A:82:SER:HB2	1:C:1885:LYS:HD3	1.86	0.57
1:C:64:ASN:OD1	1:C:122:GLN:NE2	2.35	0.57
1:C:467:GLN:NE2	1:D:1339:GLU:OE1	2.32	0.57
1:C:550:ARG:HH12	1:C:588:ASP:HB2	1.70	0.57
1:C:1191:SER:OG	1:C:1194:VAL:O	2.23	0.57
1:D:147:MET:HB2	1:D:211:SER:HB3	1.85	0.57
4:D:5107:PLX:H102	4:D:5107:PLX:H262	1.85	0.57
1:C:1293:GLN:O	1:C:1297:HIS:ND1	2.31	0.57
1:A:550:ARG:HH12	1:A:588:ASP:HB2	1.69	0.57
1:B:222:LEU:HD23	1:B:293:ARG:HH12	1.68	0.57
1:C:567:TYR:HD2	1:C:570:ASN:HB2	1.69	0.57
1:D:1191:SER:OG	1:D:1194:VAL:O	2.23	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1293:GLN:O	1:B:1297:HIS:ND1	2.31	0.57
1:C:1101:GLN:O	1:C:1101:GLN:HG2	2.04	0.57
1:D:64:ASN:OD1	1:D:122:GLN:NE2	2.35	0.57
1:D:2145:GLY:O	1:D:2151:ASN:ND2	2.38	0.57
1:B:2021:LEU:HD13	1:B:2069:LEU:HD23	1.87	0.57
1:C:85:ASP:N	1:D:1886:LYS:HB2	2.18	0.57
1:C:2145:GLY:O	1:C:2151:ASN:ND2	2.38	0.57
1:D:550:ARG:HH12	1:D:588:ASP:HB2	1.69	0.57
1:A:1101:GLN:O	1:A:1101:GLN:HG2	2.04	0.56
1:A:2145:GLY:O	1:A:2151:ASN:ND2	2.38	0.56
1:C:466:THR:OG1	1:C:468:ASN:OD1	2.22	0.56
1:A:2021:LEU:HD13	1:A:2069:LEU:HD23	1.87	0.56
1:B:443:LEU:O	1:B:447:ASN:ND2	2.31	0.56
1:B:1191:SER:OG	1:B:1194:VAL:O	2.23	0.56
1:B:2145:GLY:O	1:B:2151:ASN:ND2	2.38	0.56
1:C:2021:LEU:HD13	1:C:2069:LEU:HD23	1.87	0.56
1:A:1191:SER:OG	1:A:1194:VAL:O	2.23	0.56
1:B:768:MET:HE3	1:B:782:CYS:HA	1.87	0.56
1:D:443:LEU:O	1:D:447:ASN:ND2	2.31	0.56
1:D:654:LYS:HE2	1:D:750:LEU:HD21	1.87	0.56
1:D:1101:GLN:O	1:D:1101:GLN:HG2	2.04	0.56
1:D:2719:LEU:O	1:D:2722:GLN:HG3	2.06	0.56
1:A:2719:LEU:O	1:A:2722:GLN:HG3	2.06	0.56
1:C:1099:GLN:O	1:C:1100:VAL:HG13	2.06	0.56
1:C:2719:LEU:O	1:C:2722:GLN:HG3	2.06	0.56
1:A:2544:ARG:NH1	1:B:2547:GLY:O	2.32	0.56
1:B:1473:SER:OG	1:B:1477:LYS:NZ	2.39	0.56
1:A:808:SER:HB2	1:A:1104:VAL:CG1	2.36	0.56
1:A:1099:GLN:O	1:A:1100:VAL:HG13	2.06	0.56
1:A:1348:ARG:NH2	1:B:535:MET:O	2.39	0.56
1:A:2696:ARG:HE	1:C:2695:LEU:HD23	1.70	0.56
1:B:64:ASN:OD1	1:B:122:GLN:NE2	2.35	0.56
1:B:550:ARG:HH12	1:B:588:ASP:HB2	1.70	0.56
1:D:1406:ILE:HA	1:D:1423:TYR:HE2	1.71	0.56
1:B:1410:VAL:HG21	1:B:1450:LEU:HD21	1.88	0.56
1:C:371:ASP:OD2	1:C:389:ARG:NH1	2.36	0.56
1:C:1406:ILE:HA	1:C:1423:TYR:HE2	1.71	0.56
1:A:1473:SER:OG	1:A:1477:LYS:NZ	2.39	0.56
1:B:808:SER:HB2	1:B:1104:VAL:CG1	2.36	0.56
1:B:2394:TYR:HB2	4:B:5111:PLX:H111	1.88	0.56
1:C:768:MET:HE3	1:C:782:CYS:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:808:SER:CB	1:A:1104:VAL:CG1	2.84	0.56
1:B:808:SER:CB	1:B:1104:VAL:CG1	2.84	0.56
1:B:1099:GLN:O	1:B:1100:VAL:HG13	2.06	0.56
1:C:1473:SER:OG	1:C:1477:LYS:NZ	2.39	0.56
1:C:2394:TYR:HB2	4:C:5112:PLX:H111	1.88	0.56
1:A:1798:HIS:HA	1:A:1801:LYS:HZ3	1.71	0.56
1:C:808:SER:HB2	1:C:1104:VAL:CG1	2.36	0.56
1:A:654:LYS:HE2	1:A:750:LEU:HD21	1.87	0.55
1:B:1406:ILE:HA	1:B:1423:TYR:HE2	1.71	0.55
1:B:2719:LEU:O	1:B:2722:GLN:HG3	2.06	0.55
1:D:808:SER:HB2	1:D:1104:VAL:CG1	2.36	0.55
1:A:1406:ILE:HA	1:A:1423:TYR:HE2	1.71	0.55
1:C:654:LYS:HE2	1:C:750:LEU:HD21	1.87	0.55
1:D:1410:VAL:HG21	1:D:1450:LEU:HD21	1.88	0.55
1:D:1473:SER:OG	1:D:1477:LYS:NZ	2.39	0.55
1:A:1886:LYS:HB3	1:B:86:ALA:H	1.72	0.55
1:D:2021:LEU:HD13	1:D:2069:LEU:HD23	1.87	0.55
1:D:2706:MET:N	1:D:2706:MET:HE2	2.21	0.55
1:A:85:ASP:OD2	1:C:1884:ASN:N	2.37	0.55
1:C:242:LEU:HD12	1:C:251:LEU:HD23	1.89	0.55
1:C:808:SER:CB	1:C:1104:VAL:CG1	2.84	0.55
1:C:1107:GLN:O	1:C:1108:ASP:C	2.45	0.55
1:D:1099:GLN:O	1:D:1100:VAL:HG13	2.06	0.55
1:B:654:LYS:HE2	1:B:750:LEU:HD21	1.87	0.55
1:C:88:LEU:HA	1:C:91:LYS:HB2	1.89	0.55
1:C:1410:VAL:HG21	1:C:1450:LEU:HD21	1.88	0.55
1:D:808:SER:CB	1:D:1104:VAL:CG1	2.84	0.55
1:A:467:GLN:NE2	1:C:1339:GLU:OE1	2.32	0.55
1:A:242:LEU:HD12	1:A:251:LEU:HD23	1.89	0.55
1:B:242:LEU:HD12	1:B:251:LEU:HD23	1.89	0.55
1:B:1886:LYS:HB2	1:D:85:ASP:N	2.19	0.55
1:B:2706:MET:N	1:B:2706:MET:HE2	2.21	0.55
1:C:1627:VAL:HG12	1:C:1631:HIS:HE1	1.72	0.55
1:D:242:LEU:HD12	1:D:251:LEU:HD23	1.89	0.55
1:A:55:ASP:O	1:A:125:HIS:NE2	2.40	0.55
1:B:372:PRO:O	1:B:389:ARG:NH1	2.40	0.55
1:D:372:PRO:O	1:D:389:ARG:NH1	2.40	0.55
1:D:898:VAL:O	1:D:901:THR:OG1	2.22	0.55
1:A:1254:LEU:O	1:A:1257:LYS:HE2	2.07	0.54
1:A:1885:LYS:HG2	1:B:82:SER:H	1.72	0.54
1:B:1107:GLN:O	1:B:1108:ASP:C	2.44	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:88:LEU:HA	1:D:91:LYS:HB2	1.89	0.54
1:D:1107:GLN:O	1:D:1108:ASP:C	2.45	0.54
1:A:86:ALA:H	1:C:1886:LYS:CB	2.20	0.54
1:A:1218:LEU:HD22	1:A:1234:MET:HE3	1.88	0.54
1:A:1627:VAL:HG12	1:A:1631:HIS:HE1	1.72	0.54
1:D:1254:LEU:O	1:D:1257:LYS:HE2	2.07	0.54
1:D:1879:THR:HB	1:D:1882:LEU:HD22	1.90	0.54
1:A:1410:VAL:HG21	1:A:1450:LEU:HD21	1.88	0.54
1:B:283:GLU:HB3	1:B:306:LYS:HB3	1.89	0.54
1:C:2696:ARG:HE	1:D:2695:LEU:HD23	1.71	0.54
1:A:2695:LEU:HD11	1:B:2700:GLU:HG2	1.88	0.54
1:C:1369:SER:HB3	1:C:1370:PRO:HD3	1.90	0.54
1:C:1879:THR:HB	1:C:1882:LEU:HD22	1.90	0.54
1:B:1254:LEU:O	1:B:1257:LYS:HE2	2.08	0.54
1:D:768:MET:HE3	1:D:782:CYS:HA	1.88	0.54
1:A:1369:SER:HB3	1:A:1370:PRO:HD3	1.90	0.54
1:C:2706:MET:HE2	1:C:2706:MET:N	2.22	0.54
1:A:372:PRO:O	1:A:389:ARG:NH1	2.40	0.54
1:C:86:ALA:H	1:D:1886:LYS:CB	2.21	0.54
1:B:2695:LEU:HD23	1:D:2696:ARG:HE	1.72	0.54
1:C:372:PRO:O	1:C:389:ARG:NH1	2.40	0.54
1:A:88:LEU:HA	1:A:91:LYS:HB2	1.89	0.53
1:A:983:ASN:OD1	1:A:1085:ARG:NH2	2.41	0.53
1:A:1107:GLN:C	1:A:1109:VAL:N	2.61	0.53
1:B:88:LEU:HA	1:B:91:LYS:HB2	1.89	0.53
1:B:898:VAL:O	1:B:901:THR:OG1	2.22	0.53
1:B:983:ASN:OD1	1:B:1085:ARG:NH2	2.41	0.53
1:B:1488:THR:HG1	1:B:1536:CYS:HG	1.52	0.53
1:C:1093:VAL:HG12	1:C:1097:PHE:CE2	2.44	0.53
1:D:2283:LEU:HD11	1:D:2357:LEU:HD22	1.90	0.53
1:B:1107:GLN:C	1:B:1109:VAL:N	2.61	0.53
1:C:983:ASN:OD1	1:C:1085:ARG:NH2	2.41	0.53
1:A:283:GLU:HB3	1:A:306:LYS:HB3	1.89	0.53
1:A:1107:GLN:O	1:A:1108:ASP:C	2.45	0.53
1:B:1879:THR:HB	1:B:1882:LEU:HD22	1.90	0.53
1:B:1886:LYS:CB	1:D:86:ALA:H	2.22	0.53
1:C:283:GLU:HB3	1:C:306:LYS:HB3	1.89	0.53
1:D:1369:SER:HB3	1:D:1370:PRO:HD3	1.90	0.53
1:B:1093:VAL:HG12	1:B:1097:PHE:CE2	2.44	0.53
1:C:1218:LEU:HD22	1:C:1234:MET:HE3	1.91	0.53
1:C:1798:HIS:HA	1:C:1801:LYS:HZ3	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:VAL:HG22	1:A:149:VAL:HG22	1.91	0.53
1:A:808:SER:CB	1:A:1104:VAL:HG11	2.39	0.53
1:A:1879:THR:HB	1:A:1882:LEU:HD22	1.90	0.53
1:C:1254:LEU:O	1:C:1257:LYS:HE2	2.08	0.53
1:D:804:ALA:HB1	1:D:1102:LEU:HD22	1.91	0.53
1:A:1884:ASN:N	1:B:85:ASP:OD2	2.40	0.53
1:D:55:ASP:O	1:D:125:HIS:NE2	2.40	0.53
4:A:5108:PLX:H332	4:A:5108:PLX:H92	1.91	0.53
1:B:2283:LEU:HD11	1:B:2357:LEU:HD22	1.90	0.53
1:C:2283:LEU:HD11	1:C:2357:LEU:HD22	1.90	0.53
1:D:2439:ARG:NH2	4:D:5107:PLX:O4	2.42	0.53
1:A:1886:LYS:HB2	1:B:85:ASP:N	2.22	0.53
1:B:808:SER:CB	1:B:1104:VAL:HG11	2.39	0.53
1:B:1627:VAL:HG12	1:B:1631:HIS:HE1	1.72	0.53
1:D:983:ASN:OD1	1:D:1085:ARG:NH2	2.41	0.53
1:A:898:VAL:O	1:A:901:THR:OG1	2.22	0.53
1:B:466:THR:OG1	1:B:468:ASN:OD1	2.22	0.53
1:C:1058:ARG:NH2	1:C:1636:LEU:O	2.37	0.53
1:C:1107:GLN:C	1:C:1109:VAL:N	2.61	0.53
1:D:283:GLU:HB3	1:D:306:LYS:HB3	1.89	0.53
1:D:808:SER:OG	1:D:1104:VAL:HG12	2.09	0.53
1:D:1239:GLU:OE2	1:D:1243:ASN:ND2	2.42	0.53
1:A:1184:SER:OG	1:A:1243:ASN:ND2	2.42	0.53
1:A:2558:LYS:HE3	1:C:2533:MET:HG2	1.90	0.53
1:D:1093:VAL:HG12	1:D:1097:PHE:CE2	2.44	0.53
1:D:1627:VAL:HG12	1:D:1631:HIS:HE1	1.72	0.53
1:B:1369:SER:HB3	1:B:1370:PRO:HD3	1.90	0.52
1:D:319:ASP:OD2	1:D:322:PHE:HB3	2.09	0.52
1:D:1129:SER:HA	1:D:1132:TRP:CE2	2.44	0.52
1:A:86:ALA:H	1:C:1886:LYS:HB3	1.74	0.52
1:A:1093:VAL:HG12	1:A:1097:PHE:CE2	2.44	0.52
1:A:1239:GLU:OE2	1:A:1243:ASN:ND2	2.42	0.52
4:B:5113:PLX:H332	4:B:5113:PLX:H92	1.91	0.52
1:C:319:ASP:OD2	1:C:322:PHE:HB3	2.09	0.52
1:C:804:ALA:HB1	1:C:1102:LEU:HD22	1.91	0.52
1:C:808:SER:OG	1:C:1104:VAL:HG12	2.09	0.52
1:C:1798:HIS:HA	1:C:1801:LYS:HZ1	1.74	0.52
1:D:1107:GLN:C	1:D:1109:VAL:N	2.61	0.52
1:A:1882:LEU:HD11	1:B:92:LEU:HD21	1.92	0.52
1:B:134:VAL:HG22	1:B:149:VAL:HG22	1.91	0.52
1:C:808:SER:CB	1:C:1104:VAL:HG11	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:ASP:OD2	1:A:322:PHE:HB3	2.09	0.52
1:A:466:THR:OG1	1:A:468:ASN:OD1	2.22	0.52
1:C:1129:SER:HA	1:C:1132:TRP:CE2	2.44	0.52
1:C:1239:GLU:OE2	1:C:1243:ASN:ND2	2.43	0.52
1:A:804:ALA:HB1	1:A:1102:LEU:HD22	1.91	0.52
1:A:1408:ARG:HH12	1:B:545:ARG:HD2	1.75	0.52
1:A:2547:GLY:O	1:C:2544:ARG:NH1	2.37	0.52
1:A:2700:GLU:HG2	1:C:2695:LEU:HD11	1.92	0.52
1:B:765:LEU:HD21	1:B:835:GLN:HG3	1.92	0.52
1:D:466:THR:OG1	1:D:468:ASN:OD1	2.22	0.52
1:D:1293:GLN:O	1:D:1297:HIS:ND1	2.31	0.52
1:A:2283:LEU:HD11	1:A:2357:LEU:HD22	1.91	0.52
1:B:804:ALA:HB1	1:B:1102:LEU:HD22	1.91	0.52
1:B:1184:SER:OG	1:B:1243:ASN:ND2	2.42	0.52
1:C:535:MET:O	1:D:1348:ARG:NH2	2.42	0.52
1:C:765:LEU:HD21	1:C:835:GLN:HG3	1.92	0.52
1:C:2227:ILE:HG13	1:C:2250:LEU:HD11	1.92	0.52
1:D:808:SER:CB	1:D:1104:VAL:HG11	2.39	0.52
1:D:1184:SER:OG	1:D:1243:ASN:ND2	2.42	0.52
4:D:5112:PLX:H332	4:D:5112:PLX:H92	1.91	0.52
1:A:1129:SER:HA	1:A:1132:TRP:CE2	2.44	0.52
1:B:319:ASP:OD2	1:B:322:PHE:HB3	2.09	0.52
1:B:808:SER:OG	1:B:1104:VAL:HG12	2.09	0.52
1:C:134:VAL:HG22	1:C:149:VAL:HG22	1.91	0.52
1:A:1885:LYS:HD3	1:B:82:SER:HB2	1.92	0.52
1:C:86:ALA:H	1:D:1886:LYS:HB3	1.74	0.52
4:C:5107:PLX:H92	4:C:5107:PLX:H332	1.91	0.52
1:B:1129:SER:HA	1:B:1132:TRP:CE2	2.44	0.52
1:C:2063:ILE:HD11	1:C:2112:ILE:HG12	1.92	0.52
1:D:1218:LEU:HD22	1:D:1234:MET:HE3	1.91	0.52
1:D:2704:SER:O	1:D:2707:LYS:HB2	2.10	0.52
1:B:1421:ILE:HG13	1:B:1422:ALA:N	2.25	0.52
1:B:2227:ILE:HG13	1:B:2250:LEU:HD11	1.92	0.52
1:C:75:ALA:HB3	1:D:1879:THR:OG1	2.10	0.52
1:D:606:LEU:HD12	1:D:610:ILE:HG13	1.92	0.52
1:D:2063:ILE:HD11	1:D:2112:ILE:HG12	1.92	0.52
1:A:808:SER:OG	1:A:1104:VAL:HG12	2.09	0.51
1:A:2020:LEU:HD21	1:B:91:LYS:HB3	1.91	0.51
1:B:1348:ARG:NH2	1:D:535:MET:O	2.41	0.51
1:B:1886:LYS:HB3	1:D:86:ALA:H	1.75	0.51
1:A:2439:ARG:NH2	4:A:5110:PLX:O4	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2703:GLU:OE1	1:C:2702:LEU:HD23	2.09	0.51
1:B:578:PHE:HE1	1:B:582:GLN:HE21	1.58	0.51
1:B:1218:LEU:HD22	1:B:1234:MET:HE3	1.92	0.51
1:C:898:VAL:O	1:C:901:THR:OG1	2.22	0.51
1:A:64:ASN:OD1	1:A:122:GLN:NE2	2.35	0.51
1:A:578:PHE:HE1	1:A:582:GLN:HE21	1.58	0.51
1:B:1879:THR:OG1	1:D:75:ALA:HB3	2.09	0.51
1:B:2704:SER:O	1:B:2707:LYS:HB2	2.10	0.51
1:C:1184:SER:OG	1:C:1243:ASN:ND2	2.42	0.51
1:D:765:LEU:HD21	1:D:835:GLN:HG3	1.92	0.51
1:D:1202:GLN:HE22	1:D:1244:PHE:HA	1.75	0.51
1:A:371:ASP:OD2	1:A:389:ARG:NH1	2.36	0.51
1:A:535:MET:O	1:C:1348:ARG:NH2	2.41	0.51
1:A:1421:ILE:HG13	1:A:1422:ALA:N	2.25	0.51
1:A:2438:GLY:HA3	4:A:5112:PLX:H32	1.92	0.51
1:B:1202:GLN:HE22	1:B:1244:PHE:HA	1.75	0.51
1:A:1544:ALA:HA	1:A:1549:ILE:HD12	1.93	0.51
1:B:806:LEU:CD1	1:B:1103:LEU:C	2.79	0.51
1:C:621:LEU:HB3	1:C:630:PHE:CE2	2.45	0.51
1:C:1270:ALA:O	1:C:1274:GLN:HG3	2.10	0.51
1:C:2700:GLU:HG2	1:D:2695:LEU:HD11	1.93	0.51
1:D:134:VAL:HG22	1:D:149:VAL:HG22	1.91	0.51
1:D:806:LEU:CD1	1:D:1103:LEU:C	2.79	0.51
1:D:2227:ILE:HG13	1:D:2250:LEU:HD11	1.92	0.51
1:A:621:LEU:HB3	1:A:630:PHE:CE2	2.45	0.51
1:B:1239:GLU:OE2	1:B:1243:ASN:ND2	2.42	0.51
1:B:1507:PRO:HA	1:B:1510:VAL:HG22	1.92	0.51
1:C:55:ASP:O	1:C:125:HIS:NE2	2.40	0.51
1:C:806:LEU:CD1	1:C:1103:LEU:C	2.79	0.51
1:D:373:THR:HG23	1:D:374:THR:HG23	1.93	0.51
1:B:621:LEU:HB3	1:B:630:PHE:CE2	2.45	0.51
1:C:373:THR:HG23	1:C:374:THR:HG23	1.93	0.51
1:C:606:LEU:HD12	1:C:610:ILE:HG13	1.92	0.51
1:C:765:LEU:O	1:C:768:MET:HB2	2.11	0.51
1:D:765:LEU:O	1:D:768:MET:HB2	2.11	0.51
1:D:2448:ALA:HB2	1:D:2581:VAL:HG11	1.93	0.51
1:D:1421:ILE:HG13	1:D:1422:ALA:N	2.25	0.51
1:A:2440:PRO:HD3	1:C:2426:THR:HG21	1.93	0.51
1:B:1270:ALA:O	1:B:1274:GLN:HG3	2.10	0.51
1:B:2411:PHE:HB3	4:B:5109:PLX:H262	1.93	0.51
1:B:2695:LEU:HD11	1:D:2700:GLU:HG2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:621:LEU:HB3	1:D:630:PHE:CE2	2.45	0.51
1:D:808:SER:OG	1:D:1104:VAL:CG1	2.59	0.51
1:A:75:ALA:HB3	1:C:1879:THR:OG1	2.11	0.51
1:A:806:LEU:CD1	1:A:1103:LEU:C	2.79	0.51
1:A:1507:PRO:HA	1:A:1510:VAL:HG22	1.92	0.51
1:C:764:ILE:O	1:C:768:MET:HG2	2.12	0.51
1:C:1202:GLN:HE22	1:C:1244:PHE:HA	1.75	0.51
1:C:2437:ASN:HB2	1:C:2592:THR:HG21	1.93	0.51
1:C:2448:ALA:HB2	1:C:2581:VAL:HG11	1.93	0.51
1:C:1421:ILE:HG13	1:C:1422:ALA:N	2.25	0.50
1:C:2411:PHE:HB3	4:C:5110:PLX:H262	1.93	0.50
1:D:2437:ASN:HB2	1:D:2592:THR:HG21	1.93	0.50
1:A:2704:SER:O	1:A:2707:LYS:HB2	2.10	0.50
1:B:371:ASP:OD2	1:B:389:ARG:NH1	2.36	0.50
1:B:808:SER:OG	1:B:1104:VAL:CG1	2.59	0.50
1:B:1870:GLU:HB3	1:B:1963:ILE:HD11	1.93	0.50
1:C:808:SER:OG	1:C:1104:VAL:CG1	2.59	0.50
1:C:1507:PRO:HA	1:C:1510:VAL:HG22	1.92	0.50
1:D:1270:ALA:O	1:D:1274:GLN:HG3	2.10	0.50
1:A:91:LYS:HB3	1:C:2020:LEU:HD21	1.94	0.50
1:A:1461:ALA:O	1:A:1465:THR:HG23	2.11	0.50
1:B:375:LEU:HD13	1:D:7:SER:HA	1.92	0.50
1:B:606:LEU:HD12	1:B:610:ILE:HG13	1.92	0.50
1:B:1461:ALA:O	1:B:1465:THR:HG23	2.11	0.50
1:C:1461:ALA:O	1:C:1465:THR:HG23	2.11	0.50
1:C:2547:GLY:O	1:D:2544:ARG:NH1	2.40	0.50
1:B:765:LEU:O	1:B:768:MET:HB2	2.11	0.50
1:B:1852:LYS:NZ	1:B:1855:LYS:HE2	2.27	0.50
1:C:7:SER:HA	1:D:375:LEU:HD13	1.93	0.50
1:A:764:ILE:O	1:A:768:MET:HG2	2.11	0.50
1:A:1270:ALA:O	1:A:1274:GLN:HG3	2.10	0.50
1:B:764:ILE:O	1:B:768:MET:HG2	2.11	0.50
1:C:1100:VAL:O	1:C:1101:GLN:NE2	2.45	0.50
1:D:1461:ALA:O	1:D:1465:THR:HG23	2.11	0.50
1:A:606:LEU:HD12	1:A:610:ILE:HG13	1.92	0.50
1:A:765:LEU:HD21	1:A:835:GLN:HG3	1.92	0.50
1:A:1293:GLN:O	1:A:1297:HIS:ND1	2.31	0.50
1:A:2063:ILE:HD11	1:A:2112:ILE:HG12	1.92	0.50
1:A:2130:MET:O	1:A:2133:GLU:HG3	2.12	0.50
1:B:2437:ASN:HB2	1:B:2592:THR:HG21	1.93	0.50
1:C:1852:LYS:NZ	1:C:1855:LYS:HE2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1202:GLN:HE22	1:A:1244:PHE:HA	1.75	0.50
1:A:2227:ILE:HG13	1:A:2250:LEU:HD11	1.92	0.50
1:A:2437:ASN:HB2	1:A:2592:THR:HG21	1.93	0.50
1:B:1114:GLN:OE1	1:B:1182:ARG:NH1	2.45	0.50
1:B:1544:ALA:HA	1:B:1549:ILE:HD12	1.93	0.50
1:B:2063:ILE:HD11	1:B:2112:ILE:HG12	1.92	0.50
1:C:2130:MET:O	1:C:2133:GLU:HG3	2.12	0.50
1:D:1507:PRO:HA	1:D:1510:VAL:HG22	1.92	0.50
1:D:1852:LYS:NZ	1:D:1855:LYS:HE2	2.27	0.50
1:A:765:LEU:O	1:A:768:MET:HB2	2.11	0.50
1:A:768:MET:HE3	1:A:782:CYS:HA	1.94	0.50
1:A:993:LEU:HD12	1:A:1097:PHE:HZ	1.77	0.50
1:A:996:ILE:HG12	1:A:999:ARG:HH21	1.77	0.50
1:C:578:PHE:HE1	1:C:582:GLN:HE21	1.58	0.50
1:C:2358:GLY:HA3	1:C:2406:LEU:HD13	1.94	0.50
1:D:578:PHE:HE1	1:D:582:GLN:HE21	1.58	0.50
1:D:1870:GLU:HB3	1:D:1963:ILE:HD11	1.93	0.50
1:D:2411:PHE:HB3	4:D:5108:PLX:H262	1.94	0.50
1:A:808:SER:OG	1:A:1104:VAL:CG1	2.59	0.50
1:B:993:LEU:HD12	1:B:1097:PHE:HZ	1.77	0.50
1:B:996:ILE:HG12	1:B:999:ARG:HH21	1.77	0.50
1:B:1100:VAL:O	1:B:1101:GLN:NE2	2.45	0.50
1:B:2448:ALA:HB2	1:B:2581:VAL:HG11	1.93	0.50
1:C:524:GLN:O	1:C:528:THR:OG1	2.30	0.50
1:D:1544:ALA:HA	1:D:1549:ILE:HD12	1.93	0.50
1:D:2358:GLY:HA3	1:D:2406:LEU:HD13	1.94	0.50
1:A:1100:VAL:O	1:A:1101:GLN:NE2	2.45	0.49
1:A:1870:GLU:HB3	1:A:1963:ILE:HD11	1.93	0.49
1:B:524:GLN:O	1:B:528:THR:OG1	2.30	0.49
1:C:804:ALA:HB1	1:C:1102:LEU:HD23	1.93	0.49
1:C:996:ILE:HG12	1:C:999:ARG:HH21	1.77	0.49
1:C:2704:SER:O	1:C:2707:LYS:HB2	2.10	0.49
1:A:1101:GLN:CG	1:A:1208:MET:HE3	2.38	0.49
1:A:1879:THR:OG1	1:B:75:ALA:HB3	2.12	0.49
1:D:996:ILE:HG12	1:D:999:ARG:HH21	1.77	0.49
1:D:2654:THR:OG1	1:D:2655:GLU:OE1	2.29	0.49
1:A:373:THR:HG23	1:A:374:THR:HG23	1.93	0.49
1:A:804:ALA:HB1	1:A:1102:LEU:HD23	1.93	0.49
1:A:1114:GLN:OE1	1:A:1182:ARG:NH1	2.45	0.49
1:B:2358:GLY:HA3	1:B:2406:LEU:HD13	1.94	0.49
1:C:765:LEU:HD13	1:C:836:THR:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2544:ARG:NH1	1:D:2547:GLY:O	2.39	0.49
1:B:2654:THR:OG1	1:B:2655:GLU:OE1	2.29	0.49
1:C:1114:GLN:OE1	1:C:1182:ARG:NH1	2.45	0.49
1:C:2342:LEU:HA	1:C:2345:ILE:HG22	1.94	0.49
1:D:524:GLN:O	1:D:528:THR:OG1	2.30	0.49
1:D:764:ILE:O	1:D:768:MET:HG2	2.11	0.49
1:D:1114:GLN:OE1	1:D:1182:ARG:NH1	2.45	0.49
1:D:2130:MET:O	1:D:2133:GLU:HG3	2.12	0.49
1:D:2342:LEU:HA	1:D:2345:ILE:HG22	1.94	0.49
1:A:2448:ALA:HB2	1:A:2581:VAL:HG11	1.93	0.49
1:B:373:THR:HG23	1:B:374:THR:HG23	1.93	0.49
1:D:804:ALA:HB1	1:D:1102:LEU:HD23	1.93	0.49
1:A:1852:LYS:NZ	1:A:1855:LYS:HE2	2.27	0.49
1:A:2358:GLY:HA3	1:A:2406:LEU:HD13	1.94	0.49
1:C:993:LEU:HD12	1:C:1097:PHE:HZ	1.77	0.49
1:C:1544:ALA:HA	1:C:1549:ILE:HD12	1.93	0.49
1:D:993:LEU:HD12	1:D:1097:PHE:HZ	1.77	0.49
1:A:2654:THR:OG1	1:A:2655:GLU:OE1	2.29	0.49
1:B:804:ALA:HB1	1:B:1102:LEU:HD23	1.93	0.49
1:B:2130:MET:O	1:B:2133:GLU:HG3	2.12	0.49
1:C:1323:ILE:HG22	1:C:1326:CYS:H	1.78	0.49
1:D:897:CYS:O	1:D:901:THR:HG23	2.13	0.49
1:A:765:LEU:HD13	1:A:836:THR:HG22	1.94	0.49
1:A:2627:THR:OG1	1:A:2630:GLU:OE1	2.28	0.49
1:C:1870:GLU:HB3	1:C:1963:ILE:HD11	1.93	0.49
1:D:1100:VAL:O	1:D:1101:GLN:NE2	2.45	0.49
1:D:1106:SER:N	1:D:1108:ASP:OD2	2.45	0.49
1:A:2251:PHE:HA	1:A:2254:MET:HE2	1.95	0.49
1:C:897:CYS:O	1:C:901:THR:HG23	2.13	0.49
1:C:1101:GLN:CG	1:C:1208:MET:HE3	2.38	0.49
1:A:138:LEU:HD23	1:A:148:ARG:HH11	1.78	0.49
1:C:899:HIS:O	1:C:902:THR:OG1	2.27	0.49
1:D:808:SER:CB	1:D:1104:VAL:HG12	2.43	0.49
1:D:1103:LEU:HD22	1:D:1104:VAL:H	1.78	0.49
1:A:1323:ILE:HG22	1:A:1326:CYS:H	1.78	0.48
1:A:2588:VAL:HA	1:C:2593:PHE:CE2	2.48	0.48
1:C:138:LEU:HD23	1:C:148:ARG:HH11	1.79	0.48
1:D:1323:ILE:HG22	1:D:1326:CYS:H	1.78	0.48
1:B:55:ASP:O	1:B:125:HIS:NE2	2.40	0.48
1:C:91:LYS:HB3	1:D:2020:LEU:HD21	1.95	0.48
1:C:2023:LEU:H	1:C:2023:LEU:HD23	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:966:MET:O	1:A:970:THR:HG23	2.13	0.48
1:A:1340:ASP:OD1	1:A:1341:VAL:N	2.47	0.48
1:B:1335:VAL:HG21	1:B:1396:LYS:HE3	1.95	0.48
1:B:2020:LEU:HD21	1:D:91:LYS:HB3	1.94	0.48
1:D:765:LEU:HD13	1:D:836:THR:HG22	1.94	0.48
1:D:966:MET:O	1:D:970:THR:HG23	2.13	0.48
1:D:1335:VAL:HG21	1:D:1396:LYS:HE3	1.95	0.48
1:D:1683:MET:HE2	1:D:1799:LEU:HD22	1.94	0.48
1:A:897:CYS:O	1:A:901:THR:HG23	2.13	0.48
1:A:2702:LEU:HD23	1:B:2703:GLU:OE1	2.14	0.48
1:B:897:CYS:O	1:B:901:THR:HG23	2.13	0.48
1:C:1852:LYS:HZ1	1:C:1855:LYS:HE2	1.77	0.48
1:B:765:LEU:HD13	1:B:836:THR:HG22	1.94	0.48
1:C:1103:LEU:HD22	1:C:1104:VAL:H	1.78	0.48
1:B:138:LEU:HD23	1:B:148:ARG:HH11	1.78	0.48
1:B:808:SER:CB	1:B:1104:VAL:HG12	2.43	0.48
1:B:2342:LEU:HA	1:B:2345:ILE:HG22	1.94	0.48
1:D:9:LEU:HD11	1:D:220:ILE:HD13	1.96	0.48
1:D:2183:ASP:O	1:D:2186:LEU:N	2.47	0.48
1:D:2728:LYS:O	1:D:2731:GLN:HG3	2.14	0.48
1:B:2392:PHE:O	1:B:2396:LEU:HD23	2.14	0.48
1:D:2392:PHE:O	1:D:2396:LEU:HD23	2.14	0.48
1:A:653:CYS:O	1:A:657:LEU:HD23	2.14	0.48
1:A:988:TYR:HE2	1:A:1050:LEU:HD11	1.79	0.48
1:A:1106:SER:N	1:A:1108:ASP:OD2	2.45	0.48
1:A:2023:LEU:H	1:A:2023:LEU:HD23	1.79	0.48
1:A:2363:CYS:O	1:A:2366:ILE:HG22	2.14	0.48
1:B:1101:GLN:CG	1:B:1208:MET:HE3	2.38	0.48
1:B:1103:LEU:HD22	1:B:1104:VAL:H	1.78	0.48
1:B:1290:ARG:O	1:B:1293:GLN:HG3	2.14	0.48
1:B:1323:ILE:HG22	1:B:1326:CYS:H	1.78	0.48
1:B:2023:LEU:HD23	1:B:2023:LEU:H	1.78	0.48
1:C:9:LEU:HD11	1:C:220:ILE:HD13	1.96	0.48
1:C:808:SER:CB	1:C:1104:VAL:HG12	2.43	0.48
1:C:2662:TYR:O	1:C:2666:MET:HG2	2.14	0.48
1:C:2728:LYS:O	1:C:2731:GLN:HG3	2.14	0.48
1:A:494:VAL:HG13	1:A:495:LEU:HD22	1.96	0.48
1:A:808:SER:CB	1:A:1104:VAL:HG12	2.44	0.48
1:A:2662:TYR:O	1:A:2666:MET:HG2	2.14	0.48
1:A:2706:MET:N	1:A:2706:MET:HE2	2.29	0.48
1:B:494:VAL:HG13	1:B:495:LEU:HD22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:988:TYR:HE2	1:B:1050:LEU:HD11	1.79	0.48
1:B:1340:ASP:OD1	1:B:1341:VAL:N	2.47	0.48
1:D:653:CYS:O	1:D:657:LEU:HD23	2.14	0.48
1:A:9:LEU:HD11	1:A:220:ILE:HD13	1.96	0.48
1:A:1683:MET:HE2	1:A:1799:LEU:HD22	1.95	0.48
1:A:2034:ASN:O	1:A:2038:GLU:HG3	2.14	0.48
1:A:2342:LEU:HA	1:A:2345:ILE:HG22	1.94	0.48
1:B:2728:LYS:O	1:B:2731:GLN:HG3	2.14	0.48
1:B:9:LEU:HD11	1:B:220:ILE:HD13	1.96	0.47
1:B:2154:HIS:O	1:B:2158:ILE:HG12	2.14	0.47
1:B:2662:TYR:O	1:B:2666:MET:HG2	2.14	0.47
1:D:899:HIS:O	1:D:902:THR:OG1	2.27	0.47
1:D:988:TYR:HE2	1:D:1050:LEU:HD11	1.79	0.47
1:D:2627:THR:OG1	1:D:2630:GLU:OE1	2.29	0.47
1:D:2662:TYR:O	1:D:2666:MET:HG2	2.14	0.47
1:A:1058:ARG:NH2	1:A:1636:LEU:O	2.37	0.47
1:A:1728:GLU:O	1:A:1731:LYS:HG3	2.15	0.47
1:A:2183:ASP:O	1:A:2186:LEU:N	2.47	0.47
1:C:966:MET:O	1:C:970:THR:HG23	2.13	0.47
1:C:988:TYR:HE2	1:C:1050:LEU:HD11	1.79	0.47
1:C:1340:ASP:OD1	1:C:1341:VAL:N	2.47	0.47
1:C:2392:PHE:O	1:C:2396:LEU:HD23	2.14	0.47
1:D:138:LEU:HD23	1:D:148:ARG:HH11	1.78	0.47
1:D:1107:GLN:O	1:D:1110:ASP:N	2.47	0.47
1:A:1103:LEU:HD22	1:A:1104:VAL:H	1.78	0.47
1:A:2728:LYS:O	1:A:2731:GLN:HG3	2.14	0.47
1:B:138:LEU:HB3	1:B:148:ARG:HH11	1.80	0.47
1:B:653:CYS:O	1:B:657:LEU:HD23	2.14	0.47
1:B:1103:LEU:HD23	1:B:1103:LEU:HA	1.73	0.47
1:B:1728:GLU:O	1:B:1731:LYS:HG3	2.15	0.47
1:D:127:LYS:NZ	1:D:444:ASP:OD2	2.28	0.47
1:D:1102:LEU:HD12	1:D:1102:LEU:HA	1.79	0.47
1:A:556:CYS:O	1:A:559:VAL:HG22	2.15	0.47
1:A:1290:ARG:O	1:A:1293:GLN:HG3	2.14	0.47
1:A:1335:VAL:HG21	1:A:1396:LYS:HE3	1.95	0.47
1:B:966:MET:O	1:B:970:THR:HG23	2.13	0.47
1:B:2183:ASP:O	1:B:2186:LEU:N	2.47	0.47
1:C:138:LEU:HB3	1:C:148:ARG:HH11	1.80	0.47
1:C:1290:ARG:O	1:C:1293:GLN:HG3	2.14	0.47
1:C:2063:ILE:HA	1:C:2066:ILE:HD12	1.96	0.47
1:D:138:LEU:HB3	1:D:148:ARG:HH11	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:666:ILE:HG22	1:D:701:ARG:O	2.14	0.47
1:D:1290:ARG:O	1:D:1293:GLN:HG3	2.14	0.47
1:D:2154:HIS:O	1:D:2158:ILE:HG12	2.14	0.47
1:D:2438:GLY:HA3	4:D:5109:PLX:H32	1.96	0.47
1:A:7:SER:HA	1:C:375:LEU:HD13	1.97	0.47
1:A:162:TYR:CE1	1:A:187:VAL:HG22	2.50	0.47
1:A:1103:LEU:HD23	1:A:1103:LEU:HA	1.73	0.47
1:A:2063:ILE:HA	1:A:2066:ILE:HD12	1.96	0.47
1:A:2392:PHE:O	1:A:2396:LEU:HD23	2.14	0.47
1:B:1594:SER:O	1:B:1598:ARG:HG2	2.15	0.47
1:B:2200:ARG:NE	1:B:2206:GLU:OE2	2.28	0.47
4:B:5111:PLX:H251	4:B:5111:PLX:H51	1.64	0.47
1:D:978:LEU:O	1:D:981:ILE:HG12	2.14	0.47
1:A:2154:HIS:O	1:A:2158:ILE:HG12	2.14	0.47
1:B:666:ILE:HG22	1:B:701:ARG:O	2.14	0.47
1:B:1408:ARG:HH12	1:D:545:ARG:HD2	1.80	0.47
1:B:1685:LYS:HG3	1:B:1686:ASP:H	1.80	0.47
1:B:1806:ASN:HA	1:B:1809:ILE:HG22	1.97	0.47
1:C:666:ILE:HG22	1:C:701:ARG:O	2.14	0.47
1:C:2306:GLU:CG	1:C:2307:PRO:HD3	2.43	0.47
1:A:804:ALA:HA	1:A:1101:GLN:O	2.15	0.47
1:A:1594:SER:O	1:A:1598:ARG:HG2	2.15	0.47
1:A:1685:LYS:HG3	1:A:1686:ASP:H	1.80	0.47
1:A:1806:ASN:HA	1:A:1809:ILE:HG22	1.97	0.47
1:A:1852:LYS:HZ1	1:A:1855:LYS:HE2	1.78	0.47
1:A:2629:GLU:O	1:A:2633:LYS:NZ	2.40	0.47
1:B:556:CYS:O	1:B:559:VAL:HG22	2.15	0.47
1:B:978:LEU:O	1:B:981:ILE:HG12	2.14	0.47
1:B:2034:ASN:O	1:B:2038:GLU:HG3	2.14	0.47
1:B:2063:ILE:HA	1:B:2066:ILE:HD12	1.96	0.47
1:B:2363:CYS:O	1:B:2366:ILE:HG22	2.14	0.47
1:C:494:VAL:HG13	1:C:495:LEU:HD22	1.96	0.47
1:C:804:ALA:HA	1:C:1101:GLN:O	2.15	0.47
1:C:1107:GLN:O	1:C:1110:ASP:N	2.47	0.47
1:C:2034:ASN:O	1:C:2038:GLU:HG3	2.14	0.47
1:C:2627:THR:OG1	1:C:2630:GLU:OE1	2.28	0.47
1:D:641:MET:O	1:D:641:MET:HG2	2.15	0.47
1:D:804:ALA:HA	1:D:1101:GLN:O	2.15	0.47
4:D:5110:PLX:H251	4:D:5110:PLX:H51	1.63	0.47
1:A:978:LEU:O	1:A:981:ILE:HG12	2.14	0.47
1:B:162:TYR:CE1	1:B:187:VAL:HG22	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2629:GLU:O	1:B:2633:LYS:NZ	2.40	0.47
1:C:127:LYS:NZ	1:C:444:ASP:OD2	2.28	0.47
1:C:2183:ASP:O	1:C:2186:LEU:N	2.47	0.47
1:D:494:VAL:HG13	1:D:495:LEU:HD22	1.96	0.47
1:D:1594:SER:O	1:D:1598:ARG:HG2	2.15	0.47
1:D:2023:LEU:HD23	1:D:2023:LEU:H	1.78	0.47
1:D:2034:ASN:O	1:D:2038:GLU:HG3	2.14	0.47
1:A:666:ILE:HG22	1:A:701:ARG:O	2.14	0.47
1:C:2363:CYS:O	1:C:2366:ILE:HG22	2.14	0.47
1:A:1798:HIS:HA	1:A:1801:LYS:HZ1	1.77	0.47
1:A:1884:ASN:OD1	1:B:78:PRO:HA	2.15	0.47
1:B:807:TRP:CZ3	1:B:1102:LEU:N	2.81	0.47
1:C:978:LEU:O	1:C:981:ILE:HG12	2.14	0.47
1:C:1335:VAL:HG21	1:C:1396:LYS:HE3	1.95	0.47
1:C:2154:HIS:O	1:C:2158:ILE:HG12	2.14	0.47
1:C:2558:LYS:HE3	1:D:2533:MET:HG2	1.97	0.47
1:D:162:TYR:CE1	1:D:187:VAL:HG22	2.50	0.47
1:D:2063:ILE:HA	1:D:2066:ILE:HD12	1.96	0.47
1:D:2363:CYS:O	1:D:2366:ILE:HG22	2.14	0.47
1:A:375:LEU:HD13	1:B:7:SER:HA	1.97	0.46
1:A:641:MET:O	1:A:641:MET:HG2	2.15	0.46
1:A:2030:VAL:HG21	1:A:2084:LEU:HD13	1.97	0.46
1:B:1106:SER:N	1:B:1108:ASP:OD2	2.45	0.46
1:B:1245:CYS:SG	1:B:1255:LEU:HD12	2.56	0.46
1:B:2702:LEU:HD23	1:D:2703:GLU:OE1	2.15	0.46
1:C:653:CYS:O	1:C:657:LEU:HD23	2.14	0.46
1:C:1358:MET:SD	1:C:1362:ARG:NE	2.89	0.46
1:C:1685:LYS:HG3	1:C:1686:ASP:H	1.80	0.46
1:C:1728:GLU:O	1:C:1731:LYS:HG3	2.15	0.46
4:C:5111:PLX:H282	4:C:5111:PLX:H252	1.72	0.46
1:D:85:ASP:O	1:D:88:LEU:HD23	2.16	0.46
1:D:1685:LYS:HG3	1:D:1686:ASP:H	1.80	0.46
4:A:5109:PLX:H281	4:A:5109:PLX:H311	1.68	0.46
1:B:2152:VAL:O	1:B:2156:ILE:HG12	2.16	0.46
1:D:1277:PHE:CE1	1:D:1287:ILE:HD11	2.51	0.46
1:D:1728:GLU:O	1:D:1731:LYS:HG3	2.15	0.46
1:D:1806:ASN:HA	1:D:1809:ILE:HG22	1.97	0.46
1:D:2030:VAL:HG21	1:D:2084:LEU:HD13	1.97	0.46
1:A:1107:GLN:O	1:A:1110:ASP:N	2.47	0.46
1:B:1107:GLN:O	1:B:1110:ASP:N	2.47	0.46
1:C:2703:GLU:OE1	1:D:2702:LEU:HD23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1245:CYS:SG	1:A:1255:LEU:HD12	2.56	0.46
1:B:1358:MET:SD	1:B:1362:ARG:NE	2.89	0.46
1:B:2627:THR:OG1	1:B:2630:GLU:OE1	2.29	0.46
1:C:627:GLU:HG3	1:C:628:PRO:HD2	1.98	0.46
1:C:641:MET:O	1:C:641:MET:HG2	2.15	0.46
1:C:1447:MET:HA	1:C:1450:LEU:HD12	1.97	0.46
1:D:556:CYS:O	1:D:559:VAL:HG22	2.15	0.46
1:D:1058:ARG:NH2	1:D:1636:LEU:O	2.37	0.46
1:A:45:ASP:OD1	1:A:45:ASP:N	2.49	0.46
1:A:627:GLU:HG3	1:A:628:PRO:HD2	1.98	0.46
1:A:1447:MET:HA	1:A:1450:LEU:HD12	1.97	0.46
1:A:2152:VAL:O	1:A:2156:ILE:HG12	2.16	0.46
1:B:85:ASP:O	1:B:88:LEU:HD23	2.16	0.46
1:C:162:TYR:CE1	1:C:187:VAL:HG22	2.50	0.46
1:C:545:ARG:HD2	1:D:1408:ARG:HH12	1.80	0.46
1:C:808:SER:HB2	1:C:1104:VAL:HG12	1.97	0.46
1:C:2702:LEU:O	1:C:2706:MET:HG2	2.16	0.46
1:C:1097:PHE:O	1:C:1099:GLN:N	2.49	0.46
1:C:1277:PHE:CE1	1:C:1287:ILE:HD11	2.51	0.46
1:C:2251:PHE:HA	1:C:2254:MET:HE2	1.98	0.46
1:B:641:MET:O	1:B:641:MET:HG2	2.15	0.46
1:B:808:SER:HB2	1:B:1104:VAL:HG12	1.97	0.46
1:D:1245:CYS:SG	1:D:1255:LEU:HD12	2.56	0.46
1:D:1358:MET:SD	1:D:1362:ARG:NE	2.89	0.46
1:A:138:LEU:HB3	1:A:148:ARG:HH11	1.79	0.46
1:A:806:LEU:HD11	1:A:1104:VAL:CB	2.46	0.46
1:B:627:GLU:HG3	1:B:628:PRO:HD2	1.98	0.46
1:B:804:ALA:HA	1:B:1101:GLN:O	2.15	0.46
1:C:1468:ARG:HH21	1:C:1524:TRP:HB3	1.81	0.46
1:C:1806:ASN:HA	1:C:1809:ILE:HG22	1.97	0.46
1:D:810:ILE:N	1:D:811:PRO:HD2	2.31	0.46
1:D:1340:ASP:OD1	1:D:1341:VAL:N	2.47	0.46
1:A:78:PRO:HA	1:C:1884:ASN:OD1	2.16	0.46
1:A:545:ARG:HD2	1:C:1408:ARG:HH12	1.81	0.46
1:B:647:VAL:O	1:B:651:LEU:HD23	2.16	0.46
1:B:1058:ARG:NH2	1:B:1636:LEU:O	2.37	0.46
1:C:85:ASP:O	1:C:88:LEU:HD23	2.16	0.46
1:C:807:TRP:CZ3	1:C:1102:LEU:N	2.81	0.46
1:C:810:ILE:N	1:C:811:PRO:HD2	2.31	0.46
1:C:2654:THR:OG1	1:C:2655:GLU:OE1	2.29	0.46
1:D:1468:ARG:HH21	1:D:1524:TRP:HB3	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1097:PHE:O	1:A:1099:GLN:N	2.49	0.46
1:A:1468:ARG:HH21	1:A:1524:TRP:HB3	1.81	0.46
1:C:837:MET:HG2	1:C:873:LEU:HD13	1.98	0.46
1:C:1594:SER:O	1:C:1598:ARG:HG2	2.15	0.46
1:D:627:GLU:HG3	1:D:628:PRO:HD2	1.98	0.46
1:D:671:VAL:HB	1:D:699:PHE:HE2	1.81	0.46
1:D:2702:LEU:O	1:D:2706:MET:HG2	2.16	0.46
1:A:673:SER:HB3	1:A:695:GLU:H	1.81	0.45
1:A:1405:ASP:O	1:A:1408:ARG:HG2	2.16	0.45
1:A:2702:LEU:O	1:A:2706:MET:HG2	2.16	0.45
1:B:1283:LEU:O	1:B:1287:ILE:HG13	2.16	0.45
1:B:1468:ARG:HH21	1:B:1524:TRP:HB3	1.81	0.45
1:C:45:ASP:OD1	1:C:45:ASP:N	2.49	0.45
1:C:1245:CYS:SG	1:C:1255:LEU:HD12	2.56	0.45
1:D:2712:LEU:O	1:D:2716:LEU:HG	2.16	0.45
1:A:257:ARG:O	1:A:259:LYS:NZ	2.41	0.45
1:A:602:ASN:ND2	1:A:605:LEU:HB2	2.32	0.45
1:A:1283:LEU:O	1:A:1287:ILE:HG13	2.16	0.45
1:A:2712:LEU:O	1:A:2716:LEU:HG	2.16	0.45
1:B:837:MET:HG2	1:B:873:LEU:HD13	1.98	0.45
1:B:1407:VAL:HA	1:B:1410:VAL:HG22	1.99	0.45
1:C:1097:PHE:C	1:C:1099:GLN:N	2.70	0.45
1:C:1100:VAL:O	1:C:1101:GLN:CB	2.63	0.45
1:C:2030:VAL:HG21	1:C:2084:LEU:HD13	1.97	0.45
1:D:45:ASP:N	1:D:45:ASP:OD1	2.49	0.45
1:D:647:VAL:O	1:D:651:LEU:HD23	2.16	0.45
1:D:806:LEU:HD11	1:D:1104:VAL:CB	2.46	0.45
1:D:1097:PHE:O	1:D:1099:GLN:N	2.49	0.45
1:D:1405:ASP:O	1:D:1408:ARG:HG2	2.16	0.45
1:D:2698:LEU:HD12	1:D:2701:LYS:HE3	1.98	0.45
1:A:85:ASP:O	1:A:88:LEU:HD23	2.15	0.45
1:A:88:LEU:O	1:A:92:LEU:HG	2.17	0.45
1:A:2426:THR:HG21	1:B:2440:PRO:HD3	1.97	0.45
1:B:1097:PHE:O	1:B:1099:GLN:N	2.49	0.45
1:B:1405:ASP:O	1:B:1408:ARG:HG2	2.16	0.45
1:C:1405:ASP:O	1:C:1408:ARG:HG2	2.16	0.45
1:C:2712:LEU:O	1:C:2716:LEU:HG	2.16	0.45
1:D:19:ALA:HB2	1:D:218:TRP:CZ3	2.52	0.45
1:D:2629:GLU:O	1:D:2633:LYS:NZ	2.40	0.45
4:D:5110:PLX:H31	4:D:5110:PLX:H6	1.62	0.45
1:A:19:ALA:HB2	1:A:218:TRP:CZ3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:807:TRP:CZ3	1:A:1102:LEU:N	2.81	0.45
1:A:1885:LYS:H	1:B:85:ASP:CG	2.20	0.45
1:B:2306:GLU:CG	1:B:2307:PRO:HD3	2.43	0.45
1:B:2533:MET:HG2	1:D:2558:LYS:HE3	1.97	0.45
1:C:2152:VAL:O	1:C:2156:ILE:HG12	2.16	0.45
1:C:2698:LEU:HD12	1:C:2701:LYS:HE3	1.98	0.45
1:D:658:ASN:HB2	1:D:659:PRO:HD3	1.99	0.45
1:A:524:GLN:O	1:A:528:THR:OG1	2.30	0.45
1:B:1312:LEU:HA	1:B:1315:ILE:HG22	1.98	0.45
1:B:1447:MET:HA	1:B:1450:LEU:HD12	1.98	0.45
1:C:673:SER:HB3	1:C:695:GLU:H	1.81	0.45
1:D:88:LEU:O	1:D:92:LEU:HG	2.17	0.45
1:A:1277:PHE:CE1	1:A:1287:ILE:HD11	2.51	0.45
1:B:88:LEU:O	1:B:92:LEU:HG	2.17	0.45
1:C:85:ASP:CG	1:D:1885:LYS:H	2.19	0.45
1:C:671:VAL:HB	1:C:699:PHE:HE2	1.81	0.45
1:C:1106:SER:N	1:C:1108:ASP:OD2	2.45	0.45
1:D:1097:PHE:C	1:D:1099:GLN:N	2.70	0.45
1:D:1101:GLN:CG	1:D:1208:MET:HE3	2.38	0.45
1:A:808:SER:HB2	1:A:1104:VAL:HG12	1.98	0.45
1:A:2565:ALA:HB2	4:A:5108:PLX:H292	1.99	0.45
1:B:1277:PHE:CE1	1:B:1287:ILE:HD11	2.51	0.45
1:B:1885:LYS:H	1:D:85:ASP:CG	2.20	0.45
1:B:2030:VAL:HG21	1:B:2084:LEU:HD13	1.97	0.45
1:B:2709:VAL:HA	1:B:2712:LEU:HG	1.99	0.45
1:C:556:CYS:O	1:C:559:VAL:HG22	2.15	0.45
1:C:2557:SER:OG	1:C:2559:GLU:OE1	2.34	0.45
1:D:1447:MET:HA	1:D:1450:LEU:HD12	1.97	0.45
1:D:2152:VAL:O	1:D:2156:ILE:HG12	2.16	0.45
1:D:2276:TRP:HB2	1:D:2368:PHE:HD1	1.82	0.45
1:D:2709:VAL:HA	1:D:2712:LEU:HG	1.99	0.45
1:A:837:MET:HG2	1:A:873:LEU:HD13	1.98	0.45
1:A:2200:ARG:NE	1:A:2206:GLU:OE2	2.28	0.45
1:B:810:ILE:N	1:B:811:PRO:HD2	2.31	0.45
1:B:899:HIS:O	1:B:902:THR:OG1	2.27	0.45
1:B:1004:SER:HA	1:B:1007:GLN:HB2	1.99	0.45
1:B:2702:LEU:O	1:B:2706:MET:HG2	2.16	0.45
1:C:647:VAL:O	1:C:651:LEU:HD23	2.16	0.45
1:D:1798:HIS:HA	1:D:1801:LYS:HZ1	1.82	0.45
1:A:1407:VAL:HA	1:A:1410:VAL:HG22	1.98	0.45
1:B:673:SER:HB3	1:B:695:GLU:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:806:LEU:HD11	1:B:1104:VAL:CB	2.46	0.45
1:C:1283:LEU:O	1:C:1287:ILE:HG13	2.16	0.45
1:C:2276:TRP:HB2	1:C:2368:PHE:HD1	1.82	0.45
1:C:2715:GLN:O	1:C:2718:GLU:HG3	2.17	0.45
4:C:5110:PLX:H21	4:C:5110:PLX:H1B2	1.79	0.45
1:D:602:ASN:ND2	1:D:605:LEU:HB2	2.31	0.45
1:D:673:SER:HB3	1:D:695:GLU:H	1.81	0.45
1:D:1732:ARG:HH22	1:D:1736:LEU:HD13	1.82	0.45
1:A:13:ASP:OD1	1:A:226:TRP:N	2.50	0.45
1:A:557:TYR:OH	1:A:584:GLN:OE1	2.25	0.45
1:A:810:ILE:N	1:A:811:PRO:HD2	2.31	0.45
1:A:2411:PHE:HB3	4:A:5111:PLX:H262	1.99	0.45
1:B:19:ALA:HB2	1:B:218:TRP:CZ3	2.52	0.45
1:B:45:ASP:N	1:B:45:ASP:OD1	2.49	0.45
1:B:602:ASN:ND2	1:B:605:LEU:HB2	2.31	0.45
1:B:658:ASN:HB2	1:B:659:PRO:HD3	1.99	0.45
1:B:671:VAL:HB	1:B:699:PHE:HE2	1.81	0.45
1:C:13:ASP:OD1	1:C:226:TRP:N	2.50	0.45
1:C:2588:VAL:O	1:C:2592:THR:HG23	2.17	0.45
1:D:808:SER:HB2	1:D:1104:VAL:HG12	1.97	0.45
1:D:2306:GLU:CG	1:D:2307:PRO:HD3	2.43	0.45
1:A:2583:ASN:HB3	1:C:2586:PHE:CD2	2.52	0.44
1:A:2715:GLN:O	1:A:2718:GLU:HG3	2.17	0.44
1:B:1886:LYS:HG3	1:D:83:THR:O	2.17	0.44
1:B:2251:PHE:HA	1:B:2254:MET:HE2	1.99	0.44
1:C:88:LEU:O	1:C:92:LEU:HG	2.17	0.44
1:C:805:ARG:NH2	1:C:991:SER:OG	2.51	0.44
1:C:1106:SER:C	1:C:1108:ASP:N	2.71	0.44
1:D:837:MET:HG2	1:D:873:LEU:HD13	1.98	0.44
1:D:1312:LEU:HA	1:D:1315:ILE:HG22	1.98	0.44
1:A:85:ASP:CG	1:C:1885:LYS:H	2.19	0.44
1:A:92:LEU:HD21	1:C:1882:LEU:HD11	1.98	0.44
1:A:2276:TRP:HB2	1:A:2368:PHE:HD1	1.82	0.44
1:B:13:ASP:OD1	1:B:226:TRP:N	2.50	0.44
1:B:514:ASN:O	1:B:518:GLN:HG2	2.17	0.44
1:B:1097:PHE:C	1:B:1099:GLN:N	2.70	0.44
1:C:514:ASN:O	1:C:518:GLN:HG2	2.17	0.44
1:C:602:ASN:ND2	1:C:605:LEU:HB2	2.32	0.44
4:C:5108:PLX:H1A3	4:C:5108:PLX:H22	1.62	0.44
1:D:805:ARG:NH2	1:D:991:SER:OG	2.51	0.44
1:D:1004:SER:HA	1:D:1007:GLN:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1283:LEU:O	1:D:1287:ILE:HG13	2.16	0.44
1:D:1983:ASP:O	1:D:1987:PHE:HB2	2.17	0.44
1:A:671:VAL:HB	1:A:699:PHE:HE2	1.82	0.44
1:C:19:ALA:HB2	1:C:218:TRP:CZ3	2.52	0.44
1:C:257:ARG:O	1:C:259:LYS:NZ	2.41	0.44
1:D:2200:ARG:NE	1:D:2206:GLU:OE2	2.28	0.44
1:D:2715:GLN:O	1:D:2718:GLU:HG3	2.17	0.44
1:A:647:VAL:O	1:A:651:LEU:HD23	2.16	0.44
1:A:1732:ARG:HH22	1:A:1736:LEU:HD13	1.82	0.44
1:B:1732:ARG:HH22	1:B:1736:LEU:HD13	1.82	0.44
1:B:2588:VAL:O	1:B:2592:THR:HG23	2.17	0.44
1:B:2712:LEU:O	1:B:2716:LEU:HG	2.16	0.44
1:C:1312:LEU:HA	1:C:1315:ILE:HG22	1.98	0.44
1:D:807:TRP:CZ3	1:D:1102:LEU:N	2.81	0.44
1:D:1407:VAL:HA	1:D:1410:VAL:HG22	1.99	0.44
1:D:1621:ALA:O	1:D:1625:VAL:HG23	2.18	0.44
4:D:5108:PLX:H21	4:D:5108:PLX:H1B2	1.79	0.44
1:A:658:ASN:HB2	1:A:659:PRO:HD3	1.99	0.44
1:A:1004:SER:HA	1:A:1007:GLN:HB2	1.99	0.44
1:A:1312:LEU:HA	1:A:1315:ILE:HG22	1.98	0.44
1:A:1358:MET:SD	1:A:1362:ARG:NE	2.89	0.44
1:A:2433:SER:OG	1:A:2593:PHE:HB2	2.18	0.44
1:A:2458:VAL:HG21	4:A:5108:PLX:H151	1.99	0.44
1:A:2588:VAL:O	1:A:2592:THR:HG23	2.17	0.44
1:C:806:LEU:HD11	1:C:1104:VAL:CB	2.46	0.44
1:C:1407:VAL:HA	1:C:1410:VAL:HG22	1.98	0.44
1:C:1732:ARG:HH22	1:C:1736:LEU:HD13	1.82	0.44
1:C:1879:THR:HG22	1:C:1882:LEU:HD13	2.00	0.44
1:C:1983:ASP:O	1:C:1987:PHE:HB2	2.17	0.44
1:C:2440:PRO:HD3	1:D:2426:THR:HG21	1.99	0.44
1:D:2433:SER:OG	1:D:2593:PHE:HB2	2.18	0.44
1:A:83:THR:O	1:C:1886:LYS:HG3	2.17	0.44
1:A:805:ARG:NH2	1:A:991:SER:OG	2.51	0.44
1:A:1097:PHE:C	1:A:1099:GLN:N	2.70	0.44
1:A:1406:ILE:HA	1:A:1423:TYR:CE2	2.53	0.44
1:A:2698:LEU:HD12	1:A:2701:LYS:HE3	1.98	0.44
1:A:2709:VAL:HA	1:A:2712:LEU:HG	1.99	0.44
1:B:1621:ALA:O	1:B:1625:VAL:HG23	2.18	0.44
1:B:2426:THR:HG21	1:D:2440:PRO:HD3	1.99	0.44
1:B:2715:GLN:O	1:B:2718:GLU:HG3	2.17	0.44
1:C:1004:SER:HA	1:C:1007:GLN:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1376:ILE:O	1:C:1379:VAL:HG22	2.17	0.44
1:D:13:ASP:OD1	1:D:226:TRP:N	2.50	0.44
1:D:2251:PHE:HA	1:D:2254:MET:HE2	2.00	0.44
1:A:14:ILE:HG12	1:A:126:LEU:HD11	2.00	0.44
1:B:14:ILE:HG12	1:B:126:LEU:HD11	2.00	0.44
1:B:1102:LEU:HD12	1:B:1102:LEU:HA	1.79	0.44
1:B:1376:ILE:O	1:B:1379:VAL:HG22	2.17	0.44
1:B:1882:LEU:HD11	1:D:92:LEU:HD21	1.99	0.44
1:B:2698:LEU:HD12	1:B:2701:LYS:HE3	1.98	0.44
1:C:2709:VAL:HA	1:C:2712:LEU:HG	1.99	0.44
4:D:5107:PLX:H1B2	4:D:5107:PLX:H22	1.80	0.44
1:A:1105:THR:HG23	1:A:1108:ASP:HB2	2.00	0.44
1:B:2276:TRP:HB2	1:B:2368:PHE:HD1	1.82	0.44
1:C:2433:SER:OG	1:C:2593:PHE:HB2	2.18	0.44
1:D:514:ASN:O	1:D:518:GLN:HG2	2.17	0.44
1:D:1879:THR:HG22	1:D:1882:LEU:HD13	2.00	0.44
1:A:514:ASN:O	1:A:518:GLN:HG2	2.17	0.44
1:B:672:LEU:HD11	1:B:766:ARG:HH11	1.83	0.44
1:B:1983:ASP:O	1:B:1987:PHE:HB2	2.17	0.44
4:B:5112:PLX:H1C2	4:B:5112:PLX:H21	1.76	0.44
1:C:672:LEU:HD11	1:C:766:ARG:HH11	1.83	0.44
1:C:1107:GLN:H	1:C:1107:GLN:HG2	1.60	0.44
1:C:1683:MET:HE2	1:C:1799:LEU:HD22	1.99	0.44
1:D:1122:LEU:HD11	1:D:1217:LEU:HD12	2.00	0.44
1:D:2557:SER:OG	1:D:2559:GLU:OE1	2.34	0.44
1:D:2588:VAL:O	1:D:2592:THR:HG23	2.17	0.44
1:A:2306:GLU:CG	1:A:2307:PRO:HD3	2.43	0.43
4:A:5114:PLX:H1C2	4:A:5114:PLX:H21	1.76	0.43
1:B:1372:PHE:CZ	1:B:1419:VAL:HG22	2.53	0.43
1:B:1884:ASN:OD1	1:D:78:PRO:HA	2.17	0.43
1:B:2433:SER:OG	1:B:2593:PHE:HB2	2.18	0.43
1:D:1106:SER:C	1:D:1108:ASP:N	2.71	0.43
1:D:1376:ILE:O	1:D:1379:VAL:HG22	2.17	0.43
1:D:2083:ASP:N	1:D:2083:ASP:OD1	2.51	0.43
4:D:5111:PLX:H1C2	4:D:5111:PLX:H21	1.76	0.43
1:A:701:ARG:HG2	1:A:705:LYS:HA	2.00	0.43
1:A:1107:GLN:O	1:A:1110:ASP:OD1	2.37	0.43
1:A:1879:THR:HG22	1:A:1882:LEU:HD13	2.00	0.43
1:A:1983:ASP:O	1:A:1987:PHE:HB2	2.17	0.43
1:B:1829:ILE:HD11	1:B:1968:PRO:O	2.18	0.43
4:B:5109:PLX:H292	4:B:5109:PLX:H322	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1105:THR:HG23	1:C:1108:ASP:HB2	2.00	0.43
1:C:1372:PHE:CZ	1:C:1419:VAL:HG22	2.53	0.43
1:D:1364:ARG:HH21	1:D:1366:ASP:HB2	1.82	0.43
1:A:765:LEU:HD21	1:A:835:GLN:CG	2.49	0.43
1:A:1372:PHE:CZ	1:A:1419:VAL:HG22	2.53	0.43
1:A:2083:ASP:OD1	1:A:2083:ASP:N	2.51	0.43
1:B:2652:ASP:OD1	1:B:2652:ASP:N	2.51	0.43
1:C:83:THR:O	1:D:1886:LYS:HG3	2.17	0.43
1:C:1107:GLN:O	1:C:1110:ASP:OD1	2.37	0.43
1:D:1100:VAL:O	1:D:1101:GLN:CB	2.63	0.43
1:D:1462:CYS:O	1:D:1465:THR:OG1	2.29	0.43
1:D:2120:GLU:CD	1:D:2120:GLU:H	2.22	0.43
1:A:672:LEU:HD11	1:A:766:ARG:HH11	1.83	0.43
1:A:1376:ILE:O	1:A:1379:VAL:HG22	2.17	0.43
1:A:1621:ALA:O	1:A:1625:VAL:HG23	2.18	0.43
1:A:1829:ILE:HD11	1:A:1968:PRO:O	2.18	0.43
1:B:1364:ARG:HH21	1:B:1366:ASP:HB2	1.83	0.43
1:B:1728:GLU:HG2	1:B:1731:LYS:HE3	2.00	0.43
1:C:765:LEU:HD21	1:C:835:GLN:CG	2.49	0.43
1:C:1621:ALA:O	1:C:1625:VAL:HG23	2.18	0.43
1:C:1728:GLU:HG2	1:C:1731:LYS:HE3	2.00	0.43
1:C:1829:ILE:HD11	1:C:1968:PRO:O	2.18	0.43
1:D:996:ILE:HG12	1:D:999:ARG:NH2	2.34	0.43
1:D:1829:ILE:HD11	1:D:1968:PRO:O	2.18	0.43
1:A:672:LEU:HD11	1:A:766:ARG:NH1	2.34	0.43
1:B:765:LEU:HD21	1:B:835:GLN:CG	2.49	0.43
1:B:1879:THR:HG22	1:B:1882:LEU:HD13	1.99	0.43
1:C:14:ILE:HG12	1:C:126:LEU:HD11	2.00	0.43
1:C:701:ARG:HG2	1:C:705:LYS:HA	2.00	0.43
1:C:1122:LEU:HD11	1:C:1217:LEU:HD12	2.01	0.43
1:D:14:ILE:HG12	1:D:126:LEU:HD11	2.00	0.43
1:D:1103:LEU:HD23	1:D:1103:LEU:HA	1.73	0.43
4:D:5112:PLX:H1B2	4:D:5112:PLX:H22	1.80	0.43
1:A:411:GLU:OE2	1:A:411:GLU:N	2.52	0.43
1:A:1064:LEU:HB3	1:A:1083:LEU:HG	2.01	0.43
1:A:1886:LYS:HB2	1:B:86:ALA:H	1.84	0.43
4:A:5113:PLX:H51	4:A:5113:PLX:H251	1.63	0.43
1:B:411:GLU:OE2	1:B:411:GLU:N	2.52	0.43
1:B:2083:ASP:N	1:B:2083:ASP:OD1	2.51	0.43
1:B:2730:LYS:HD2	1:B:2733:ILE:HD11	2.01	0.43
1:C:658:ASN:HB2	1:C:659:PRO:HD3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1214:VAL:HG21	1:C:1240:PHE:CE2	2.54	0.43
4:C:5109:PLX:H1B2	4:C:5109:PLX:H22	1.80	0.43
1:B:805:ARG:NH2	1:B:991:SER:OG	2.51	0.43
1:B:2120:GLU:CD	1:B:2120:GLU:H	2.22	0.43
1:C:1364:ARG:HH21	1:C:1366:ASP:HB2	1.82	0.43
1:D:672:LEU:HD11	1:D:766:ARG:NH1	2.34	0.43
1:D:2730:LYS:HD2	1:D:2733:ILE:HD11	2.01	0.43
4:A:5114:PLX:H122	4:A:5114:PLX:H91	1.80	0.43
1:B:1304:ARG:HB3	1:B:1374:TYR:CE1	2.53	0.43
1:B:1379:VAL:HG23	1:B:1422:ALA:HB1	2.01	0.43
1:C:618:PHE:O	1:C:622:VAL:HG23	2.18	0.43
1:C:996:ILE:HG12	1:C:999:ARG:NH2	2.34	0.43
1:C:1520:TYR:HA	1:C:1525:LEU:HD11	2.01	0.43
1:C:2083:ASP:OD1	1:C:2083:ASP:N	2.51	0.43
1:C:2200:ARG:NE	1:C:2206:GLU:OE2	2.28	0.43
1:D:618:PHE:O	1:D:622:VAL:HG23	2.18	0.43
1:D:1379:VAL:HG23	1:D:1422:ALA:HB1	2.01	0.43
1:D:2365:LYS:HD2	1:D:2365:LYS:HA	1.76	0.43
1:D:2709:VAL:O	1:D:2712:LEU:HG	2.18	0.43
1:A:1095:GLN:O	1:A:1099:GLN:HG2	2.19	0.43
1:B:1064:LEU:HB3	1:B:1083:LEU:HG	2.01	0.43
1:C:672:LEU:HD11	1:C:766:ARG:NH1	2.34	0.43
1:C:1095:GLN:O	1:C:1099:GLN:HG2	2.19	0.43
1:C:1379:VAL:HG23	1:C:1422:ALA:HB1	2.01	0.43
4:C:5110:PLX:H322	4:C:5110:PLX:H292	1.78	0.43
1:D:672:LEU:HD11	1:D:766:ARG:HH11	1.83	0.43
1:D:974:ILE:HA	1:D:977:ILE:HD12	2.01	0.43
1:D:1058:ARG:HD3	1:D:1744:TYR:O	2.19	0.43
1:D:1064:LEU:HB3	1:D:1083:LEU:HG	2.01	0.43
1:D:1372:PHE:CZ	1:D:1419:VAL:HG22	2.53	0.43
1:A:241:ARG:NH2	1:A:276:THR:HG23	2.34	0.43
1:A:884:LEU:HD23	1:A:884:LEU:HA	1.94	0.43
1:A:1122:LEU:HD11	1:A:1217:LEU:HD12	2.00	0.43
1:A:1364:ARG:HH21	1:A:1366:ASP:HB2	1.82	0.43
1:A:1728:GLU:HG2	1:A:1731:LYS:HE3	2.00	0.43
1:A:2040:LEU:HA	1:A:2043:TYR:CD2	2.54	0.43
1:B:673:SER:HA	1:B:697:TRP:CZ3	2.54	0.43
1:B:1214:VAL:HG21	1:B:1240:PHE:CE2	2.54	0.43
1:B:1406:ILE:HA	1:B:1423:TYR:CE2	2.53	0.43
1:B:2709:VAL:O	1:B:2712:LEU:HG	2.18	0.43
1:C:92:LEU:HD21	1:D:1882:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1103:LEU:HA	1:C:1103:LEU:HD23	1.73	0.43
4:C:5113:PLX:H122	4:C:5113:PLX:H91	1.80	0.43
1:D:257:ARG:O	1:D:259:LYS:NZ	2.41	0.43
1:D:1105:THR:HG23	1:D:1108:ASP:HB2	2.00	0.43
1:D:1214:VAL:HG21	1:D:1240:PHE:CE2	2.54	0.43
1:A:618:PHE:O	1:A:622:VAL:HG23	2.18	0.42
1:A:1106:SER:C	1:A:1108:ASP:N	2.71	0.42
1:A:1214:VAL:HG21	1:A:1240:PHE:CE2	2.54	0.42
1:A:1304:ARG:HB3	1:A:1374:TYR:CE1	2.54	0.42
1:A:2424:GLU:OE2	1:B:2439:ARG:NH2	2.51	0.42
1:B:996:ILE:HG12	1:B:999:ARG:NH2	2.34	0.42
1:B:1058:ARG:HD3	1:B:1744:TYR:O	2.19	0.42
1:C:1058:ARG:HD3	1:C:1744:TYR:O	2.19	0.42
1:C:1097:PHE:C	1:C:1099:GLN:H	2.23	0.42
1:D:1109:VAL:O	1:D:1113:LYS:HG2	2.19	0.42
1:D:1198:ARG:HH12	1:D:1200:GLN:H	1.66	0.42
1:D:2040:LEU:HA	1:D:2043:TYR:CD2	2.54	0.42
1:D:2196:ILE:HG23	1:D:2210:PHE:HE1	1.84	0.42
4:D:5106:PLX:H362	4:D:5106:PLX:H332	1.76	0.42
1:B:618:PHE:O	1:B:622:VAL:HG23	2.18	0.42
1:B:884:LEU:HD23	1:B:884:LEU:HA	1.94	0.42
1:B:1093:VAL:HG12	1:B:1097:PHE:HE2	1.85	0.42
1:B:1520:TYR:HA	1:B:1525:LEU:HD11	2.01	0.42
1:C:78:PRO:HA	1:D:1884:ASN:OD1	2.18	0.42
1:C:1064:LEU:HB3	1:C:1083:LEU:HG	2.01	0.42
1:C:1109:VAL:O	1:C:1113:LYS:HG2	2.19	0.42
1:C:1406:ILE:HA	1:C:1423:TYR:CE2	2.53	0.42
1:D:701:ARG:HG2	1:D:705:LYS:HA	2.00	0.42
1:B:1095:GLN:O	1:B:1099:GLN:HG2	2.19	0.42
1:B:1122:LEU:HD11	1:B:1217:LEU:HD12	2.00	0.42
1:B:1798:HIS:HA	1:B:1801:LYS:HZ1	1.83	0.42
1:B:2557:SER:OG	1:B:2559:GLU:OE1	2.34	0.42
4:B:5107:PLX:H311	4:B:5107:PLX:H281	1.68	0.42
4:B:5111:PLX:H6	4:B:5111:PLX:H31	1.62	0.42
1:C:503:ASN:O	1:C:507:GLN:HG3	2.20	0.42
1:C:1089:GLN:O	1:C:1092:GLU:HG2	2.20	0.42
1:C:2120:GLU:H	1:C:2120:GLU:CD	2.22	0.42
1:C:2652:ASP:OD1	1:C:2652:ASP:N	2.51	0.42
1:C:2709:VAL:O	1:C:2712:LEU:HG	2.18	0.42
1:D:673:SER:HA	1:D:697:TRP:CZ3	2.54	0.42
1:D:1304:ARG:HB3	1:D:1374:TYR:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:5106:PLX:H311	4:D:5106:PLX:H281	1.68	0.42
1:A:974:ILE:HA	1:A:977:ILE:HD12	2.01	0.42
1:B:1106:SER:C	1:B:1108:ASP:N	2.71	0.42
1:B:1669:GLU:HG2	1:B:1670:LYS:N	2.35	0.42
1:B:2339:SER:O	1:B:2342:LEU:HG	2.20	0.42
4:B:5107:PLX:H22	4:B:5107:PLX:H1A3	1.62	0.42
1:C:967:VAL:O	1:C:970:THR:OG1	2.31	0.42
1:C:2716:LEU:HD23	1:C:2719:LEU:HD21	2.01	0.42
4:D:5109:PLX:H21	4:D:5109:PLX:H1C3	1.78	0.42
1:A:1876:THR:OG1	1:A:1957:LEU:HD21	2.20	0.42
1:B:2357:LEU:HD23	1:B:2357:LEU:HA	1.86	0.42
1:C:241:ARG:NH2	1:C:276:THR:HG23	2.34	0.42
1:C:974:ILE:HA	1:C:977:ILE:HD12	2.01	0.42
1:C:2040:LEU:HA	1:C:2043:TYR:CD2	2.54	0.42
1:D:1095:GLN:O	1:D:1099:GLN:HG2	2.19	0.42
1:A:986:LEU:HD21	1:A:1092:GLU:HG3	2.02	0.42
1:A:1109:VAL:O	1:A:1113:LYS:HG2	2.19	0.42
1:A:1520:TYR:HA	1:A:1525:LEU:HD11	2.01	0.42
1:A:2339:SER:O	1:A:2342:LEU:HG	2.20	0.42
1:A:2652:ASP:OD1	1:A:2652:ASP:N	2.51	0.42
1:B:1105:THR:HG23	1:B:1108:ASP:HB2	2.00	0.42
1:B:1198:ARG:HH12	1:B:1200:GLN:H	1.67	0.42
1:B:2196:ILE:HG23	1:B:2210:PHE:HE1	1.84	0.42
1:B:2716:LEU:HD23	1:B:2719:LEU:HD21	2.01	0.42
1:C:74:LYS:HE3	1:D:1879:THR:OG1	2.19	0.42
1:C:673:SER:HA	1:C:697:TRP:CZ3	2.54	0.42
1:C:1255:LEU:HD23	1:C:1255:LEU:HA	1.85	0.42
1:C:1304:ARG:HB3	1:C:1374:TYR:CE1	2.54	0.42
1:C:1628:ASP:OD2	1:C:1737:ARG:NE	2.52	0.42
1:A:74:LYS:HE3	1:C:1879:THR:OG1	2.19	0.42
1:B:246:GLU:OE2	1:D:168:LYS:N	2.53	0.42
1:C:1618:LEU:HG	1:C:1736:LEU:HD22	2.02	0.42
1:C:2339:SER:O	1:C:2342:LEU:HG	2.20	0.42
1:D:1089:GLN:O	1:D:1092:GLU:HG2	2.19	0.42
1:D:1805:SER:HB2	1:D:1843:PHE:CE1	2.55	0.42
1:A:673:SER:HA	1:A:697:TRP:CZ3	2.54	0.42
1:A:776:ASP:OD1	1:A:776:ASP:N	2.53	0.42
1:A:2120:GLU:H	1:A:2120:GLU:CD	2.22	0.42
1:A:2409:HIS:CD2	4:A:5111:PLX:H51	2.54	0.42
1:A:2709:VAL:O	1:A:2712:LEU:HG	2.18	0.42
1:A:2716:LEU:HD23	1:A:2719:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2730:LYS:HD2	1:A:2733:ILE:HD11	2.01	0.42
1:B:672:LEU:HD11	1:B:766:ARG:NH1	2.34	0.42
1:B:1089:GLN:O	1:B:1092:GLU:HG2	2.19	0.42
1:B:2040:LEU:HA	1:B:2043:TYR:CD2	2.54	0.42
1:B:2365:LYS:HA	1:B:2365:LYS:HD2	1.76	0.42
4:B:5107:PLX:H362	4:B:5107:PLX:H332	1.76	0.42
1:C:411:GLU:OE2	1:C:411:GLU:N	2.52	0.42
1:C:2730:LYS:HD2	1:C:2733:ILE:HD11	2.01	0.42
1:D:1107:GLN:O	1:D:1110:ASP:OD1	2.37	0.42
1:D:1669:GLU:HG2	1:D:1670:LYS:N	2.35	0.42
1:D:1728:GLU:HG2	1:D:1731:LYS:HE3	2.00	0.42
1:A:996:ILE:HG12	1:A:999:ARG:NH2	2.34	0.42
1:A:1058:ARG:HD3	1:A:1744:TYR:O	2.19	0.42
1:A:1097:PHE:C	1:A:1099:GLN:H	2.23	0.42
1:B:1107:GLN:O	1:B:1110:ASP:OD1	2.37	0.42
1:C:168:LYS:N	1:D:246:GLU:OE2	2.52	0.42
1:D:241:ARG:NH2	1:D:276:THR:HG23	2.34	0.42
1:D:1957:LEU:O	1:D:1957:LEU:HD12	2.20	0.42
1:D:2409:HIS:CD2	4:D:5108:PLX:H51	2.55	0.42
1:A:1089:GLN:O	1:A:1092:GLU:HG2	2.19	0.42
1:A:1093:VAL:HG12	1:A:1097:PHE:HE2	1.85	0.42
1:A:1198:ARG:HH12	1:A:1200:GLN:H	1.67	0.42
1:A:2207:GLN:HE21	1:A:2207:GLN:HB3	1.72	0.42
4:A:5110:PLX:H22	4:A:5110:PLX:H1B2	1.80	0.42
1:B:241:ARG:NH2	1:B:276:THR:HG23	2.34	0.42
1:B:503:ASN:O	1:B:507:GLN:HG3	2.20	0.42
4:B:5112:PLX:H122	4:B:5112:PLX:H91	1.80	0.42
1:C:231:ASP:OD1	1:C:231:ASP:N	2.53	0.42
1:C:776:ASP:OD1	1:C:776:ASP:N	2.53	0.42
1:C:1283:LEU:HD23	1:C:1283:LEU:HA	1.88	0.42
4:C:5113:PLX:H21	4:C:5113:PLX:H1C2	1.76	0.42
1:D:765:LEU:HD21	1:D:835:GLN:CG	2.49	0.42
1:A:1379:VAL:HG23	1:A:1422:ALA:HB1	2.01	0.41
4:A:5111:PLX:H322	4:A:5111:PLX:H292	1.78	0.41
1:B:1097:PHE:C	1:B:1099:GLN:H	2.23	0.41
1:C:1102:LEU:HD12	1:C:1102:LEU:HA	1.79	0.41
1:C:1198:ARG:HH12	1:C:1200:GLN:H	1.66	0.41
1:C:1805:SER:HB2	1:C:1843:PHE:CE1	2.55	0.41
1:C:1957:LEU:HD12	1:C:1957:LEU:O	2.20	0.41
4:C:5111:PLX:H1C3	4:C:5111:PLX:H21	1.78	0.41
4:C:5112:PLX:H251	4:C:5112:PLX:H51	1.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:318:VAL:HG22	1:D:353:TYR:CE1	2.55	0.41
1:D:986:LEU:HD21	1:D:1092:GLU:HG3	2.02	0.41
1:D:1520:TYR:HA	1:D:1525:LEU:HD11	2.01	0.41
1:A:1618:LEU:HG	1:A:1736:LEU:HD22	2.02	0.41
1:A:2196:ILE:HG23	1:A:2210:PHE:HE1	1.84	0.41
1:B:302:LEU:HD22	1:B:393:LEU:HD22	2.02	0.41
1:B:318:VAL:HG22	1:B:353:TYR:CE1	2.55	0.41
1:B:749:TYR:OH	1:B:793:ASP:OD2	2.37	0.41
1:B:974:ILE:HA	1:B:977:ILE:HD12	2.01	0.41
1:B:1401:LEU:HD23	1:B:1426:PHE:HE2	1.85	0.41
1:B:1805:SER:HB2	1:B:1843:PHE:CE1	2.55	0.41
1:C:1249:GLN:HE21	1:C:1249:GLN:HB3	1.74	0.41
1:C:2196:ILE:HG23	1:C:2210:PHE:HE1	1.84	0.41
1:D:698:LEU:HD21	1:D:715:LEU:HD22	2.02	0.41
1:D:881:PHE:O	1:D:885:LEU:HD23	2.21	0.41
1:D:1249:GLN:HE21	1:D:1249:GLN:HB3	1.74	0.41
1:D:1628:ASP:OD2	1:D:1737:ARG:NE	2.52	0.41
1:D:2357:LEU:HD23	1:D:2357:LEU:HA	1.86	0.41
1:D:2716:LEU:HD23	1:D:2719:LEU:HD21	2.01	0.41
1:A:1805:SER:HB2	1:A:1843:PHE:CE1	2.55	0.41
1:B:701:ARG:HG2	1:B:705:LYS:HA	2.00	0.41
1:B:993:LEU:HA	1:B:993:LEU:HD23	1.82	0.41
1:B:1109:VAL:O	1:B:1113:LYS:HG2	2.19	0.41
1:B:1685:LYS:HD2	1:B:1685:LYS:HA	1.83	0.41
1:B:1876:THR:OG1	1:B:1957:LEU:HD21	2.20	0.41
4:B:5108:PLX:H1B2	4:B:5108:PLX:H22	1.80	0.41
1:C:1876:THR:OG1	1:C:1957:LEU:HD21	2.20	0.41
1:D:503:ASN:O	1:D:507:GLN:HG3	2.20	0.41
1:D:1787:ARG:NH1	1:D:1789:GLU:HA	2.36	0.41
1:D:2365:LYS:HE2	1:D:2398:TYR:CD2	2.56	0.41
1:A:231:ASP:OD1	1:A:231:ASP:N	2.53	0.41
1:B:698:LEU:HD21	1:B:715:LEU:HD22	2.02	0.41
1:B:2020:LEU:HD12	1:B:2023:LEU:HD21	2.03	0.41
1:D:302:LEU:HD22	1:D:393:LEU:HD22	2.02	0.41
1:D:2020:LEU:HD12	1:D:2023:LEU:HD21	2.03	0.41
1:D:2652:ASP:N	1:D:2652:ASP:OD1	2.51	0.41
1:A:503:ASN:O	1:A:507:GLN:HG3	2.20	0.41
1:A:1348:ARG:HD3	1:A:1348:ARG:H	1.85	0.41
1:A:2020:LEU:HD12	1:A:2023:LEU:HD21	2.03	0.41
1:B:1628:ASP:OD2	1:B:1737:ARG:NE	2.52	0.41
1:C:1334:LEU:HB2	1:C:1342:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2020:LEU:HD12	1:C:2023:LEU:HD21	2.03	0.41
1:A:168:LYS:N	1:C:246:GLU:OE2	2.53	0.41
1:A:318:VAL:HG22	1:A:353:TYR:CE1	2.55	0.41
1:B:1382:LEU:HD23	1:B:1382:LEU:HA	1.93	0.41
1:C:1787:ARG:NH1	1:C:1789:GLU:HA	2.35	0.41
1:D:982:LEU:HD22	1:D:985:ARG:HH21	1.86	0.41
1:D:1618:LEU:HG	1:D:1736:LEU:HD22	2.02	0.41
1:D:1876:THR:OG1	1:D:1957:LEU:HD21	2.20	0.41
1:D:2119:LYS:O	1:D:2122:VAL:N	2.54	0.41
1:D:2339:SER:O	1:D:2342:LEU:HG	2.20	0.41
1:A:1102:LEU:HD12	1:A:1102:LEU:HA	1.79	0.41
1:A:1879:THR:O	1:A:1882:LEU:HB3	2.21	0.41
1:A:2327:LEU:N	1:A:2328:PRO:HD2	2.36	0.41
1:A:2458:VAL:HG11	4:A:5108:PLX:H131	2.03	0.41
1:A:2533:MET:HG2	1:B:2558:LYS:HE3	2.03	0.41
4:A:5109:PLX:H22	4:A:5109:PLX:H1A3	1.62	0.41
1:B:364:ILE:O	1:B:367:ILE:HG22	2.21	0.41
1:B:805:ARG:NH2	1:B:987:ASP:OD1	2.44	0.41
1:B:1107:GLN:H	1:B:1107:GLN:HG2	1.60	0.41
1:B:1787:ARG:NH1	1:B:1789:GLU:HA	2.36	0.41
1:C:555:LEU:O	1:C:559:VAL:HG13	2.21	0.41
1:C:1216:GLU:OE1	1:C:1216:GLU:N	2.54	0.41
1:C:1669:GLU:HG2	1:C:1670:LYS:N	2.35	0.41
1:C:1879:THR:O	1:C:1882:LEU:HB3	2.21	0.41
1:D:1066:HIS:O	1:D:1070:HIS:NE2	2.54	0.41
1:D:1097:PHE:C	1:D:1099:GLN:H	2.23	0.41
1:A:698:LEU:HD21	1:A:715:LEU:HD22	2.02	0.41
1:A:881:PHE:O	1:A:885:LEU:HD23	2.21	0.41
1:A:1066:HIS:O	1:A:1070:HIS:NE2	2.54	0.41
1:A:1107:GLN:H	1:A:1107:GLN:HG2	1.60	0.41
1:A:1669:GLU:HG2	1:A:1670:LYS:N	2.35	0.41
1:B:1288:ASN:OD1	1:B:1289:GLU:N	2.54	0.41
1:B:1334:LEU:HB2	1:B:1342:LEU:HD21	2.02	0.41
1:B:1342:LEU:HD12	1:B:1344:PHE:CZ	2.55	0.41
1:B:1348:ARG:H	1:B:1348:ARG:HD3	1.85	0.41
1:B:1506:GLN:N	1:B:1507:PRO:HD2	2.36	0.41
1:B:1879:THR:O	1:B:1882:LEU:HB3	2.21	0.41
1:B:2119:LYS:O	1:B:2122:VAL:N	2.54	0.41
1:C:302:LEU:HD22	1:C:393:LEU:HD22	2.02	0.41
1:C:1342:LEU:HD12	1:C:1344:PHE:CZ	2.55	0.41
1:C:2716:LEU:HA	1:C:2719:LEU:HG	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1342:LEU:HD12	1:D:1344:PHE:CZ	2.55	0.41
1:D:1722:PRO:HG2	1:D:1723:PRO:HD3	2.03	0.41
4:D:5108:PLX:H292	4:D:5108:PLX:H322	1.77	0.41
1:A:982:LEU:HD22	1:A:985:ARG:HH21	1.86	0.41
1:A:1094:LEU:HA	1:A:1097:PHE:HD2	1.86	0.41
1:A:1342:LEU:HD12	1:A:1344:PHE:CZ	2.55	0.41
1:A:1882:LEU:HD21	1:B:92:LEU:HD11	2.02	0.41
1:A:1885:LYS:HB2	1:B:85:ASP:CG	2.41	0.41
1:A:1998:ASN:ND2	1:A:2001:CYS:SG	2.94	0.41
1:A:2365:LYS:HE2	1:A:2398:TYR:CD2	2.56	0.41
1:B:578:PHE:HA	1:B:581:MET:HG2	2.03	0.41
1:B:839:PHE:O	1:B:842:GLU:HG3	2.21	0.41
1:B:881:PHE:O	1:B:885:LEU:HD23	2.21	0.41
1:B:986:LEU:HD21	1:B:1092:GLU:HG3	2.02	0.41
4:B:5113:PLX:H1B2	4:B:5113:PLX:H22	1.80	0.41
1:C:143:GLU:OE1	1:C:146:ALA:N	2.54	0.41
1:C:364:ILE:O	1:C:367:ILE:HG22	2.21	0.41
1:C:698:LEU:HD21	1:C:715:LEU:HD22	2.02	0.41
1:C:997:PHE:CZ	1:C:1604:LEU:HB3	2.56	0.41
1:C:2119:LYS:O	1:C:2122:VAL:N	2.54	0.41
1:C:2327:LEU:N	1:C:2328:PRO:HD2	2.36	0.41
1:C:2436:ARG:HD3	1:C:2596:LEU:HD11	2.03	0.41
1:C:2588:VAL:HA	1:D:2593:PHE:CE2	2.56	0.41
1:C:2625:THR:HG23	1:C:2626:VAL:N	2.25	0.41
1:D:143:GLU:OE1	1:D:146:ALA:N	2.54	0.41
1:D:555:LEU:O	1:D:559:VAL:HG13	2.21	0.41
1:D:768:MET:CE	1:D:782:CYS:HA	2.51	0.41
1:D:1125:ILE:HA	1:D:1128:LYS:HG2	2.03	0.41
1:D:1401:LEU:HD23	1:D:1426:PHE:HE2	1.85	0.41
1:D:1871:ILE:HG13	1:D:1963:ILE:HD12	2.03	0.41
1:D:2327:LEU:N	1:D:2328:PRO:HD2	2.36	0.41
1:A:318:VAL:HA	1:A:353:TYR:HD1	1.86	0.41
1:A:808:SER:HB2	1:A:1104:VAL:HG11	2.02	0.41
1:A:839:PHE:O	1:A:842:GLU:HG3	2.21	0.41
1:A:997:PHE:CZ	1:A:1604:LEU:HB3	2.56	0.41
1:A:1251:ASN:O	1:A:1254:LEU:HG	2.21	0.41
1:A:1506:GLN:N	1:A:1507:PRO:HD2	2.36	0.41
1:A:1613:ASP:O	1:A:1616:ARG:HG2	2.21	0.41
1:A:2119:LYS:O	1:A:2122:VAL:N	2.54	0.41
4:A:5109:PLX:H282	4:A:5109:PLX:H251	1.96	0.41
1:B:2327:LEU:N	1:B:2328:PRO:HD2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:5110:PLX:H282	4:B:5110:PLX:H252	1.72	0.41
1:C:318:VAL:HG22	1:C:353:TYR:CE1	2.55	0.41
1:C:805:ARG:NH2	1:C:987:ASP:OD1	2.44	0.41
1:C:881:PHE:O	1:C:885:LEU:HD23	2.21	0.41
1:C:1685:LYS:HA	1:C:1685:LYS:HD2	1.83	0.41
1:C:1871:ILE:HG13	1:C:1963:ILE:HD12	2.03	0.41
1:C:1998:ASN:ND2	1:C:2001:CYS:SG	2.94	0.41
1:C:2070:ILE:CD1	1:C:2096:LEU:HD12	2.51	0.41
1:D:773:LEU:HD13	1:D:777:LEU:HD23	2.03	0.41
1:D:2093:SER:O	1:D:2097:LEU:HD23	2.21	0.41
1:D:2436:ARG:HD3	1:D:2596:LEU:HD11	2.03	0.41
4:D:5109:PLX:H282	4:D:5109:PLX:H252	1.72	0.41
4:D:5111:PLX:H91	4:D:5111:PLX:H122	1.80	0.41
1:A:1174:ARG:HG3	1:A:1175:VAL:N	2.36	0.40
1:A:1216:GLU:OE1	1:A:1216:GLU:N	2.54	0.40
1:A:1287:ILE:HG22	1:A:1288:ASN:O	2.21	0.40
1:A:1722:PRO:HG2	1:A:1723:PRO:HD3	2.03	0.40
1:A:1787:ARG:NH1	1:A:1789:GLU:HA	2.36	0.40
1:A:2593:PHE:CE2	1:B:2588:VAL:HA	2.56	0.40
1:B:1174:ARG:HG3	1:B:1175:VAL:N	2.37	0.40
1:B:1722:PRO:HG2	1:B:1723:PRO:HD3	2.03	0.40
1:B:1852:LYS:HZ1	1:B:1855:LYS:HE2	1.85	0.40
1:C:354:SER:HA	1:C:419:GLY:HA2	2.03	0.40
1:C:456:ILE:HD13	1:C:456:ILE:HA	1.96	0.40
1:C:768:MET:CE	1:C:782:CYS:HA	2.51	0.40
1:C:1198:ARG:HD2	1:C:1198:ARG:HA	1.95	0.40
1:C:1401:LEU:HD23	1:C:1426:PHE:HE2	1.85	0.40
1:C:2365:LYS:HE2	1:C:2398:TYR:CD2	2.56	0.40
1:D:578:PHE:HA	1:D:581:MET:HG2	2.03	0.40
1:D:835:GLN:HA	1:D:838:GLU:HG2	2.03	0.40
1:D:1251:ASN:O	1:D:1254:LEU:HG	2.21	0.40
1:D:2630:GLU:HA	1:D:2633:LYS:HG2	2.03	0.40
1:A:578:PHE:HA	1:A:581:MET:HG2	2.03	0.40
1:A:1482:ILE:O	1:A:1486:ILE:HG22	2.21	0.40
1:A:1957:LEU:HD12	1:A:1957:LEU:O	2.20	0.40
1:A:2133:GLU:HB3	1:A:2150:ARG:NH2	2.36	0.40
1:B:967:VAL:O	1:B:970:THR:OG1	2.31	0.40
1:B:1125:ILE:HA	1:B:1128:LYS:HG2	2.03	0.40
1:B:1957:LEU:HD12	1:B:1957:LEU:O	2.20	0.40
1:B:2593:PHE:CE2	1:D:2588:VAL:HA	2.56	0.40
1:C:501:LYS:HA	1:C:502:PRO:HD3	1.96	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:986:LEU:HD21	1:C:1092:GLU:HG3	2.02	0.40
1:C:2133:GLU:HB3	1:C:2150:ARG:NH2	2.36	0.40
1:C:2579:ILE:HD13	1:C:2579:ILE:HA	1.98	0.40
1:D:1174:ARG:HG3	1:D:1175:VAL:N	2.36	0.40
1:D:1406:ILE:HA	1:D:1423:TYR:CE2	2.53	0.40
1:A:602:ASN:C	1:A:603:ARG:HD3	2.42	0.40
1:A:2093:SER:O	1:A:2097:LEU:HD23	2.21	0.40
1:B:657:LEU:HA	1:B:660:THR:OG1	2.21	0.40
1:B:1287:ILE:HG22	1:B:1288:ASN:O	2.21	0.40
1:B:1618:LEU:HG	1:B:1736:LEU:HD22	2.02	0.40
1:B:2365:LYS:HE2	1:B:2398:TYR:CD2	2.56	0.40
1:C:578:PHE:HA	1:C:581:MET:HG2	2.03	0.40
1:C:839:PHE:O	1:C:842:GLU:HG3	2.21	0.40
1:C:982:LEU:HD22	1:C:985:ARG:HH21	1.86	0.40
1:C:1722:PRO:HG2	1:C:1723:PRO:HD3	2.03	0.40
1:D:364:ILE:O	1:D:367:ILE:HG22	2.21	0.40
1:D:1216:GLU:OE1	1:D:1216:GLU:N	2.54	0.40
1:D:1288:ASN:OD1	1:D:1289:GLU:N	2.54	0.40
1:D:2133:GLU:HB3	1:D:2150:ARG:NH2	2.36	0.40
1:A:354:SER:HA	1:A:419:GLY:HA2	2.03	0.40
1:A:657:LEU:HA	1:A:660:THR:OG1	2.21	0.40
1:A:1334:LEU:HB2	1:A:1342:LEU:HD21	2.02	0.40
1:A:2557:SER:OG	1:A:2559:GLU:OE1	2.34	0.40
1:A:2630:GLU:HA	1:A:2633:LYS:HG2	2.03	0.40
1:B:555:LEU:O	1:B:559:VAL:HG13	2.21	0.40
1:B:1482:ILE:O	1:B:1486:ILE:HG22	2.22	0.40
1:B:1879:THR:OG1	1:D:74:LYS:HE3	2.20	0.40
1:B:2026:ASN:O	1:B:2030:VAL:HG13	2.22	0.40
1:C:668:THR:CG2	1:C:698:LEU:HB2	2.52	0.40
1:C:2200:ARG:HB2	1:C:2206:GLU:OE2	2.22	0.40
1:D:1506:GLN:N	1:D:1507:PRO:HD2	2.36	0.40
4:D:5111:PLX:H302	4:D:5111:PLX:H272	1.78	0.40
1:A:1255:LEU:HA	1:A:1255:LEU:HD23	1.85	0.40
1:A:1401:LEU:HD23	1:A:1426:PHE:HE2	1.85	0.40
1:A:1871:ILE:HG13	1:A:1963:ILE:HD12	2.03	0.40
1:A:2013:SER:HB3	1:B:65:ARG:NH2	2.36	0.40
1:A:2070:ILE:CD1	1:A:2096:LEU:HD12	2.51	0.40
1:A:2732:ARG:HH12	1:C:302:LEU:HD21	1.87	0.40
1:B:231:ASP:N	1:B:231:ASP:OD1	2.53	0.40
1:B:982:LEU:HD22	1:B:985:ARG:HH21	1.86	0.40
1:B:1066:HIS:O	1:B:1070:HIS:NE2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:835:GLN:HA	1:C:838:GLU:HG2	2.03	0.40
1:C:2430:VAL:O	1:C:2433:SER:HB3	2.21	0.40
4:C:5108:PLX:H281	4:C:5108:PLX:H311	1.68	0.40
1:D:411:GLU:OE2	1:D:411:GLU:N	2.52	0.40
1:D:997:PHE:CZ	1:D:1604:LEU:HB3	2.56	0.40
1:D:1613:ASP:O	1:D:1616:ARG:HG2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2351/2750 (86%)	2245 (96%)	97 (4%)	9 (0%)	34	67
1	B	2351/2750 (86%)	2244 (95%)	98 (4%)	9 (0%)	34	67
1	C	2351/2750 (86%)	2245 (96%)	97 (4%)	9 (0%)	34	67
1	D	2351/2750 (86%)	2244 (95%)	98 (4%)	9 (0%)	34	67
All	All	9404/11000 (86%)	8978 (96%)	390 (4%)	36 (0%)	38	67

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	811	PRO
1	A	1101	GLN
1	A	1102	LEU
1	A	1108	ASP
1	A	2307	PRO
1	A	2625	THR
1	B	811	PRO
1	B	1101	GLN
1	B	1102	LEU

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Mol	Chain	Res	Type
1	B	1108	ASP
1	B	2307	PRO
1	B	2625	THR
1	C	811	PRO
1	C	1101	GLN
1	C	1102	LEU
1	C	1108	ASP
1	C	2307	PRO
1	C	2625	THR
1	D	811	PRO
1	D	1101	GLN
1	D	1102	LEU
1	D	1108	ASP
1	D	2307	PRO
1	D	2625	THR
1	A	1100	VAL
1	A	1105	THR
1	A	1369	SER
1	B	1100	VAL
1	B	1105	THR
1	B	1369	SER
1	C	1100	VAL
1	C	1105	THR
1	C	1369	SER
1	D	1100	VAL
1	D	1105	THR
1	D	1369	SER

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2154/2459 (88%)	2137 (99%)	17 (1%)	81	89
1	B	2154/2459 (88%)	2137 (99%)	17 (1%)	81	89
1	C	2154/2459 (88%)	2137 (99%)	17 (1%)	81	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	2154/2459 (88%)	2137 (99%)	17 (1%)	81	89
All	All	8616/9836 (88%)	8548 (99%)	68 (1%)	82	89

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	LYS
1	A	77	LYS
1	A	629	ARG
1	A	886	ARG
1	A	1099	GLN
1	A	1100	VAL
1	A	1101	GLN
1	A	1103	LEU
1	A	1104	VAL
1	A	1105	THR
1	A	1249	GLN
1	A	1348	ARG
1	A	1587	ARG
1	A	1731	LYS
1	A	2045	GLN
1	A	2207	GLN
1	A	2701	LYS
1	B	74	LYS
1	B	77	LYS
1	B	629	ARG
1	B	886	ARG
1	B	1099	GLN
1	B	1100	VAL
1	B	1101	GLN
1	B	1103	LEU
1	B	1104	VAL
1	B	1105	THR
1	B	1249	GLN
1	B	1348	ARG
1	B	1587	ARG
1	B	1731	LYS
1	B	2045	GLN
1	B	2207	GLN
1	B	2701	LYS
1	C	74	LYS
1	C	77	LYS

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Mol	Chain	Res	Type
1	C	629	ARG
1	C	886	ARG
1	C	1099	GLN
1	C	1100	VAL
1	C	1101	GLN
1	C	1103	LEU
1	C	1104	VAL
1	C	1105	THR
1	C	1249	GLN
1	C	1348	ARG
1	C	1587	ARG
1	C	1731	LYS
1	C	2045	GLN
1	C	2207	GLN
1	C	2701	LYS
1	D	74	LYS
1	D	77	LYS
1	D	629	ARG
1	D	886	ARG
1	D	1099	GLN
1	D	1100	VAL
1	D	1101	GLN
1	D	1103	LEU
1	D	1104	VAL
1	D	1105	THR
1	D	1249	GLN
1	D	1348	ARG
1	D	1587	ARG
1	D	1731	LYS
1	D	2045	GLN
1	D	2207	GLN
1	D	2701	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1005	ASN
1	A	1202	GLN
1	A	1558	GLN
1	A	1868	GLN
1	A	1998	ASN
1	A	2699	GLN

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Mol	Chain	Res	Type
1	B	1005	ASN
1	B	1202	GLN
1	B	1558	GLN
1	B	1868	GLN
1	B	1998	ASN
1	B	2699	GLN
1	C	1005	ASN
1	C	1202	GLN
1	C	1558	GLN
1	C	1868	GLN
1	C	1998	ASN
1	C	2699	GLN
1	D	1005	ASN
1	D	1202	GLN
1	D	1558	GLN
1	D	1868	GLN
1	D	1998	ASN
1	D	2699	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 52 ligands modelled in this entry, 24 are monoatomic - leaving 28 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$
4	PLX	A	5108	-	45,45,51	1.14	5 (11%)	49,53,59	0.78	0
4	PLX	D	5112	-	45,45,51	1.14	5 (11%)	49,53,59	0.78	0
4	PLX	D	5109	-	35,35,51	1.20	3 (8%)	39,43,59	0.76	1 (2%)
4	PLX	A	5113	-	38,38,51	1.17	3 (7%)	42,46,59	0.80	0
4	PLX	C	5110	-	36,36,51	1.14	4 (11%)	40,44,59	1.22	2 (5%)
4	PLX	A	5110	-	39,39,51	1.18	4 (10%)	43,47,59	0.74	0
4	PLX	C	5111	-	35,35,51	1.20	3 (8%)	39,43,59	0.76	1 (2%)
4	PLX	B	5109	-	36,36,51	1.15	4 (11%)	40,44,59	1.22	2 (5%)
4	PLX	A	5114	-	37,37,51	1.20	4 (10%)	41,45,59	0.75	0
4	PLX	B	5113	-	45,45,51	1.13	5 (11%)	49,53,59	0.77	0
4	PLX	D	5110	-	38,38,51	1.16	4 (10%)	42,46,59	0.80	0
4	PLX	C	5113	-	37,37,51	1.19	4 (10%)	41,45,59	0.75	0
4	PLX	B	5108	-	39,39,51	1.18	4 (10%)	43,47,59	0.74	0
4	PLX	D	5108	-	36,36,51	1.14	4 (11%)	40,44,59	1.22	2 (5%)
4	PLX	C	5109	-	39,39,51	1.18	4 (10%)	43,47,59	0.74	0
4	PLX	A	5109	-	44,44,51	1.15	2 (4%)	48,52,59	0.77	0
4	PLX	B	5107	-	44,44,51	1.15	2 (4%)	48,52,59	0.77	0
4	PLX	B	5110	-	35,35,51	1.20	3 (8%)	39,43,59	0.76	1 (2%)
4	PLX	D	5106	-	44,44,51	1.16	2 (4%)	48,52,59	0.77	0
4	PLX	B	5112	-	37,37,51	1.20	4 (10%)	41,45,59	0.75	0
4	PLX	A	5111	-	36,36,51	1.15	4 (11%)	40,44,59	1.23	2 (5%)
4	PLX	C	5112	-	38,38,51	1.16	4 (10%)	42,46,59	0.80	0
4	PLX	B	5111	-	38,38,51	1.17	3 (7%)	42,46,59	0.80	0
4	PLX	A	5112	-	35,35,51	1.20	3 (8%)	39,43,59	0.76	1 (2%)
4	PLX	D	5107	-	39,39,51	1.19	4 (10%)	43,47,59	0.74	0
4	PLX	C	5107	-	45,45,51	1.14	5 (11%)	49,53,59	0.77	0
4	PLX	C	5108	-	44,44,51	1.15	2 (4%)	48,52,59	0.77	0
4	PLX	D	5111	-	37,37,51	1.20	3 (8%)	41,45,59	0.75	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
4	PLX	A	5108	-	-	30/49/49/55	-
4	PLX	D	5112	-	-	30/49/49/55	-
4	PLX	D	5109	-	-	26/39/39/55	-
4	PLX	A	5113	-	-	19/42/42/55	-
4	PLX	C	5110	-	-	18/40/40/55	-
4	PLX	A	5110	-	-	20/43/43/55	-
4	PLX	C	5111	-	-	26/39/39/55	-
4	PLX	B	5109	-	-	18/40/40/55	-
4	PLX	A	5114	-	-	14/41/41/55	-
4	PLX	B	5113	-	-	30/49/49/55	-
4	PLX	D	5110	-	-	19/42/42/55	-
4	PLX	C	5113	-	-	14/41/41/55	-
4	PLX	B	5108	-	-	19/43/43/55	-
4	PLX	D	5108	-	-	18/40/40/55	-
4	PLX	C	5109	-	-	20/43/43/55	-
4	PLX	A	5109	-	-	24/48/48/55	-
4	PLX	B	5107	-	-	24/48/48/55	-
4	PLX	B	5110	-	-	26/39/39/55	-
4	PLX	D	5106	-	-	24/48/48/55	-
4	PLX	B	5112	-	-	14/41/41/55	-
4	PLX	A	5111	-	-	18/40/40/55	-
4	PLX	C	5112	-	-	19/42/42/55	-
4	PLX	B	5111	-	-	19/42/42/55	-
4	PLX	A	5112	-	-	26/39/39/55	-
4	PLX	D	5107	-	-	19/43/43/55	-
4	PLX	C	5107	-	-	30/49/49/55	-
4	PLX	C	5108	-	-	24/48/48/55	-
4	PLX	D	5111	-	-	14/41/41/55	-

All (101) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	5106	PLX	O6-C4	-3.59	1.39	1.44
4	D	5111	PLX	O6-C4	-3.52	1.39	1.44
4	A	5109	PLX	O6-C4	-3.52	1.39	1.44
4	B	5107	PLX	O6-C4	-3.52	1.39	1.44
4	C	5108	PLX	O6-C4	-3.52	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	5112	PLX	O6-C4	-3.52	1.39	1.44
4	D	5107	PLX	O6-C4	-3.47	1.39	1.44
4	A	5114	PLX	O6-C4	-3.46	1.39	1.44
4	B	5108	PLX	O6-C4	-3.45	1.40	1.44
4	C	5113	PLX	O6-C4	-3.42	1.40	1.44
4	A	5110	PLX	O6-C4	-3.39	1.40	1.44
4	C	5109	PLX	O6-C4	-3.39	1.40	1.44
4	C	5107	PLX	O6-C4	-3.35	1.40	1.44
4	B	5113	PLX	O6-C4	-3.29	1.40	1.44
4	A	5108	PLX	O6-C4	-3.28	1.40	1.44
4	D	5112	PLX	O6-C4	-3.28	1.40	1.44
4	B	5110	PLX	O6-C4	-3.20	1.40	1.44
4	A	5112	PLX	O6-C4	-3.15	1.40	1.44
4	D	5109	PLX	O6-C4	-3.14	1.40	1.44
4	C	5111	PLX	O6-C4	-3.14	1.40	1.44
4	A	5113	PLX	O6-C4	-3.02	1.40	1.44
4	B	5111	PLX	O6-C4	-3.02	1.40	1.44
4	D	5110	PLX	O6-C4	-3.02	1.40	1.44
4	C	5112	PLX	O6-C4	-2.97	1.40	1.44
4	B	5109	PLX	O6-C4	-2.57	1.41	1.44
4	A	5111	PLX	O6-C4	-2.56	1.41	1.44
4	C	5110	PLX	O6-C4	-2.54	1.41	1.44
4	D	5108	PLX	O6-C4	-2.45	1.41	1.44
4	C	5108	PLX	P1-O4	2.43	1.69	1.59
4	A	5109	PLX	P1-O4	2.42	1.69	1.59
4	B	5107	PLX	P1-O4	2.42	1.69	1.59
4	D	5106	PLX	P1-O4	2.40	1.69	1.59
4	D	5107	PLX	P1-O4	2.35	1.68	1.59
4	B	5108	PLX	P1-O4	2.35	1.68	1.59
4	C	5109	PLX	P1-O4	2.35	1.68	1.59
4	C	5113	PLX	P1-O4	2.34	1.68	1.59
4	A	5110	PLX	P1-O4	2.33	1.68	1.59
4	A	5114	PLX	P1-O4	2.32	1.68	1.59
4	B	5112	PLX	P1-O4	2.32	1.68	1.59
4	D	5111	PLX	P1-O4	2.32	1.68	1.59
4	A	5108	PLX	P1-O4	2.31	1.68	1.59
4	C	5107	PLX	P1-O4	2.31	1.68	1.59
4	A	5111	PLX	P1-O4	2.31	1.68	1.59
4	D	5108	PLX	P1-O4	2.31	1.68	1.59
4	B	5109	PLX	P1-O4	2.31	1.68	1.59
4	C	5110	PLX	P1-O4	2.31	1.68	1.59
4	B	5113	PLX	P1-O4	2.30	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	5112	PLX	P1-O4	2.30	1.68	1.59
4	A	5113	PLX	P1-O4	2.28	1.68	1.59
4	C	5112	PLX	P1-O4	2.28	1.68	1.59
4	B	5111	PLX	P1-O4	2.28	1.68	1.59
4	D	5110	PLX	P1-O4	2.27	1.68	1.59
4	B	5110	PLX	P1-O4	2.26	1.68	1.59
4	A	5112	PLX	P1-O4	2.25	1.68	1.59
4	C	5111	PLX	P1-O4	2.25	1.68	1.59
4	D	5109	PLX	P1-O4	2.24	1.68	1.59
4	D	5108	PLX	C7-C6	2.17	1.55	1.50
4	A	5111	PLX	C7-C6	2.16	1.55	1.50
4	B	5109	PLX	C7-C6	2.16	1.55	1.50
4	A	5108	PLX	C7-C6	2.14	1.55	1.50
4	B	5113	PLX	C7-C6	2.14	1.55	1.50
4	C	5107	PLX	C7-C6	2.14	1.55	1.50
4	D	5112	PLX	C7-C6	2.14	1.55	1.50
4	C	5110	PLX	C7-C6	2.11	1.55	1.50
4	A	5112	PLX	C1A-N1	-2.10	1.43	1.50
4	A	5113	PLX	C1A-N1	-2.08	1.43	1.50
4	D	5109	PLX	C1A-N1	-2.08	1.43	1.50
4	B	5113	PLX	C1A-N1	-2.07	1.44	1.50
4	B	5110	PLX	C1A-N1	-2.07	1.44	1.50
4	C	5111	PLX	C1A-N1	-2.07	1.44	1.50
4	D	5112	PLX	C1A-N1	-2.06	1.44	1.50
4	D	5107	PLX	C1A-N1	-2.05	1.44	1.50
4	A	5108	PLX	C1A-N1	-2.05	1.44	1.50
4	C	5112	PLX	C1A-N1	-2.05	1.44	1.50
4	A	5110	PLX	C1A-N1	-2.05	1.44	1.50
4	D	5110	PLX	C1A-N1	-2.05	1.44	1.50
4	B	5111	PLX	C1A-N1	-2.05	1.44	1.50
4	A	5111	PLX	C1A-N1	-2.04	1.44	1.50
4	B	5109	PLX	C1A-N1	-2.04	1.44	1.50
4	A	5114	PLX	C7-C6	2.04	1.55	1.50
4	D	5111	PLX	C7-C6	2.04	1.55	1.50
4	C	5107	PLX	C1A-N1	-2.04	1.44	1.50
4	B	5112	PLX	C1A-N1	-2.04	1.44	1.50
4	C	5110	PLX	C1A-N1	-2.04	1.44	1.50
4	B	5112	PLX	C7-C6	2.03	1.55	1.50
4	C	5113	PLX	C7-C6	2.03	1.55	1.50
4	D	5108	PLX	C1A-N1	-2.02	1.44	1.50
4	C	5112	PLX	C7-C6	2.02	1.55	1.50
4	D	5112	PLX	P1-O1	2.02	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	5114	PLX	C1A-N1	-2.02	1.44	1.50
4	C	5113	PLX	C1A-N1	-2.02	1.44	1.50
4	B	5108	PLX	C1A-N1	-2.01	1.44	1.50
4	C	5109	PLX	C1A-N1	-2.01	1.44	1.50
4	A	5108	PLX	P1-O1	2.01	1.67	1.59
4	C	5107	PLX	P1-O1	2.01	1.67	1.59
4	A	5110	PLX	C7-C6	2.01	1.55	1.50
4	C	5109	PLX	C7-C6	2.01	1.55	1.50
4	D	5107	PLX	C7-C6	2.01	1.55	1.50
4	B	5108	PLX	C7-C6	2.01	1.55	1.50
4	B	5113	PLX	P1-O1	2.01	1.67	1.59
4	D	5110	PLX	C7-C6	2.01	1.55	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	5111	PLX	C6-O6-C4	5.24	125.67	115.20
4	B	5109	PLX	C6-O6-C4	5.24	125.66	115.20
4	D	5108	PLX	C6-O6-C4	5.21	125.59	115.20
4	C	5110	PLX	C6-O6-C4	5.21	125.59	115.20
4	C	5110	PLX	O6-C4-C3	2.53	117.02	109.03
4	D	5108	PLX	O6-C4-C3	2.51	116.97	109.03
4	B	5109	PLX	O6-C4-C3	2.51	116.96	109.03
4	A	5111	PLX	O6-C4-C3	2.51	116.95	109.03
4	B	5110	PLX	C8-C7-C6	-2.07	108.59	113.38
4	A	5112	PLX	C8-C7-C6	-2.06	108.61	113.38
4	C	5111	PLX	C8-C7-C6	-2.06	108.61	113.38
4	D	5109	PLX	C8-C7-C6	-2.06	108.61	113.38

There are no chirality outliers.

All (602) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	5108	PLX	O7-C6-O6-C4
4	A	5108	PLX	C3-O4-P1-O2
4	A	5108	PLX	C3-O4-P1-O3
4	A	5108	PLX	C2-O1-P1-O2
4	A	5108	PLX	C2-O1-P1-O3
4	A	5108	PLX	C25-C24-O8-C5
4	A	5108	PLX	O9-C24-C25-C26
4	A	5109	PLX	O7-C6-O6-C4
4	A	5109	PLX	C3-O4-P1-O3

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Mol	Chain	Res	Type	Atoms
4	A	5109	PLX	C25-C24-O8-C5
4	A	5110	PLX	C3-O4-P1-O2
4	A	5110	PLX	C3-O4-P1-O3
4	A	5110	PLX	N1-C1-C2-O1
4	A	5110	PLX	O9-C24-C25-C26
4	A	5111	PLX	O7-C6-O6-C4
4	A	5111	PLX	C3-C4-O6-C6
4	A	5111	PLX	C3-O4-P1-O2
4	A	5111	PLX	C3-O4-P1-O3
4	A	5111	PLX	C2-O1-P1-O2
4	A	5112	PLX	O7-C6-O6-C4
4	A	5112	PLX	C3-O4-P1-O2
4	A	5112	PLX	C3-O4-P1-O3
4	A	5112	PLX	N1-C1-C2-O1
4	A	5113	PLX	C3-C4-O6-C6
4	A	5113	PLX	C3-O4-P1-O2
4	A	5113	PLX	C3-O4-P1-O3
4	A	5113	PLX	C2-O1-P1-O2
4	A	5113	PLX	C2-O1-P1-O3
4	A	5114	PLX	C3-O4-P1-O2
4	A	5114	PLX	C3-O4-P1-O3
4	B	5107	PLX	O7-C6-O6-C4
4	B	5107	PLX	C3-O4-P1-O3
4	B	5107	PLX	C25-C24-O8-C5
4	B	5108	PLX	C3-O4-P1-O2
4	B	5108	PLX	C3-O4-P1-O3
4	B	5108	PLX	N1-C1-C2-O1
4	B	5108	PLX	O9-C24-C25-C26
4	B	5109	PLX	O7-C6-O6-C4
4	B	5109	PLX	C3-C4-O6-C6
4	B	5109	PLX	C3-O4-P1-O2
4	B	5109	PLX	C3-O4-P1-O3
4	B	5109	PLX	C2-O1-P1-O2
4	B	5110	PLX	O7-C6-O6-C4
4	B	5110	PLX	C3-O4-P1-O2
4	B	5110	PLX	C3-O4-P1-O3
4	B	5110	PLX	N1-C1-C2-O1
4	B	5111	PLX	C3-C4-O6-C6
4	B	5111	PLX	C3-O4-P1-O2
4	B	5111	PLX	C3-O4-P1-O3
4	B	5111	PLX	C2-O1-P1-O2
4	B	5111	PLX	C2-O1-P1-O3

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Mol	Chain	Res	Type	Atoms
4	B	5112	PLX	C3-O4-P1-O2
4	B	5112	PLX	C3-O4-P1-O3
4	B	5113	PLX	O7-C6-O6-C4
4	B	5113	PLX	C3-O4-P1-O2
4	B	5113	PLX	C3-O4-P1-O3
4	B	5113	PLX	C2-O1-P1-O2
4	B	5113	PLX	C2-O1-P1-O3
4	B	5113	PLX	C25-C24-O8-C5
4	B	5113	PLX	O9-C24-C25-C26
4	C	5107	PLX	O7-C6-O6-C4
4	C	5107	PLX	C3-O4-P1-O2
4	C	5107	PLX	C3-O4-P1-O3
4	C	5107	PLX	C2-O1-P1-O2
4	C	5107	PLX	C2-O1-P1-O3
4	C	5107	PLX	C25-C24-O8-C5
4	C	5107	PLX	O9-C24-C25-C26
4	C	5108	PLX	O7-C6-O6-C4
4	C	5108	PLX	C3-O4-P1-O3
4	C	5108	PLX	C25-C24-O8-C5
4	C	5109	PLX	C3-O4-P1-O2
4	C	5109	PLX	C3-O4-P1-O3
4	C	5109	PLX	N1-C1-C2-O1
4	C	5109	PLX	O9-C24-C25-C26
4	C	5110	PLX	O7-C6-O6-C4
4	C	5110	PLX	C3-C4-O6-C6
4	C	5110	PLX	C3-O4-P1-O2
4	C	5110	PLX	C3-O4-P1-O3
4	C	5110	PLX	C2-O1-P1-O2
4	C	5111	PLX	O7-C6-O6-C4
4	C	5111	PLX	C3-O4-P1-O2
4	C	5111	PLX	C3-O4-P1-O3
4	C	5111	PLX	N1-C1-C2-O1
4	C	5112	PLX	C3-C4-O6-C6
4	C	5112	PLX	C3-O4-P1-O2
4	C	5112	PLX	C3-O4-P1-O3
4	C	5112	PLX	C2-O1-P1-O2
4	C	5112	PLX	C2-O1-P1-O3
4	C	5113	PLX	C3-O4-P1-O2
4	C	5113	PLX	C3-O4-P1-O3
4	D	5106	PLX	O7-C6-O6-C4
4	D	5106	PLX	C3-O4-P1-O3
4	D	5106	PLX	C25-C24-O8-C5

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Mol	Chain	Res	Type	Atoms
4	D	5107	PLX	C3-O4-P1-O2
4	D	5107	PLX	C3-O4-P1-O3
4	D	5107	PLX	N1-C1-C2-O1
4	D	5107	PLX	O9-C24-C25-C26
4	D	5108	PLX	O7-C6-O6-C4
4	D	5108	PLX	C3-C4-O6-C6
4	D	5108	PLX	C3-O4-P1-O2
4	D	5108	PLX	C3-O4-P1-O3
4	D	5108	PLX	C2-O1-P1-O2
4	D	5109	PLX	O7-C6-O6-C4
4	D	5109	PLX	C3-O4-P1-O2
4	D	5109	PLX	C3-O4-P1-O3
4	D	5109	PLX	N1-C1-C2-O1
4	D	5110	PLX	C3-C4-O6-C6
4	D	5110	PLX	C3-O4-P1-O2
4	D	5110	PLX	C3-O4-P1-O3
4	D	5110	PLX	C2-O1-P1-O2
4	D	5110	PLX	C2-O1-P1-O3
4	D	5111	PLX	C3-O4-P1-O2
4	D	5111	PLX	C3-O4-P1-O3
4	D	5112	PLX	O7-C6-O6-C4
4	D	5112	PLX	C3-O4-P1-O2
4	D	5112	PLX	C3-O4-P1-O3
4	D	5112	PLX	C2-O1-P1-O2
4	D	5112	PLX	C2-O1-P1-O3
4	D	5112	PLX	C25-C24-O8-C5
4	D	5112	PLX	O9-C24-C25-C26
4	A	5109	PLX	C28-C29-C30-C31
4	B	5107	PLX	C28-C29-C30-C31
4	C	5108	PLX	C28-C29-C30-C31
4	D	5106	PLX	C28-C29-C30-C31
4	A	5109	PLX	C33-C34-C35-C36
4	B	5107	PLX	C33-C34-C35-C36
4	C	5108	PLX	C33-C34-C35-C36
4	D	5106	PLX	C33-C34-C35-C36
4	A	5108	PLX	C3-O4-P1-O1
4	A	5109	PLX	C3-O4-P1-O1
4	A	5109	PLX	C2-O1-P1-O4
4	A	5110	PLX	C3-O4-P1-O1
4	A	5110	PLX	C2-O1-P1-O4
4	A	5111	PLX	C3-O4-P1-O1
4	A	5111	PLX	C2-O1-P1-O4

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Mol	Chain	Res	Type	Atoms
4	A	5112	PLX	C3-O4-P1-O1
4	A	5112	PLX	C2-O1-P1-O4
4	A	5113	PLX	C3-O4-P1-O1
4	A	5113	PLX	C2-O1-P1-O4
4	A	5114	PLX	C3-O4-P1-O1
4	B	5107	PLX	C3-O4-P1-O1
4	B	5107	PLX	C2-O1-P1-O4
4	B	5108	PLX	C3-O4-P1-O1
4	B	5108	PLX	C2-O1-P1-O4
4	B	5109	PLX	C3-O4-P1-O1
4	B	5109	PLX	C2-O1-P1-O4
4	B	5110	PLX	C3-O4-P1-O1
4	B	5110	PLX	C2-O1-P1-O4
4	B	5111	PLX	C3-O4-P1-O1
4	B	5111	PLX	C2-O1-P1-O4
4	B	5112	PLX	C3-O4-P1-O1
4	B	5113	PLX	C3-O4-P1-O1
4	C	5107	PLX	C3-O4-P1-O1
4	C	5108	PLX	C3-O4-P1-O1
4	C	5108	PLX	C2-O1-P1-O4
4	C	5109	PLX	C3-O4-P1-O1
4	C	5109	PLX	C2-O1-P1-O4
4	C	5110	PLX	C3-O4-P1-O1
4	C	5110	PLX	C2-O1-P1-O4
4	C	5111	PLX	C3-O4-P1-O1
4	C	5111	PLX	C2-O1-P1-O4
4	C	5112	PLX	C3-O4-P1-O1
4	C	5112	PLX	C2-O1-P1-O4
4	C	5113	PLX	C3-O4-P1-O1
4	D	5106	PLX	C3-O4-P1-O1
4	D	5106	PLX	C2-O1-P1-O4
4	D	5107	PLX	C3-O4-P1-O1
4	D	5107	PLX	C2-O1-P1-O4
4	D	5108	PLX	C3-O4-P1-O1
4	D	5108	PLX	C2-O1-P1-O4
4	D	5109	PLX	C3-O4-P1-O1
4	D	5109	PLX	C2-O1-P1-O4
4	D	5110	PLX	C3-O4-P1-O1
4	D	5110	PLX	C2-O1-P1-O4
4	D	5111	PLX	C3-O4-P1-O1
4	D	5112	PLX	C3-O4-P1-O1
4	A	5109	PLX	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
4	B	5107	PLX	C10-C11-C12-C13
4	B	5113	PLX	C35-C36-C37-C38
4	C	5108	PLX	C10-C11-C12-C13
4	D	5106	PLX	C10-C11-C12-C13
4	A	5108	PLX	C11-C10-C9-C8
4	A	5108	PLX	C34-C35-C36-C37
4	A	5108	PLX	C35-C36-C37-C38
4	A	5110	PLX	C11-C10-C9-C8
4	A	5112	PLX	C25-C26-C27-C28
4	B	5108	PLX	C11-C10-C9-C8
4	B	5110	PLX	C25-C26-C27-C28
4	B	5113	PLX	C11-C10-C9-C8
4	C	5107	PLX	C11-C10-C9-C8
4	C	5107	PLX	C35-C36-C37-C38
4	C	5109	PLX	C11-C10-C9-C8
4	C	5111	PLX	C25-C26-C27-C28
4	D	5107	PLX	C11-C10-C9-C8
4	D	5109	PLX	C25-C26-C27-C28
4	D	5112	PLX	C11-C10-C9-C8
4	D	5112	PLX	C34-C35-C36-C37
4	D	5112	PLX	C35-C36-C37-C38
4	B	5113	PLX	C34-C35-C36-C37
4	C	5107	PLX	C34-C35-C36-C37
4	A	5112	PLX	C30-C31-C32-C33
4	B	5107	PLX	C30-C31-C32-C33
4	B	5110	PLX	C30-C31-C32-C33
4	C	5111	PLX	C30-C31-C32-C33
4	D	5109	PLX	C30-C31-C32-C33
4	A	5109	PLX	C30-C31-C32-C33
4	C	5108	PLX	C30-C31-C32-C33
4	D	5106	PLX	C30-C31-C32-C33
4	D	5108	PLX	C7-C8-C9-C10
4	A	5109	PLX	C11-C12-C13-C14
4	A	5110	PLX	C30-C31-C32-C33
4	A	5111	PLX	C9-C10-C11-C12
4	A	5111	PLX	C7-C8-C9-C10
4	A	5111	PLX	C27-C28-C29-C30
4	B	5108	PLX	C30-C31-C32-C33
4	B	5109	PLX	C9-C10-C11-C12
4	B	5109	PLX	C7-C8-C9-C10
4	B	5109	PLX	C27-C28-C29-C30
4	B	5113	PLX	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
4	C	5109	PLX	C30-C31-C32-C33
4	C	5110	PLX	C9-C10-C11-C12
4	C	5110	PLX	C7-C8-C9-C10
4	C	5110	PLX	C27-C28-C29-C30
4	D	5107	PLX	C30-C31-C32-C33
4	D	5108	PLX	C9-C10-C11-C12
4	D	5108	PLX	C27-C28-C29-C30
4	A	5108	PLX	C10-C11-C12-C13
4	A	5108	PLX	C30-C31-C32-C33
4	B	5107	PLX	C11-C12-C13-C14
4	B	5113	PLX	C10-C11-C12-C13
4	C	5107	PLX	C10-C11-C12-C13
4	C	5107	PLX	C30-C31-C32-C33
4	C	5108	PLX	C11-C12-C13-C14
4	D	5106	PLX	C11-C12-C13-C14
4	D	5112	PLX	C10-C11-C12-C13
4	D	5112	PLX	C30-C31-C32-C33
4	A	5108	PLX	C25-C26-C27-C28
4	B	5113	PLX	C25-C26-C27-C28
4	C	5107	PLX	C25-C26-C27-C28
4	D	5112	PLX	C25-C26-C27-C28
4	A	5109	PLX	C11-C10-C9-C8
4	B	5107	PLX	C27-C28-C29-C30
4	C	5108	PLX	C11-C10-C9-C8
4	D	5106	PLX	C11-C10-C9-C8
4	A	5111	PLX	O7-C6-C7-C8
4	A	5111	PLX	O9-C24-C25-C26
4	B	5109	PLX	O7-C6-C7-C8
4	B	5109	PLX	O9-C24-C25-C26
4	C	5110	PLX	O7-C6-C7-C8
4	C	5110	PLX	O9-C24-C25-C26
4	D	5108	PLX	O7-C6-C7-C8
4	D	5108	PLX	O9-C24-C25-C26
4	A	5109	PLX	C27-C28-C29-C30
4	A	5113	PLX	C25-C26-C27-C28
4	B	5107	PLX	C11-C10-C9-C8
4	C	5108	PLX	C27-C28-C29-C30
4	D	5106	PLX	C27-C28-C29-C30
4	D	5110	PLX	C25-C26-C27-C28
4	B	5111	PLX	C25-C26-C27-C28
4	C	5112	PLX	C25-C26-C27-C28
4	A	5108	PLX	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
4	A	5114	PLX	C28-C29-C30-C31
4	B	5112	PLX	C28-C29-C30-C31
4	B	5113	PLX	C26-C27-C28-C29
4	C	5107	PLX	C26-C27-C28-C29
4	C	5113	PLX	C28-C29-C30-C31
4	D	5111	PLX	C28-C29-C30-C31
4	D	5112	PLX	C26-C27-C28-C29
4	A	5110	PLX	C25-C26-C27-C28
4	A	5112	PLX	C27-C28-C29-C30
4	B	5108	PLX	C25-C26-C27-C28
4	C	5109	PLX	C25-C26-C27-C28
4	C	5111	PLX	C27-C28-C29-C30
4	D	5107	PLX	C25-C26-C27-C28
4	B	5110	PLX	C27-C28-C29-C30
4	D	5109	PLX	C27-C28-C29-C30
4	A	5111	PLX	C26-C27-C28-C29
4	B	5109	PLX	C26-C27-C28-C29
4	C	5110	PLX	C26-C27-C28-C29
4	D	5108	PLX	C26-C27-C28-C29
4	A	5109	PLX	C35-C36-C37-C38
4	B	5107	PLX	C35-C36-C37-C38
4	C	5108	PLX	C35-C36-C37-C38
4	D	5106	PLX	C35-C36-C37-C38
4	A	5113	PLX	C26-C27-C28-C29
4	B	5111	PLX	C26-C27-C28-C29
4	C	5112	PLX	C26-C27-C28-C29
4	D	5110	PLX	C26-C27-C28-C29
4	A	5110	PLX	O6-C4-C5-O8
4	B	5108	PLX	O6-C4-C5-O8
4	C	5109	PLX	O6-C4-C5-O8
4	D	5107	PLX	O6-C4-C5-O8
4	B	5111	PLX	C13-C14-C15-C16
4	A	5113	PLX	C13-C14-C15-C16
4	C	5112	PLX	C13-C14-C15-C16
4	D	5110	PLX	C13-C14-C15-C16
4	A	5108	PLX	C2-O1-P1-O4
4	B	5113	PLX	C2-O1-P1-O4
4	C	5107	PLX	C2-O1-P1-O4
4	D	5112	PLX	C2-O1-P1-O4
4	A	5109	PLX	C4-C3-O4-P1
4	B	5107	PLX	C4-C3-O4-P1
4	C	5108	PLX	C4-C3-O4-P1

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Mol	Chain	Res	Type	Atoms
4	D	5106	PLX	C4-C3-O4-P1
4	A	5108	PLX	O4-C3-C4-C5
4	A	5110	PLX	O4-C3-C4-C5
4	A	5112	PLX	O4-C3-C4-C5
4	A	5114	PLX	O4-C3-C4-C5
4	B	5108	PLX	O4-C3-C4-C5
4	B	5110	PLX	O4-C3-C4-C5
4	B	5112	PLX	O4-C3-C4-C5
4	B	5113	PLX	O4-C3-C4-C5
4	C	5107	PLX	O4-C3-C4-C5
4	C	5109	PLX	O4-C3-C4-C5
4	C	5111	PLX	O4-C3-C4-C5
4	C	5113	PLX	O4-C3-C4-C5
4	D	5107	PLX	O4-C3-C4-C5
4	D	5109	PLX	O4-C3-C4-C5
4	D	5111	PLX	O4-C3-C4-C5
4	D	5112	PLX	O4-C3-C4-C5
4	B	5107	PLX	C32-C33-C34-C35
4	D	5106	PLX	C32-C33-C34-C35
4	A	5109	PLX	C32-C33-C34-C35
4	C	5108	PLX	C32-C33-C34-C35
4	A	5114	PLX	C27-C28-C29-C30
4	C	5113	PLX	C27-C28-C29-C30
4	D	5111	PLX	C27-C28-C29-C30
4	B	5112	PLX	C27-C28-C29-C30
4	A	5108	PLX	C3-C4-C5-O8
4	B	5113	PLX	C3-C4-C5-O8
4	C	5107	PLX	C3-C4-C5-O8
4	D	5112	PLX	C3-C4-C5-O8
4	A	5110	PLX	C31-C32-C33-C34
4	B	5108	PLX	C31-C32-C33-C34
4	C	5109	PLX	C31-C32-C33-C34
4	D	5107	PLX	C31-C32-C33-C34
4	A	5108	PLX	O6-C6-C7-C8
4	B	5113	PLX	O6-C6-C7-C8
4	C	5107	PLX	O6-C6-C7-C8
4	D	5112	PLX	O6-C6-C7-C8
4	A	5108	PLX	C27-C28-C29-C30
4	B	5113	PLX	C27-C28-C29-C30
4	C	5107	PLX	C27-C28-C29-C30
4	D	5112	PLX	C27-C28-C29-C30
4	C	5112	PLX	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
4	D	5110	PLX	C27-C28-C29-C30
4	A	5113	PLX	C27-C28-C29-C30
4	B	5111	PLX	C27-C28-C29-C30
4	A	5110	PLX	C3-C4-C5-O8
4	A	5113	PLX	C3-C4-C5-O8
4	B	5108	PLX	C3-C4-C5-O8
4	B	5111	PLX	C3-C4-C5-O8
4	C	5109	PLX	C3-C4-C5-O8
4	C	5112	PLX	C3-C4-C5-O8
4	D	5107	PLX	C3-C4-C5-O8
4	D	5110	PLX	C3-C4-C5-O8
4	A	5111	PLX	C10-C11-C12-C13
4	B	5109	PLX	C10-C11-C12-C13
4	D	5108	PLX	C10-C11-C12-C13
4	C	5110	PLX	C10-C11-C12-C13
4	A	5112	PLX	C3-C4-O6-C6
4	A	5112	PLX	C5-C4-O6-C6
4	B	5110	PLX	C3-C4-O6-C6
4	B	5110	PLX	C5-C4-O6-C6
4	C	5111	PLX	C3-C4-O6-C6
4	C	5111	PLX	C5-C4-O6-C6
4	D	5109	PLX	C3-C4-O6-C6
4	D	5109	PLX	C5-C4-O6-C6
4	A	5109	PLX	O7-C6-C7-C8
4	A	5112	PLX	O9-C24-C25-C26
4	B	5107	PLX	O7-C6-C7-C8
4	B	5110	PLX	O9-C24-C25-C26
4	C	5108	PLX	O7-C6-C7-C8
4	C	5111	PLX	O9-C24-C25-C26
4	D	5106	PLX	O7-C6-C7-C8
4	D	5109	PLX	O9-C24-C25-C26
4	A	5108	PLX	O4-C3-C4-O6
4	A	5112	PLX	O4-C3-C4-O6
4	B	5110	PLX	O4-C3-C4-O6
4	B	5113	PLX	O4-C3-C4-O6
4	C	5107	PLX	O4-C3-C4-O6
4	C	5111	PLX	O4-C3-C4-O6
4	D	5109	PLX	O4-C3-C4-O6
4	D	5112	PLX	O4-C3-C4-O6
4	A	5114	PLX	C30-C31-C32-C33
4	B	5112	PLX	C30-C31-C32-C33
4	D	5111	PLX	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
4	C	5113	PLX	C30-C31-C32-C33
4	A	5114	PLX	C29-C30-C31-C32
4	B	5112	PLX	C29-C30-C31-C32
4	C	5113	PLX	C29-C30-C31-C32
4	D	5111	PLX	C29-C30-C31-C32
4	A	5114	PLX	C10-C11-C12-C13
4	A	5112	PLX	C7-C8-C9-C10
4	B	5110	PLX	C7-C8-C9-C10
4	B	5112	PLX	C10-C11-C12-C13
4	C	5111	PLX	C7-C8-C9-C10
4	C	5113	PLX	C10-C11-C12-C13
4	D	5109	PLX	C7-C8-C9-C10
4	D	5111	PLX	C10-C11-C12-C13
4	A	5108	PLX	O8-C24-C25-C26
4	A	5110	PLX	O8-C24-C25-C26
4	A	5111	PLX	O6-C6-C7-C8
4	B	5108	PLX	O8-C24-C25-C26
4	B	5109	PLX	O6-C6-C7-C8
4	B	5113	PLX	O8-C24-C25-C26
4	C	5107	PLX	O8-C24-C25-C26
4	C	5109	PLX	O8-C24-C25-C26
4	C	5110	PLX	O6-C6-C7-C8
4	D	5107	PLX	O8-C24-C25-C26
4	D	5108	PLX	O6-C6-C7-C8
4	D	5112	PLX	O8-C24-C25-C26
4	B	5108	PLX	C7-C8-C9-C10
4	A	5110	PLX	O4-C3-C4-O6
4	A	5113	PLX	O4-C3-C4-O6
4	B	5108	PLX	O4-C3-C4-O6
4	B	5111	PLX	O4-C3-C4-O6
4	C	5109	PLX	O4-C3-C4-O6
4	C	5112	PLX	O4-C3-C4-O6
4	D	5107	PLX	O4-C3-C4-O6
4	D	5110	PLX	O4-C3-C4-O6
4	D	5107	PLX	C7-C8-C9-C10
4	A	5110	PLX	C7-C8-C9-C10
4	C	5109	PLX	C7-C8-C9-C10
4	A	5109	PLX	C24-C25-C26-C27
4	B	5107	PLX	C24-C25-C26-C27
4	C	5108	PLX	C24-C25-C26-C27
4	D	5106	PLX	C24-C25-C26-C27
4	A	5108	PLX	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
4	B	5113	PLX	C28-C29-C30-C31
4	C	5107	PLX	C28-C29-C30-C31
4	D	5112	PLX	C28-C29-C30-C31
4	D	5112	PLX	C9-C10-C11-C12
4	A	5112	PLX	C4-C3-O4-P1
4	B	5110	PLX	C4-C3-O4-P1
4	C	5111	PLX	C4-C3-O4-P1
4	D	5109	PLX	C4-C3-O4-P1
4	B	5113	PLX	C9-C10-C11-C12
4	C	5107	PLX	C9-C10-C11-C12
4	A	5109	PLX	C2-O1-P1-O2
4	A	5109	PLX	C2-O1-P1-O3
4	A	5110	PLX	C2-O1-P1-O3
4	A	5111	PLX	C2-O1-P1-O3
4	A	5112	PLX	C2-O1-P1-O3
4	B	5107	PLX	C2-O1-P1-O2
4	B	5107	PLX	C2-O1-P1-O3
4	B	5108	PLX	C2-O1-P1-O3
4	B	5109	PLX	C2-O1-P1-O3
4	B	5110	PLX	C2-O1-P1-O3
4	C	5108	PLX	C2-O1-P1-O2
4	C	5108	PLX	C2-O1-P1-O3
4	C	5109	PLX	C2-O1-P1-O3
4	C	5110	PLX	C2-O1-P1-O3
4	C	5111	PLX	C2-O1-P1-O3
4	D	5106	PLX	C2-O1-P1-O2
4	D	5106	PLX	C2-O1-P1-O3
4	D	5107	PLX	C2-O1-P1-O3
4	D	5108	PLX	C2-O1-P1-O3
4	D	5109	PLX	C2-O1-P1-O3
4	A	5108	PLX	C9-C10-C11-C12
4	A	5113	PLX	O4-C3-C4-C5
4	B	5111	PLX	O4-C3-C4-C5
4	C	5112	PLX	O4-C3-C4-C5
4	D	5110	PLX	O4-C3-C4-C5
4	A	5110	PLX	C25-C24-O8-C5
4	A	5114	PLX	C25-C24-O8-C5
4	B	5108	PLX	C25-C24-O8-C5
4	B	5112	PLX	C25-C24-O8-C5
4	C	5109	PLX	C25-C24-O8-C5
4	C	5113	PLX	C25-C24-O8-C5
4	D	5107	PLX	C25-C24-O8-C5

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Mol	Chain	Res	Type	Atoms
4	D	5111	PLX	C25-C24-O8-C5
4	D	5109	PLX	C11-C10-C9-C8
4	B	5110	PLX	C11-C10-C9-C8
4	A	5112	PLX	C11-C10-C9-C8
4	C	5111	PLX	C11-C10-C9-C8
4	A	5108	PLX	N1-C1-C2-O1
4	A	5112	PLX	C3-C4-C5-O8
4	A	5113	PLX	N1-C1-C2-O1
4	A	5114	PLX	N1-C1-C2-O1
4	B	5110	PLX	C3-C4-C5-O8
4	B	5111	PLX	N1-C1-C2-O1
4	B	5112	PLX	N1-C1-C2-O1
4	B	5113	PLX	N1-C1-C2-O1
4	C	5107	PLX	N1-C1-C2-O1
4	C	5111	PLX	C3-C4-C5-O8
4	C	5112	PLX	N1-C1-C2-O1
4	C	5113	PLX	N1-C1-C2-O1
4	D	5109	PLX	C3-C4-C5-O8
4	D	5110	PLX	N1-C1-C2-O1
4	D	5111	PLX	N1-C1-C2-O1
4	D	5112	PLX	N1-C1-C2-O1
4	A	5112	PLX	O6-C4-C5-O8
4	A	5113	PLX	O6-C4-C5-O8
4	B	5110	PLX	O6-C4-C5-O8
4	B	5111	PLX	O6-C4-C5-O8
4	C	5111	PLX	O6-C4-C5-O8
4	C	5112	PLX	O6-C4-C5-O8
4	D	5109	PLX	O6-C4-C5-O8
4	D	5110	PLX	O6-C4-C5-O8
4	B	5112	PLX	O7-C6-C7-C8
4	C	5113	PLX	O7-C6-C7-C8
4	D	5111	PLX	O7-C6-C7-C8
4	A	5108	PLX	C7-C8-C9-C10
4	B	5113	PLX	C7-C8-C9-C10
4	D	5112	PLX	C7-C8-C9-C10
4	C	5107	PLX	C7-C8-C9-C10
4	A	5114	PLX	O4-C3-C4-O6
4	B	5112	PLX	O4-C3-C4-O6
4	C	5113	PLX	O4-C3-C4-O6
4	D	5111	PLX	O4-C3-C4-O6
4	A	5108	PLX	O6-C4-C5-O8
4	B	5113	PLX	O6-C4-C5-O8

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Mol	Chain	Res	Type	Atoms
4	C	5107	PLX	O6-C4-C5-O8
4	D	5112	PLX	O6-C4-C5-O8
4	A	5111	PLX	C24-C25-C26-C27
4	B	5109	PLX	C24-C25-C26-C27
4	C	5110	PLX	C24-C25-C26-C27
4	D	5108	PLX	C24-C25-C26-C27
4	A	5112	PLX	C24-C25-C26-C27
4	A	5113	PLX	C6-C7-C8-C9
4	A	5114	PLX	C24-C25-C26-C27
4	B	5110	PLX	C24-C25-C26-C27
4	B	5111	PLX	C6-C7-C8-C9
4	B	5112	PLX	C24-C25-C26-C27
4	C	5111	PLX	C24-C25-C26-C27
4	C	5112	PLX	C6-C7-C8-C9
4	C	5113	PLX	C24-C25-C26-C27
4	D	5109	PLX	C24-C25-C26-C27
4	D	5110	PLX	C6-C7-C8-C9
4	D	5111	PLX	C24-C25-C26-C27
4	C	5111	PLX	C28-C29-C30-C31
4	D	5109	PLX	C28-C29-C30-C31
4	A	5112	PLX	C28-C29-C30-C31
4	A	5110	PLX	C6-C7-C8-C9
4	B	5108	PLX	C6-C7-C8-C9
4	C	5109	PLX	C6-C7-C8-C9
4	D	5107	PLX	C6-C7-C8-C9
4	B	5110	PLX	C28-C29-C30-C31
4	A	5112	PLX	O8-C24-C25-C26
4	B	5110	PLX	O8-C24-C25-C26
4	C	5111	PLX	O8-C24-C25-C26
4	D	5109	PLX	O8-C24-C25-C26
4	A	5109	PLX	C12-C13-C14-C15
4	B	5107	PLX	C12-C13-C14-C15
4	C	5108	PLX	C12-C13-C14-C15
4	D	5106	PLX	C12-C13-C14-C15
4	A	5113	PLX	C24-C25-C26-C27
4	B	5111	PLX	C24-C25-C26-C27
4	C	5112	PLX	C24-C25-C26-C27
4	D	5110	PLX	C24-C25-C26-C27
4	B	5113	PLX	C32-C33-C34-C35
4	C	5107	PLX	C32-C33-C34-C35
4	D	5112	PLX	C32-C33-C34-C35
4	A	5108	PLX	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
4	A	5109	PLX	C5-C4-O6-C6
4	B	5107	PLX	C5-C4-O6-C6
4	C	5108	PLX	C5-C4-O6-C6
4	D	5106	PLX	C5-C4-O6-C6
4	A	5114	PLX	O7-C6-C7-C8
4	A	5109	PLX	C3-C4-C5-O8
4	B	5107	PLX	C3-C4-C5-O8
4	C	5108	PLX	C3-C4-C5-O8
4	D	5106	PLX	C3-C4-C5-O8
4	A	5109	PLX	O8-C24-C25-C26
4	B	5107	PLX	O8-C24-C25-C26
4	C	5108	PLX	O8-C24-C25-C26
4	D	5106	PLX	O8-C24-C25-C26
4	A	5108	PLX	C11-C12-C13-C14
4	D	5112	PLX	C11-C12-C13-C14
4	B	5113	PLX	C11-C12-C13-C14
4	C	5107	PLX	C11-C12-C13-C14
4	C	5112	PLX	C7-C8-C9-C10
4	D	5110	PLX	C7-C8-C9-C10
4	A	5113	PLX	C7-C8-C9-C10
4	B	5111	PLX	C7-C8-C9-C10
4	C	5110	PLX	C29-C30-C31-C32
4	D	5108	PLX	C29-C30-C31-C32
4	B	5109	PLX	C29-C30-C31-C32
4	A	5111	PLX	C29-C30-C31-C32
4	A	5108	PLX	C24-C25-C26-C27
4	A	5112	PLX	C6-C7-C8-C9
4	B	5110	PLX	C6-C7-C8-C9
4	B	5113	PLX	C24-C25-C26-C27
4	C	5107	PLX	C24-C25-C26-C27
4	C	5111	PLX	C6-C7-C8-C9
4	D	5109	PLX	C6-C7-C8-C9
4	D	5112	PLX	C24-C25-C26-C27
4	A	5109	PLX	C1-C2-O1-P1
4	A	5112	PLX	C1-C2-O1-P1
4	A	5112	PLX	C25-C24-O8-C5
4	B	5107	PLX	C1-C2-O1-P1
4	B	5110	PLX	C1-C2-O1-P1
4	B	5110	PLX	C25-C24-O8-C5
4	C	5108	PLX	C1-C2-O1-P1
4	C	5111	PLX	C1-C2-O1-P1
4	C	5111	PLX	C25-C24-O8-C5

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Mol	Chain	Res	Type	Atoms
4	D	5106	PLX	C1-C2-O1-P1
4	D	5109	PLX	C1-C2-O1-P1
4	D	5109	PLX	C25-C24-O8-C5
4	A	5110	PLX	C9-C10-C11-C12
4	C	5109	PLX	C9-C10-C11-C12

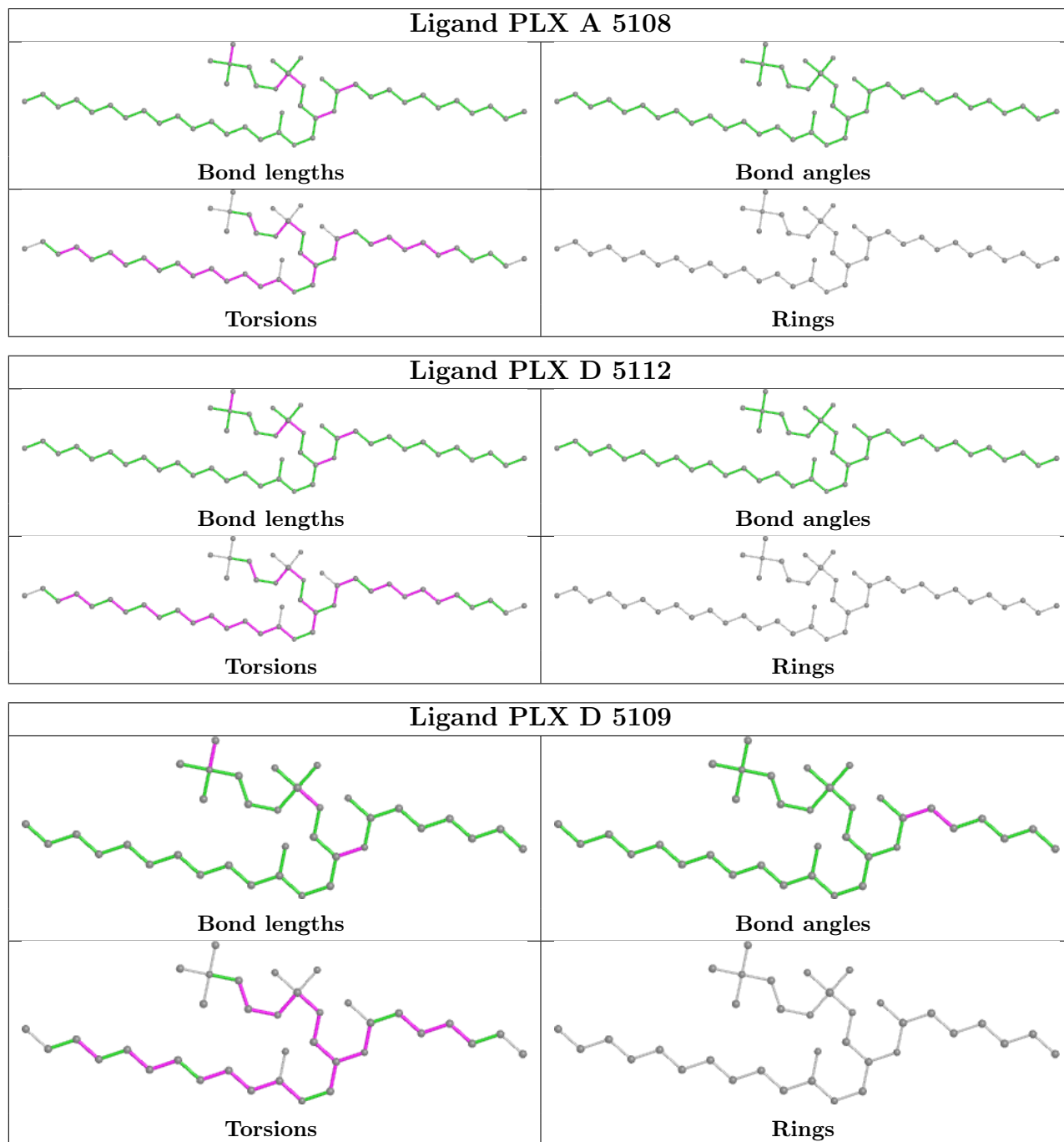
There are no ring outliers.

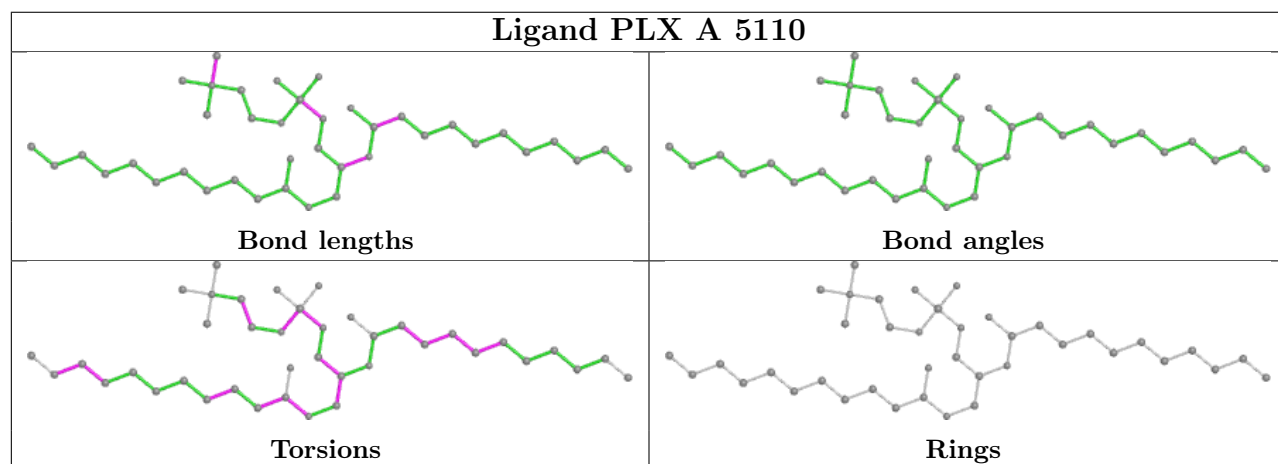
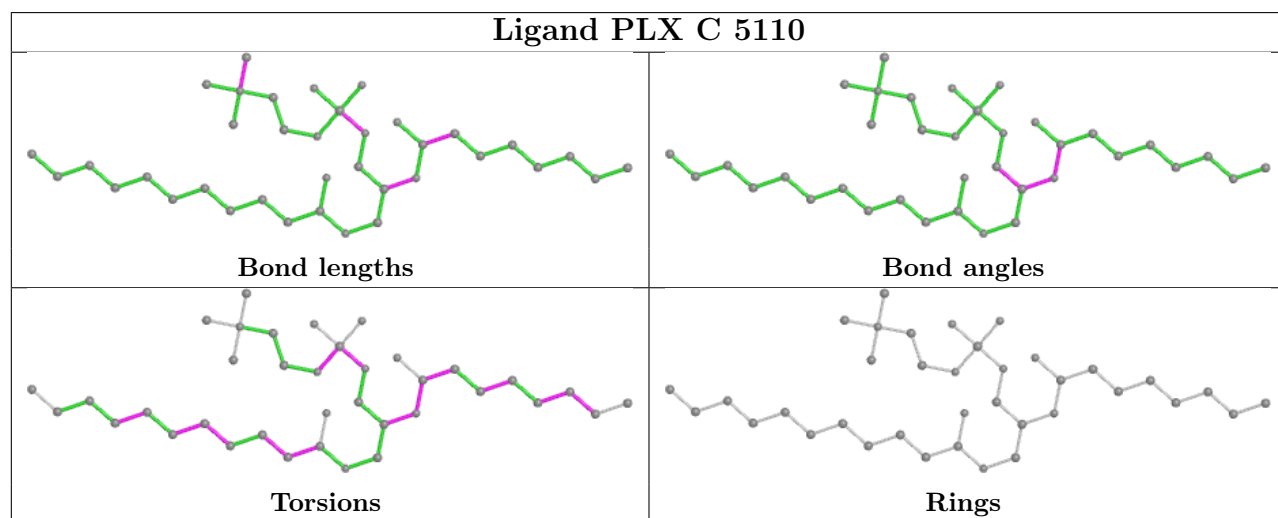
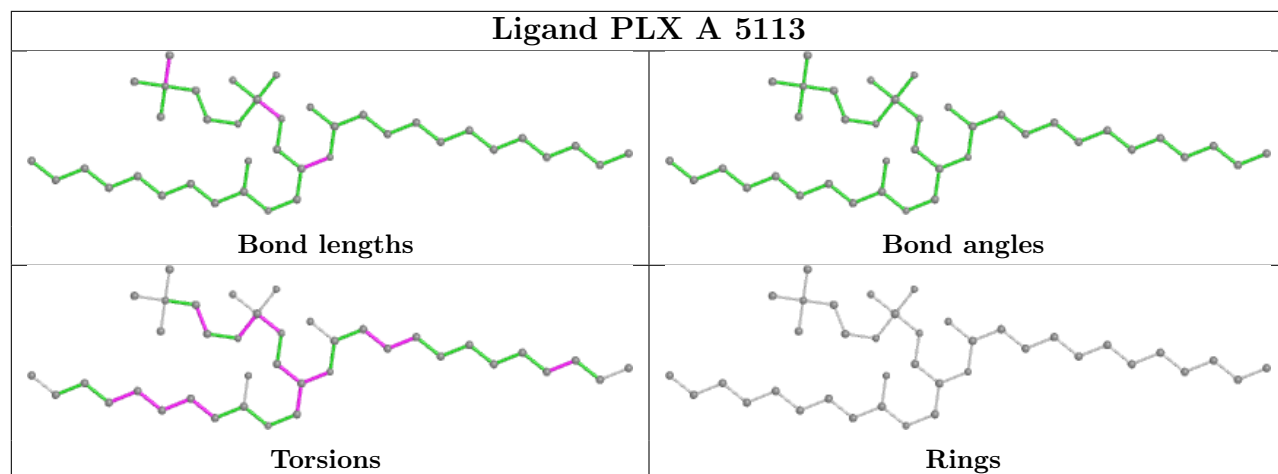
28 monomers are involved in 83 short contacts:

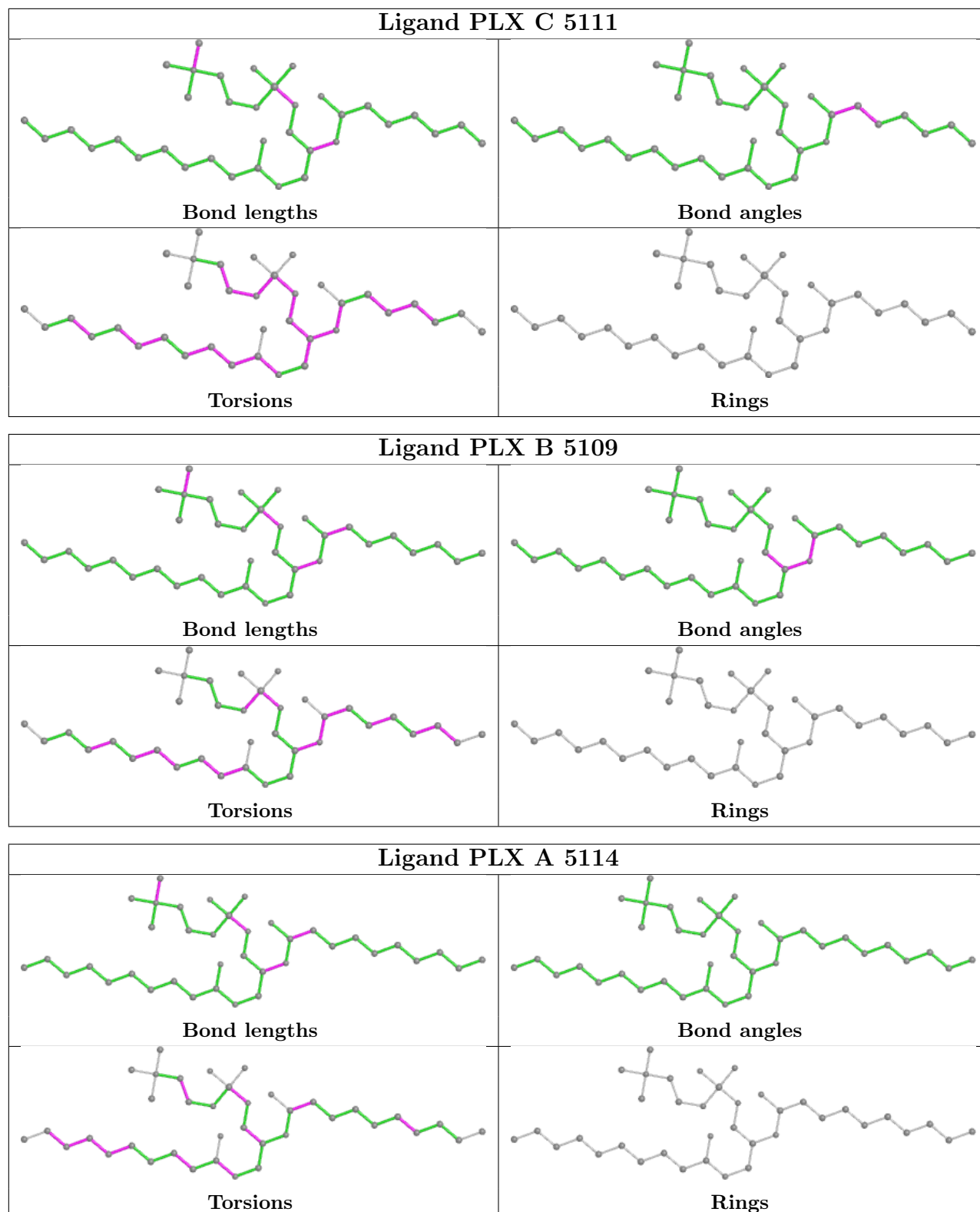
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	5108	PLX	4	0
4	D	5112	PLX	2	0
4	D	5109	PLX	3	0
4	A	5113	PLX	2	0
4	C	5110	PLX	4	0
4	A	5110	PLX	3	0
4	C	5111	PLX	3	0
4	B	5109	PLX	3	0
4	A	5114	PLX	3	0
4	B	5113	PLX	2	0
4	D	5110	PLX	3	0
4	C	5113	PLX	3	0
4	B	5108	PLX	3	0
4	D	5108	PLX	5	0
4	C	5109	PLX	3	0
4	A	5109	PLX	4	0
4	B	5107	PLX	4	0
4	B	5110	PLX	2	0
4	D	5106	PLX	3	0
4	B	5112	PLX	3	0
4	A	5111	PLX	4	0
4	C	5112	PLX	2	0
4	B	5111	PLX	3	0
4	A	5112	PLX	1	0
4	D	5107	PLX	3	0
4	C	5107	PLX	1	0
4	C	5108	PLX	3	0
4	D	5111	PLX	4	0

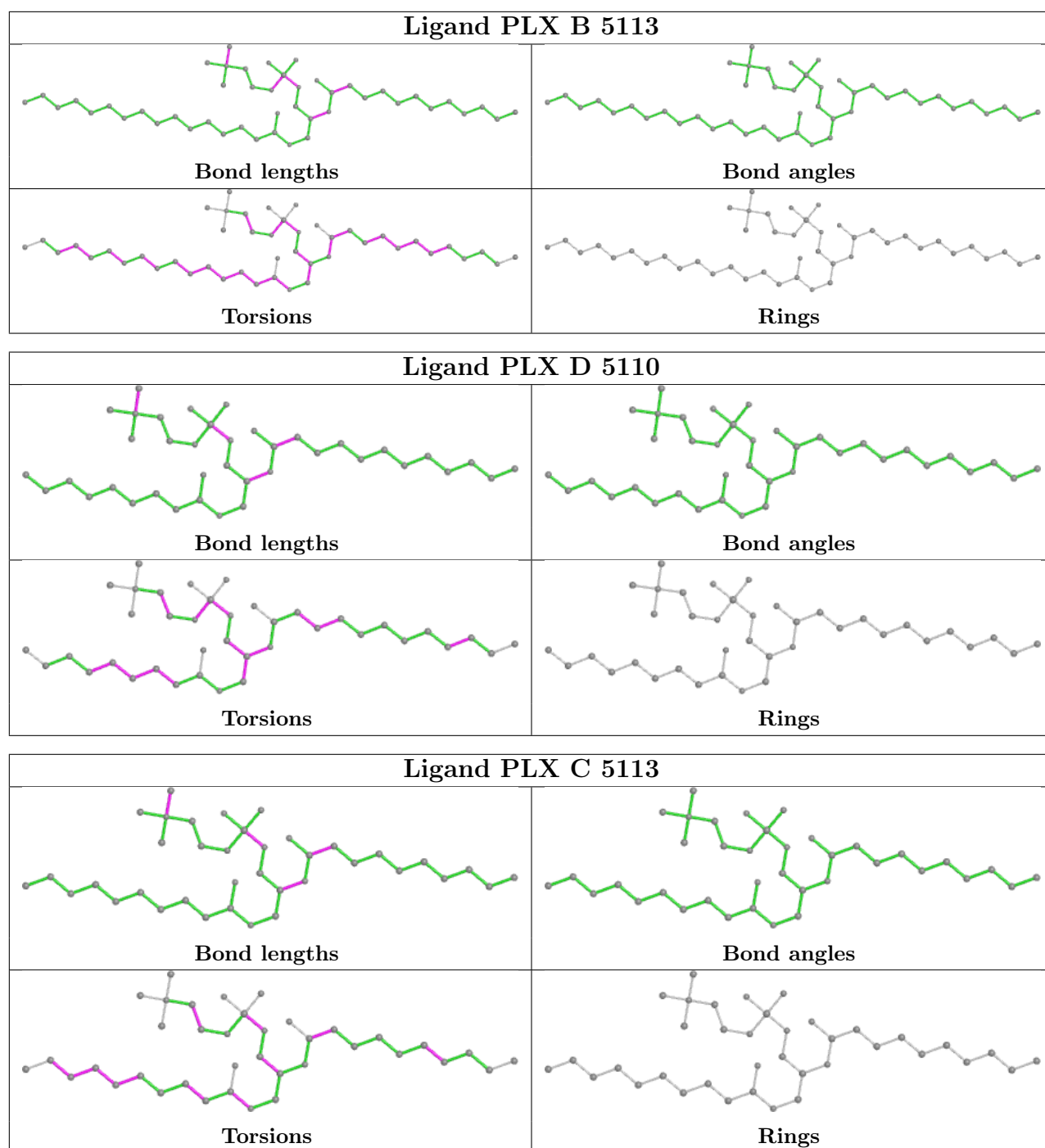
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

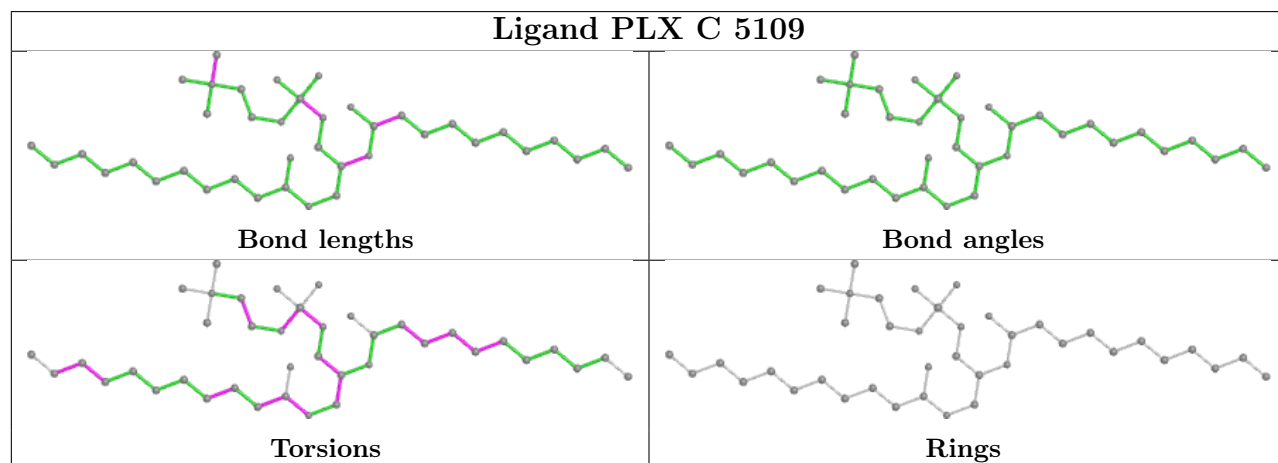
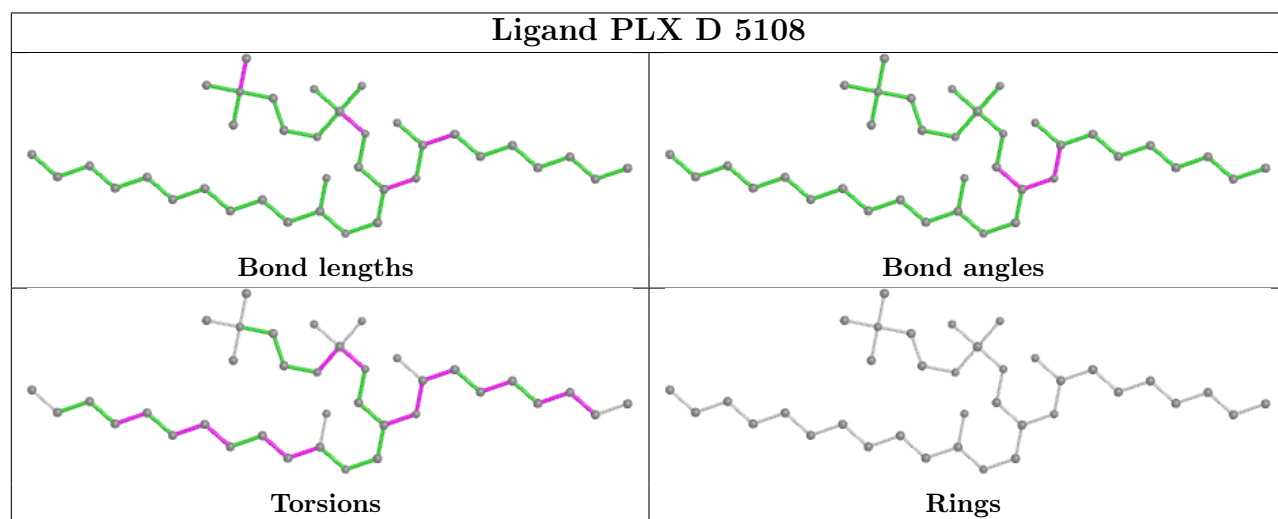
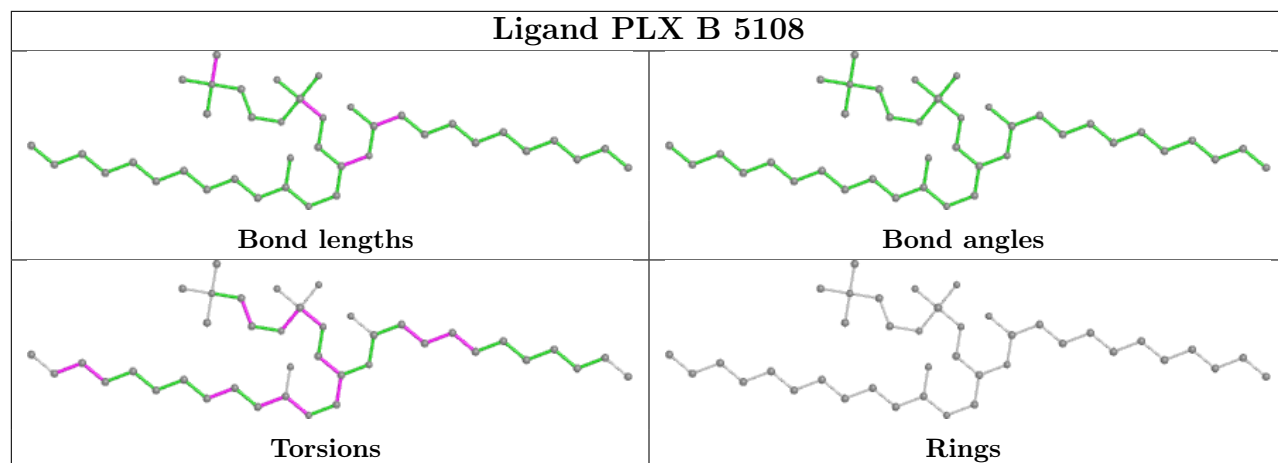
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

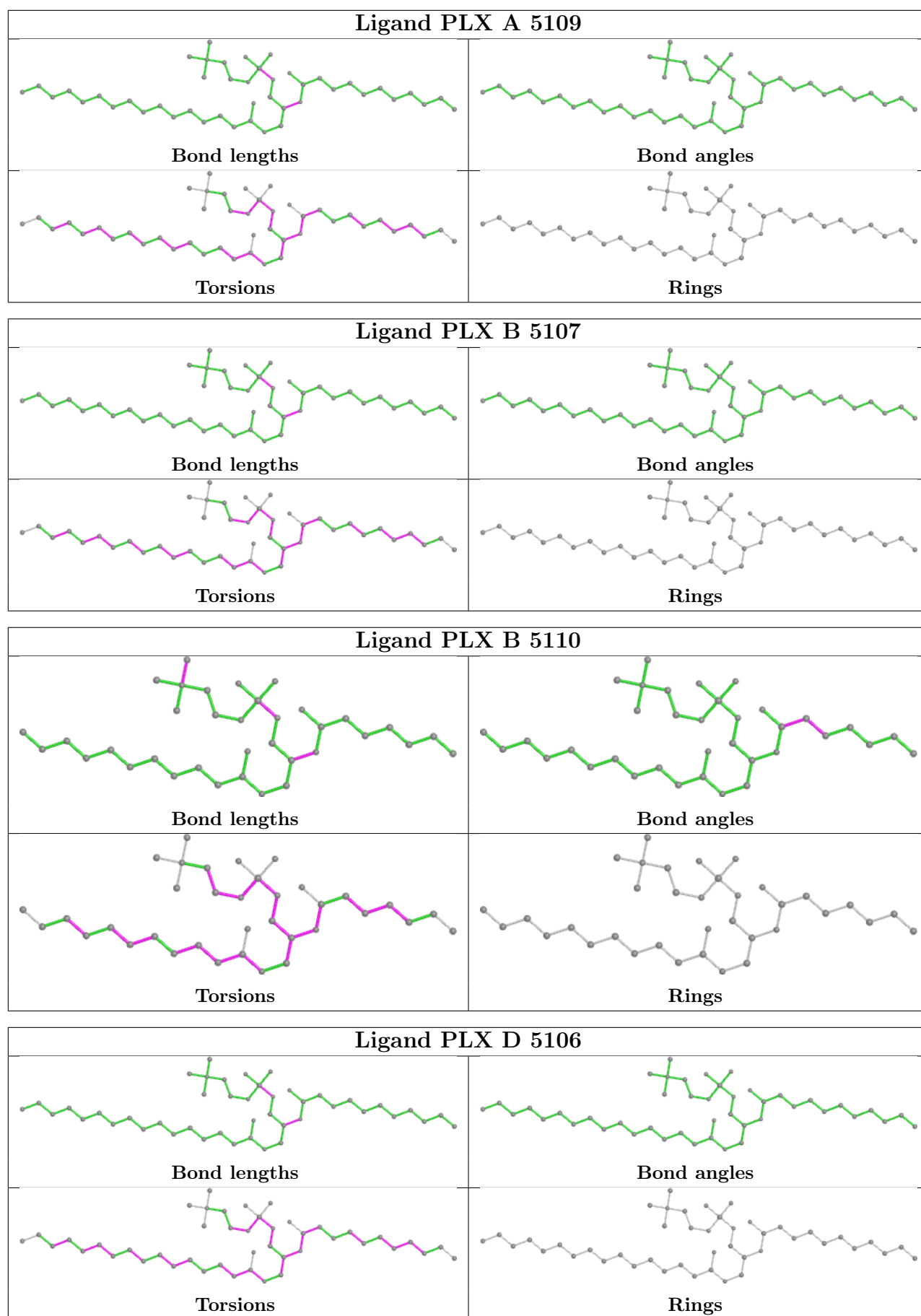


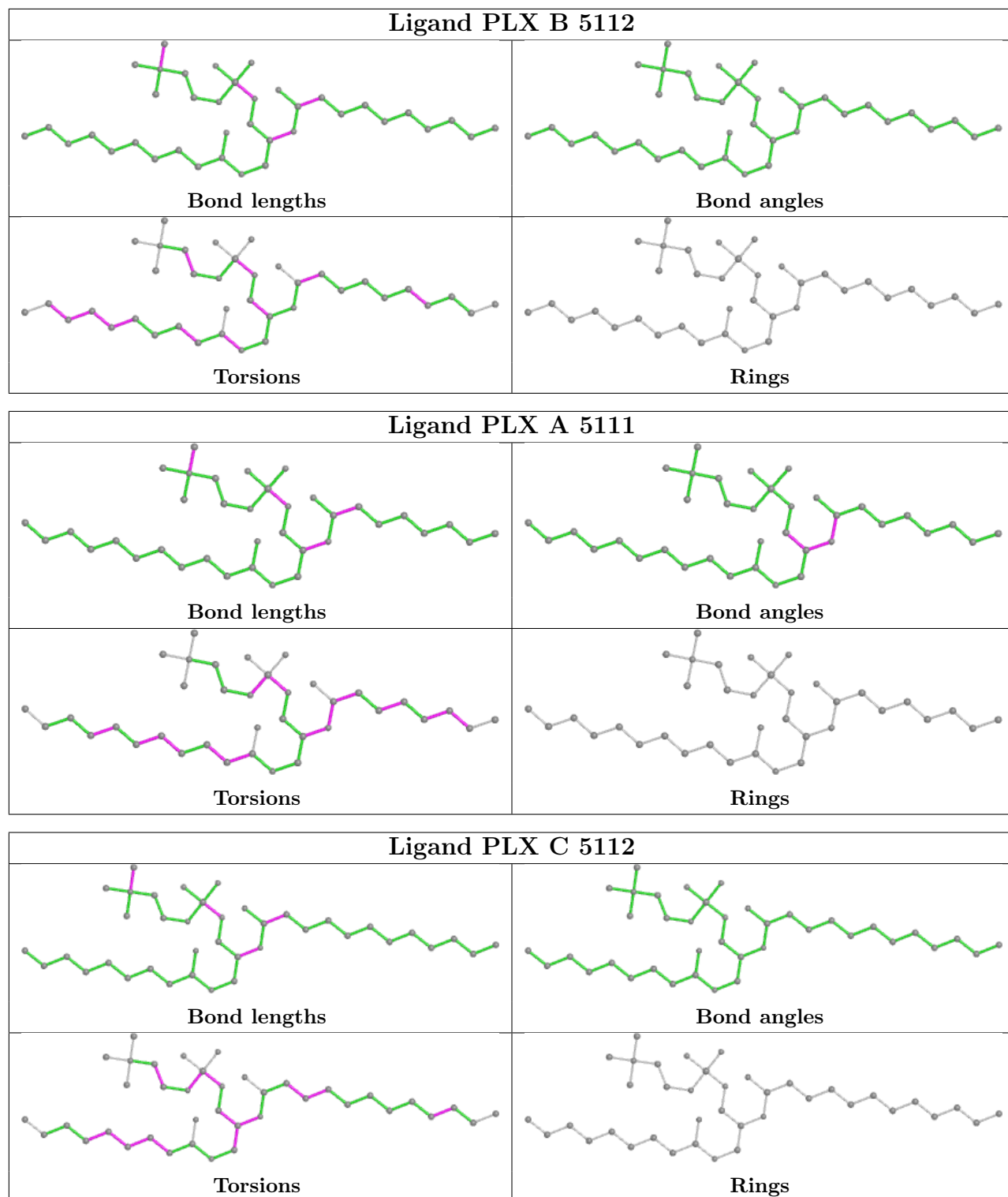


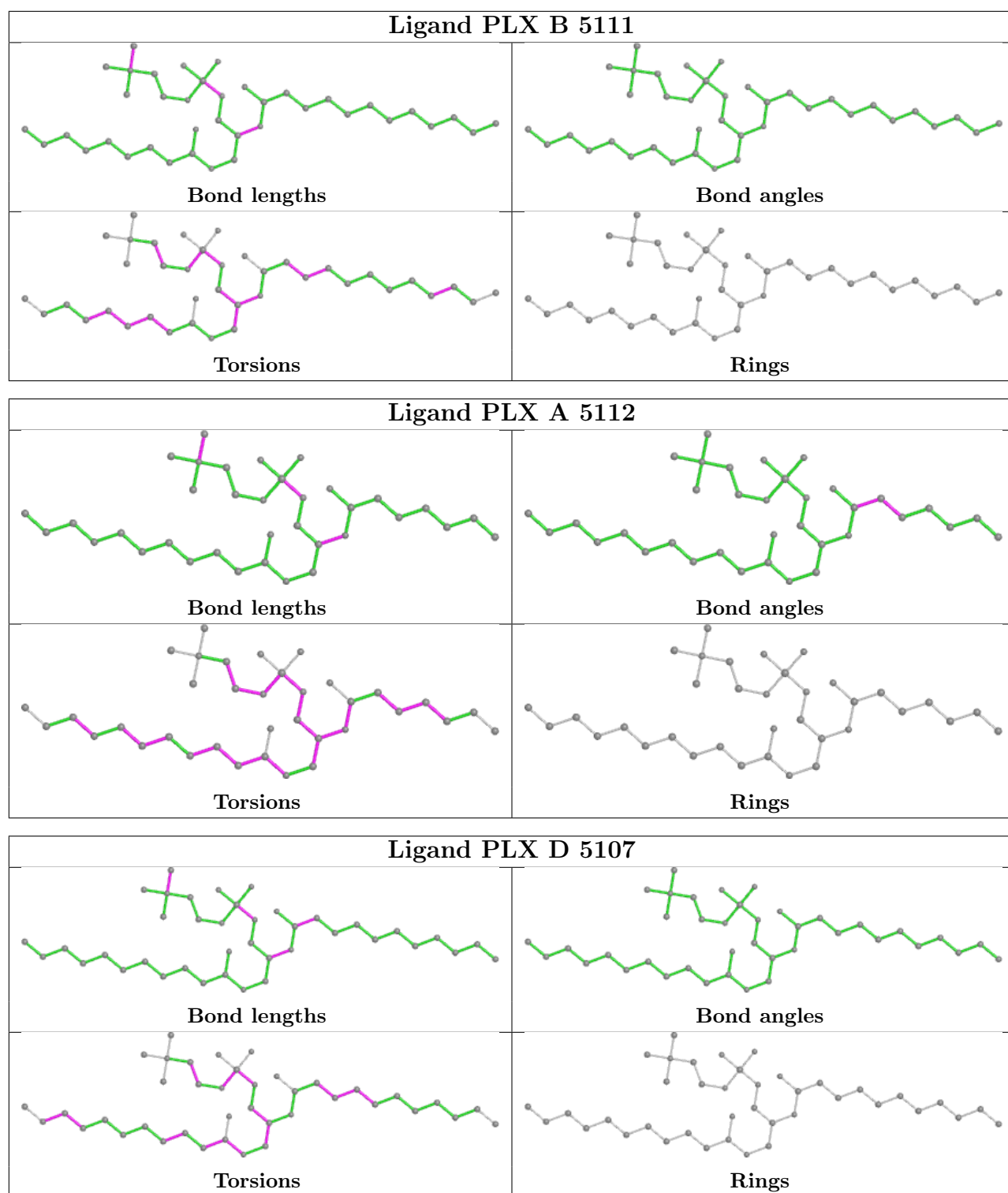


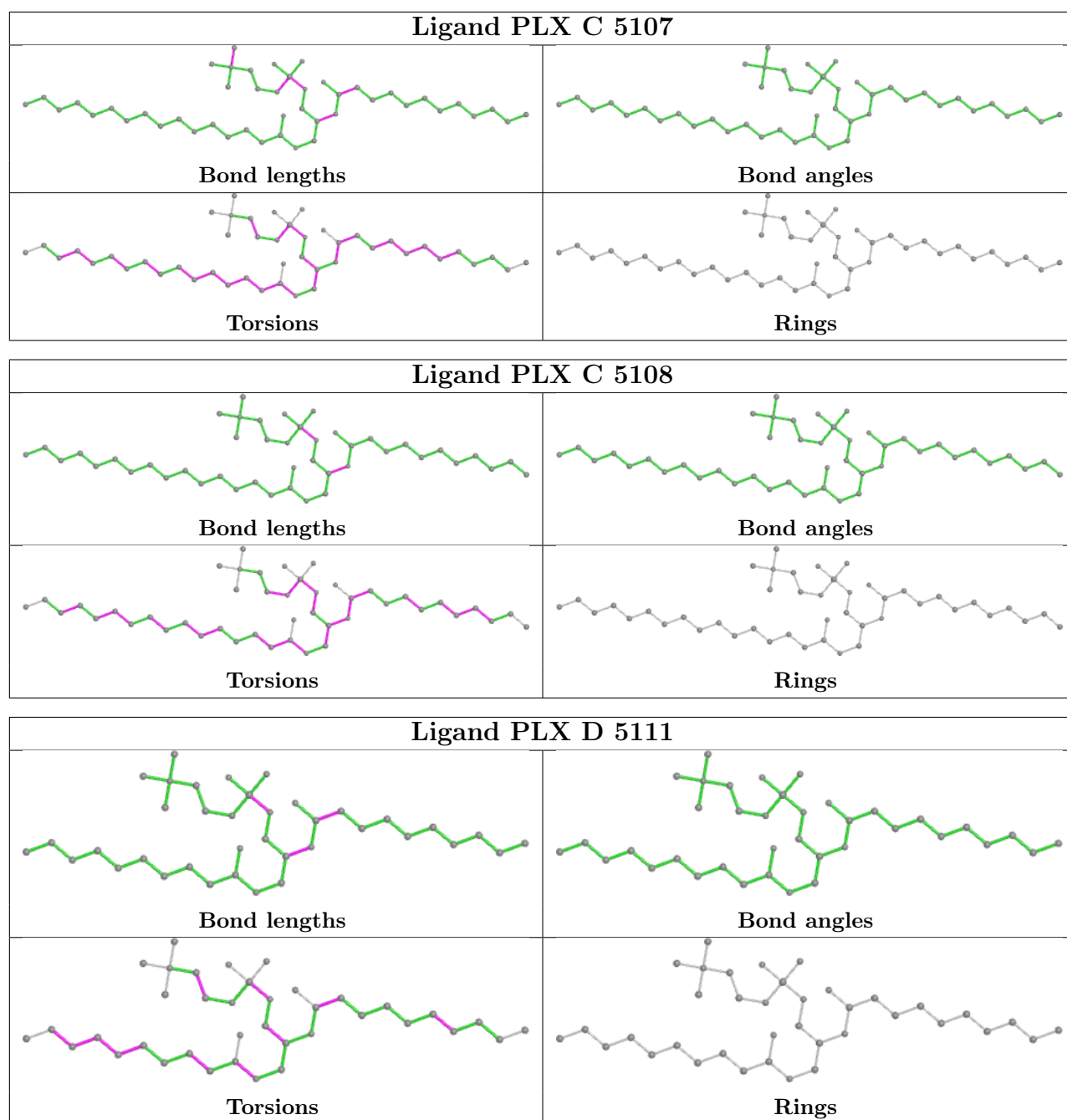












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

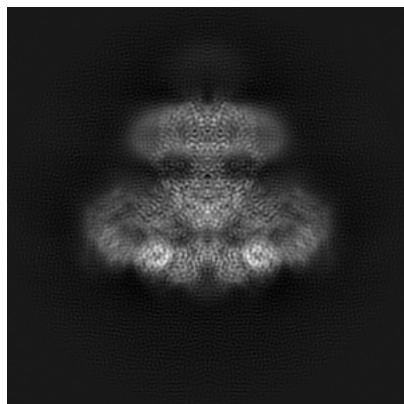
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27982. These allow visual inspection of the internal detail of the map and identification of artifacts.

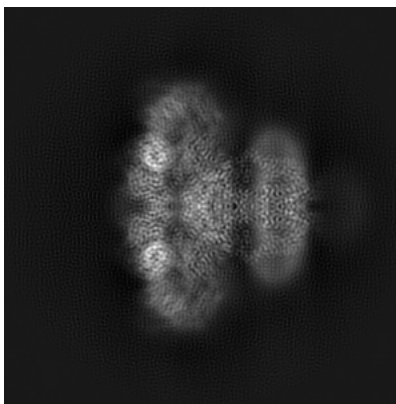
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

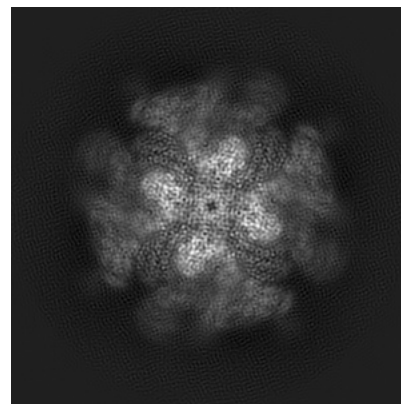
6.1.1 Primary map



X

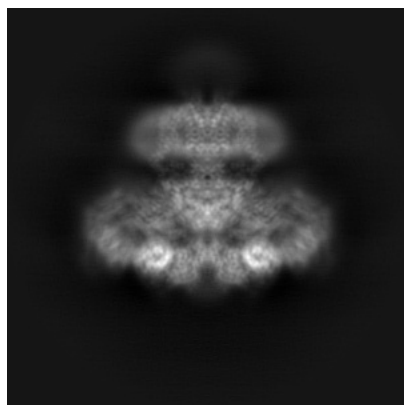


Y

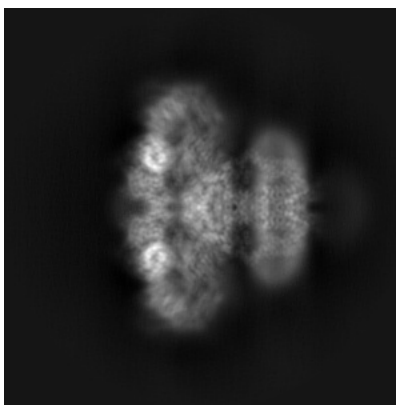


Z

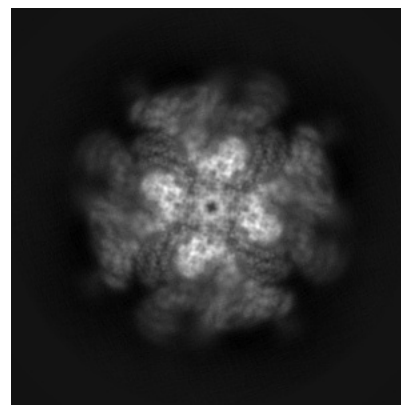
6.1.2 Raw map



X



Y

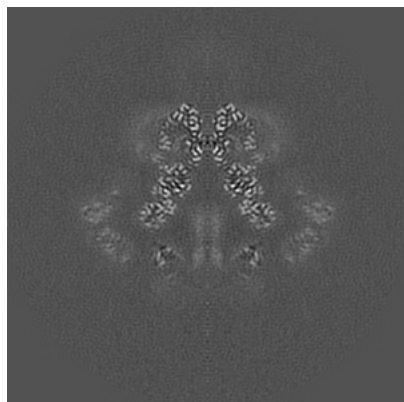


Z

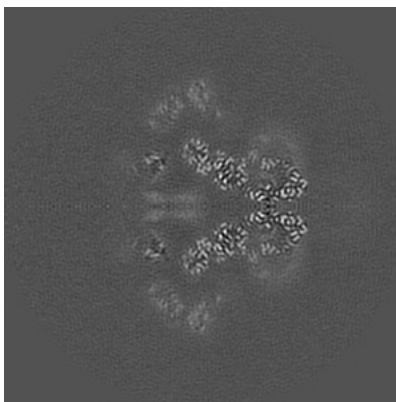
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

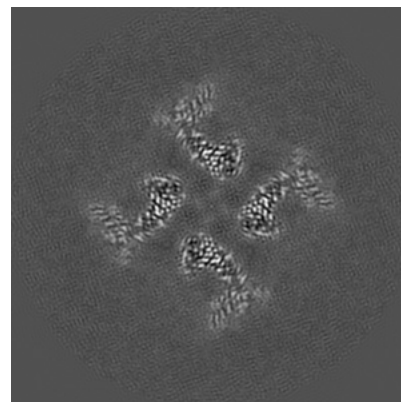
6.2.1 Primary map



X Index: 168

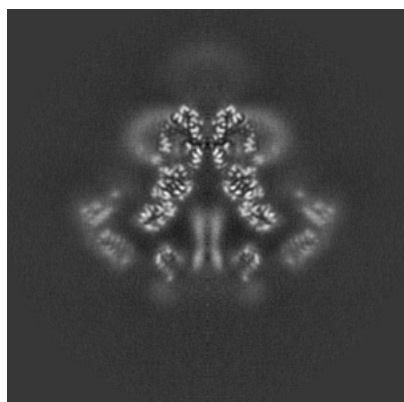


Y Index: 168

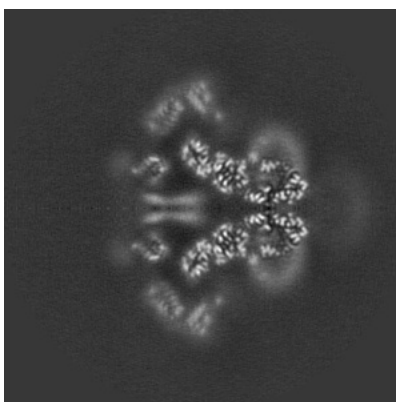


Z Index: 168

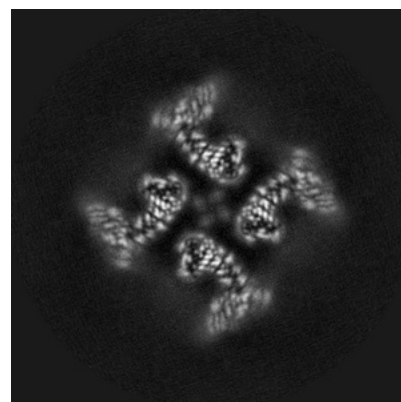
6.2.2 Raw map



X Index: 168



Y Index: 168

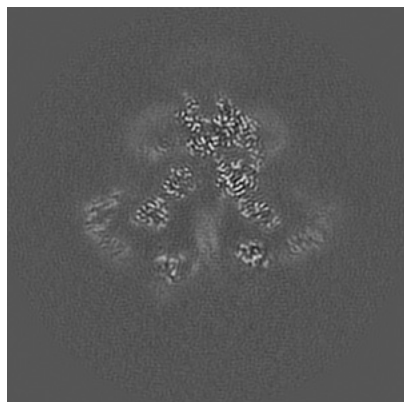


Z Index: 168

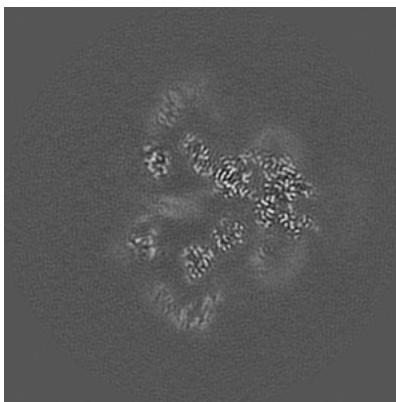
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

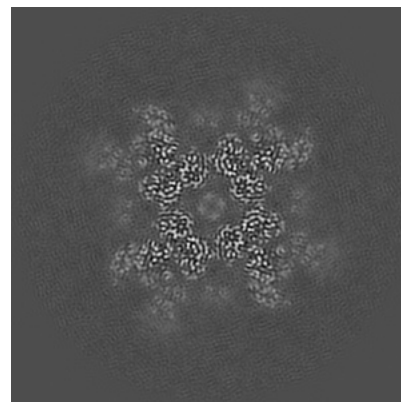
6.3.1 Primary map



X Index: 173

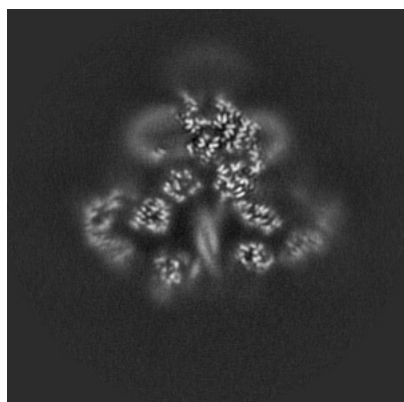


Y Index: 163

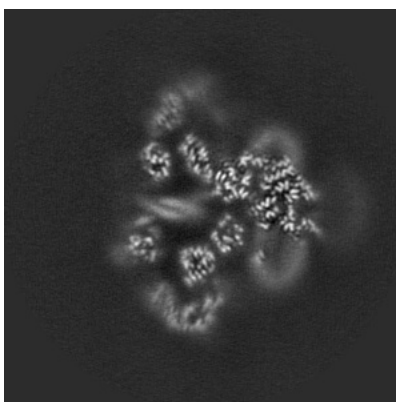


Z Index: 123

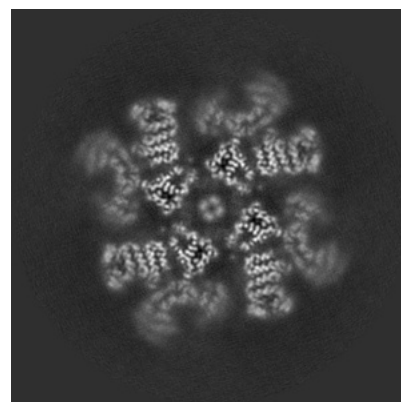
6.3.2 Raw map



X Index: 174



Y Index: 162

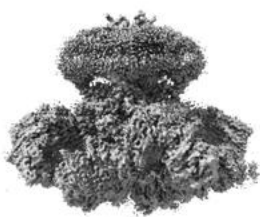


Z Index: 131

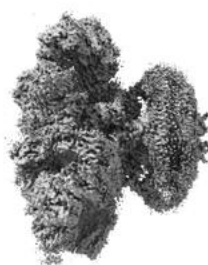
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

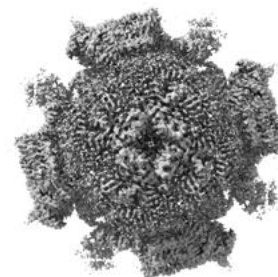
6.4.1 Primary map



X



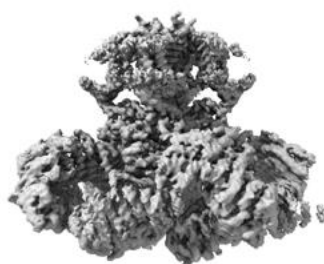
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0118. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

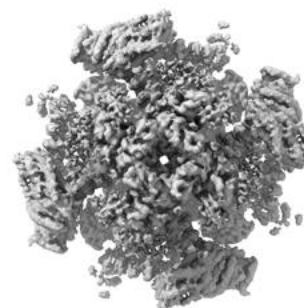
6.4.2 Raw map



X



Y



Z

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.

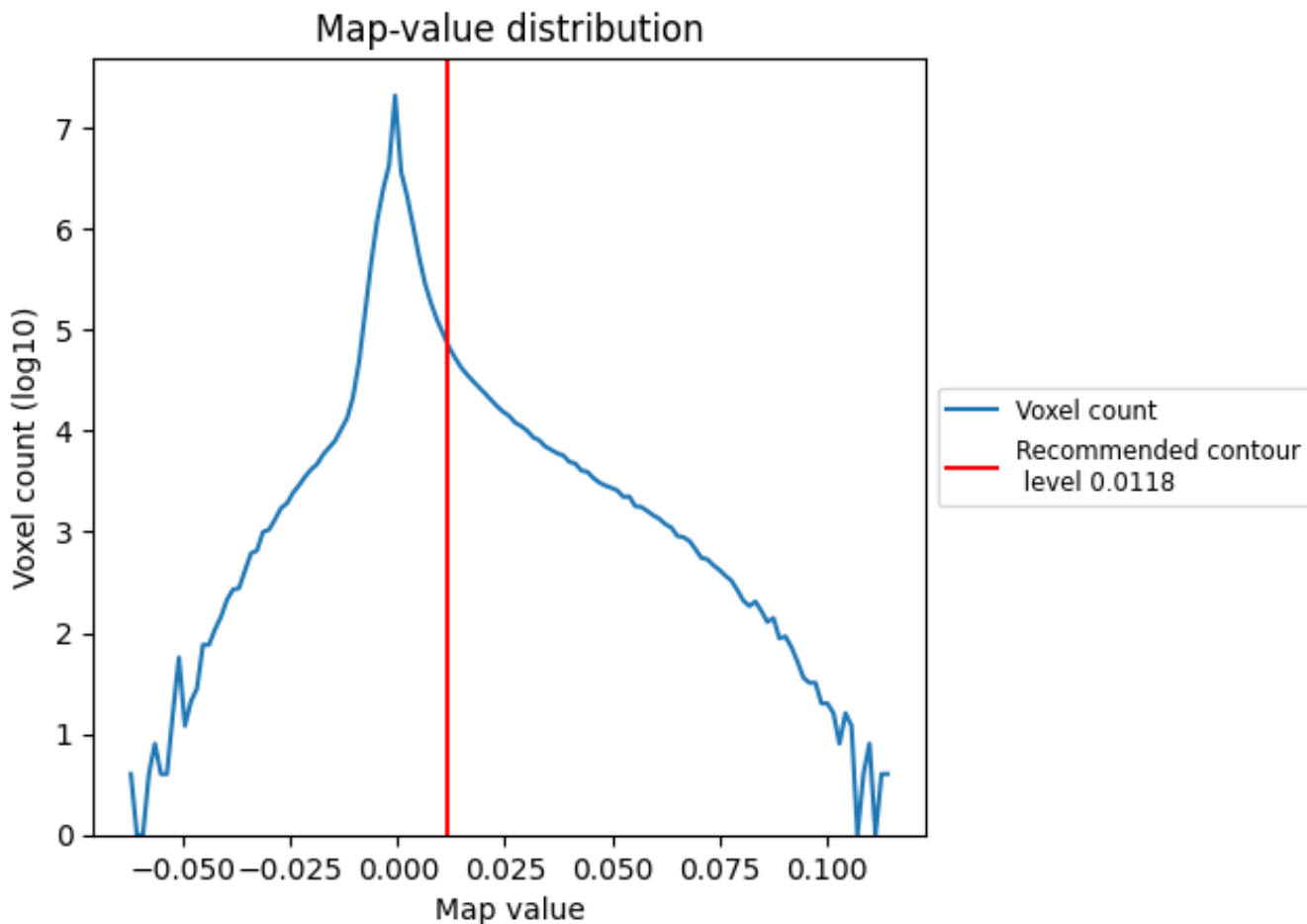
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

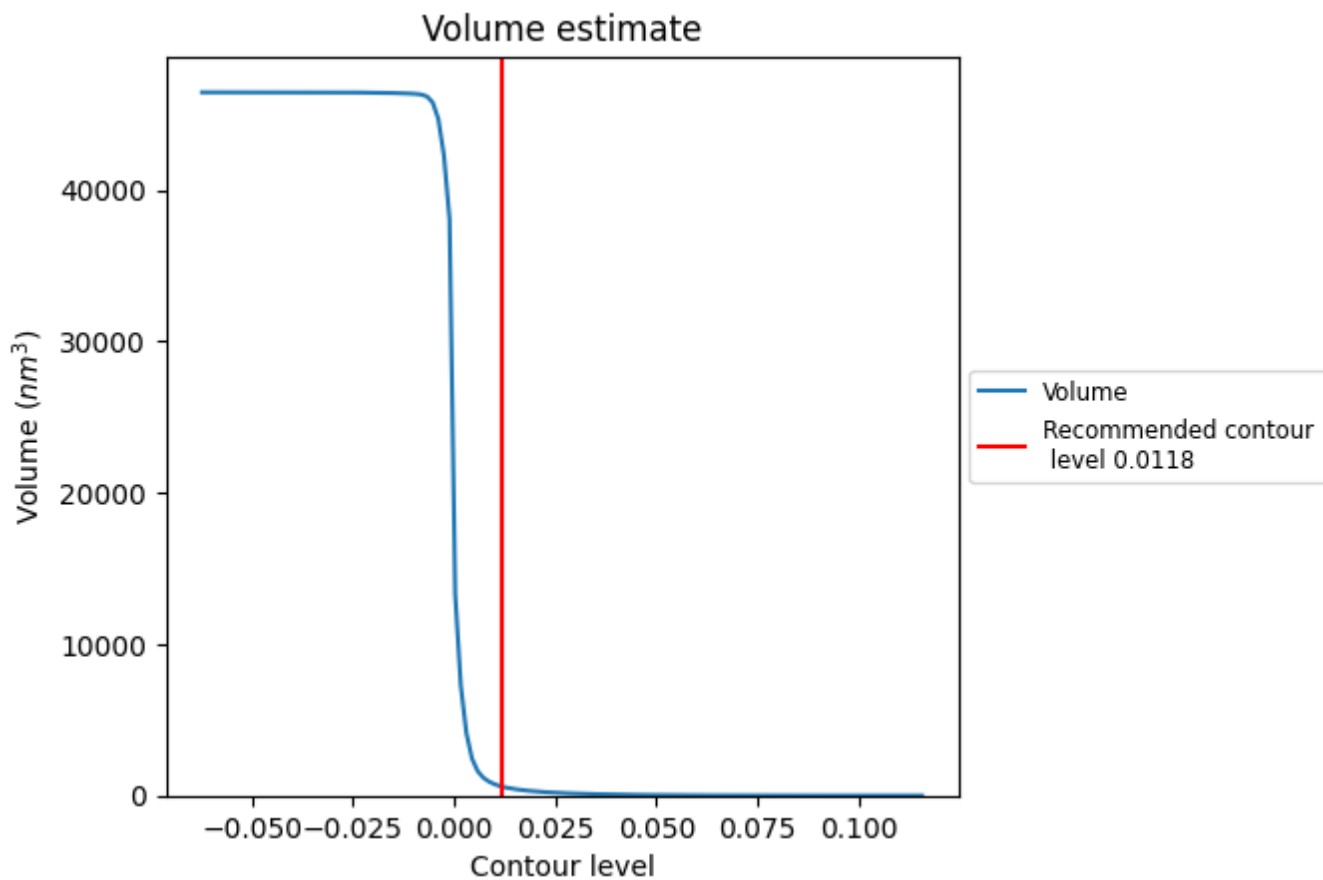
This section contains the results of statistical analysis of the map.

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.

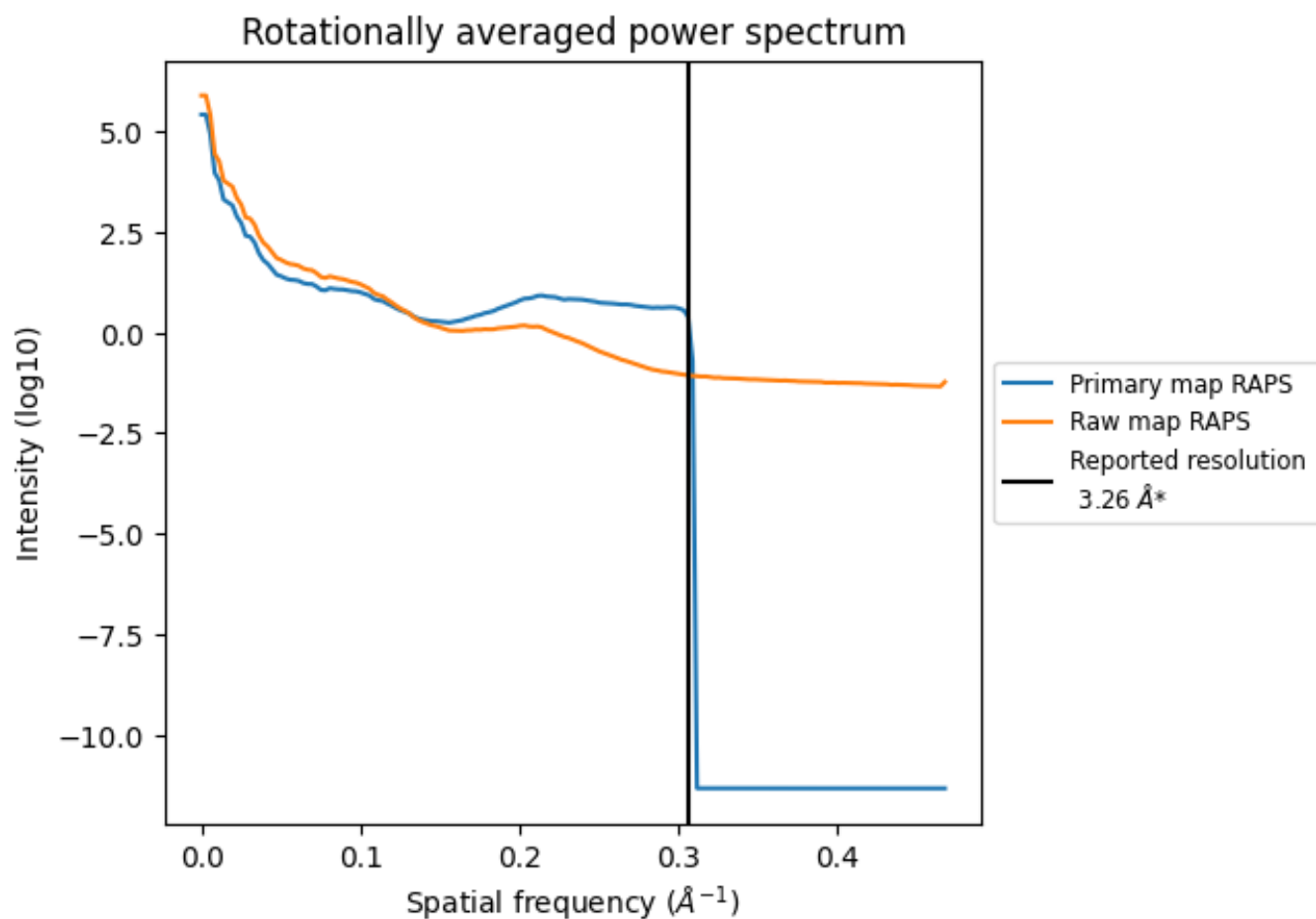
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 600 nm^3 ; this corresponds to an approximate mass of 542 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 [i](#)

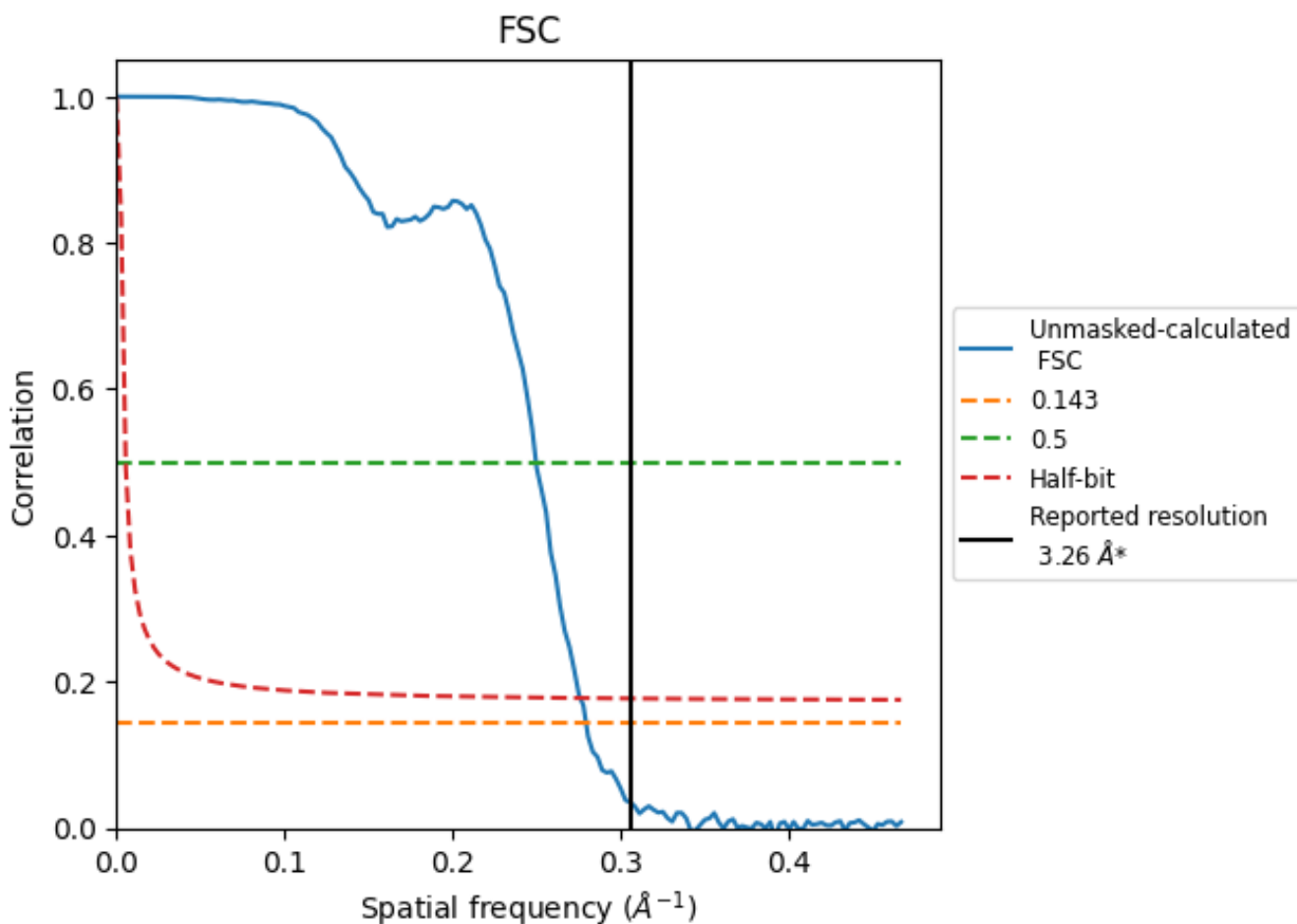


*Reported resolution corresponds to spatial frequency of 0.307 Å⁻¹

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 0.307\AA^{-1}

8.2 Resolution estimates [i](#)

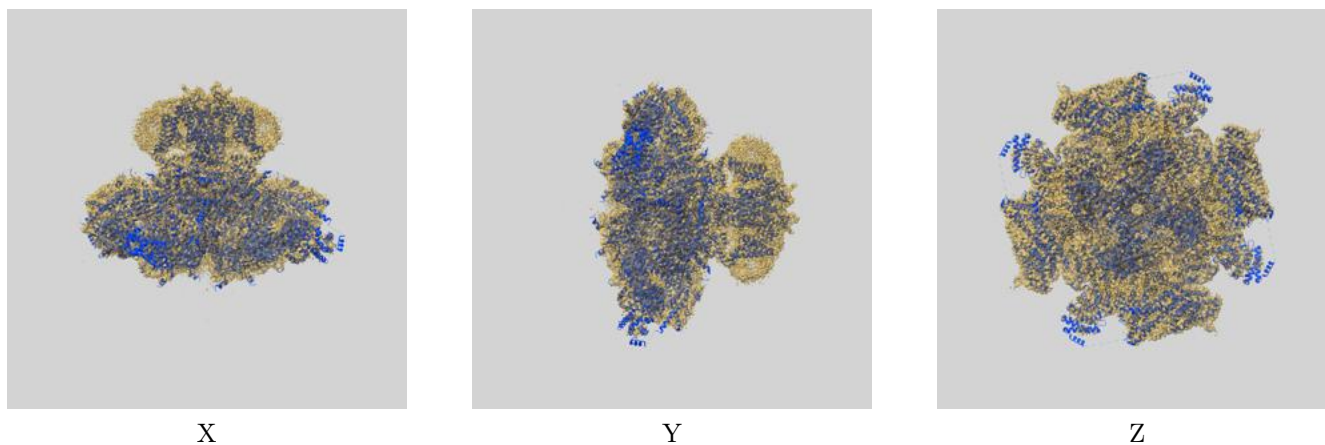
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.26	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.58	4.00	3.62

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

9 Map-model fit [i](#)

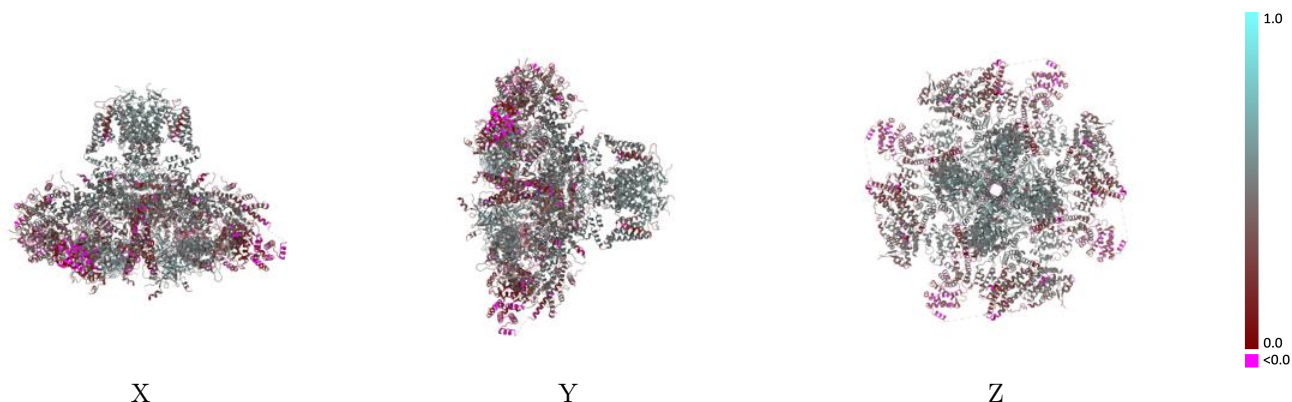
This section contains information regarding the fit between EMDB map EMD-27982 and PDB model 8EAQ. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



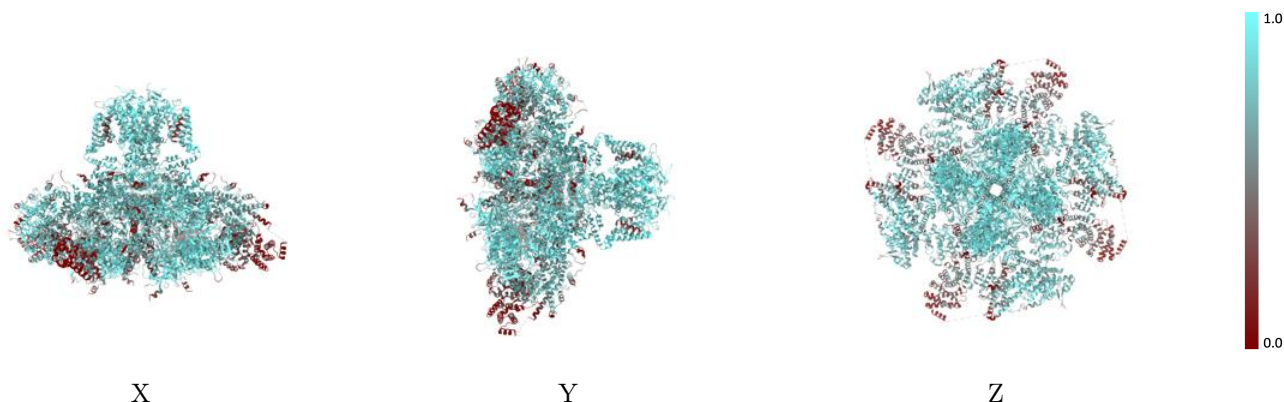
The images above show the 3D surface view of the map at the recommended contour level 0.0118 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



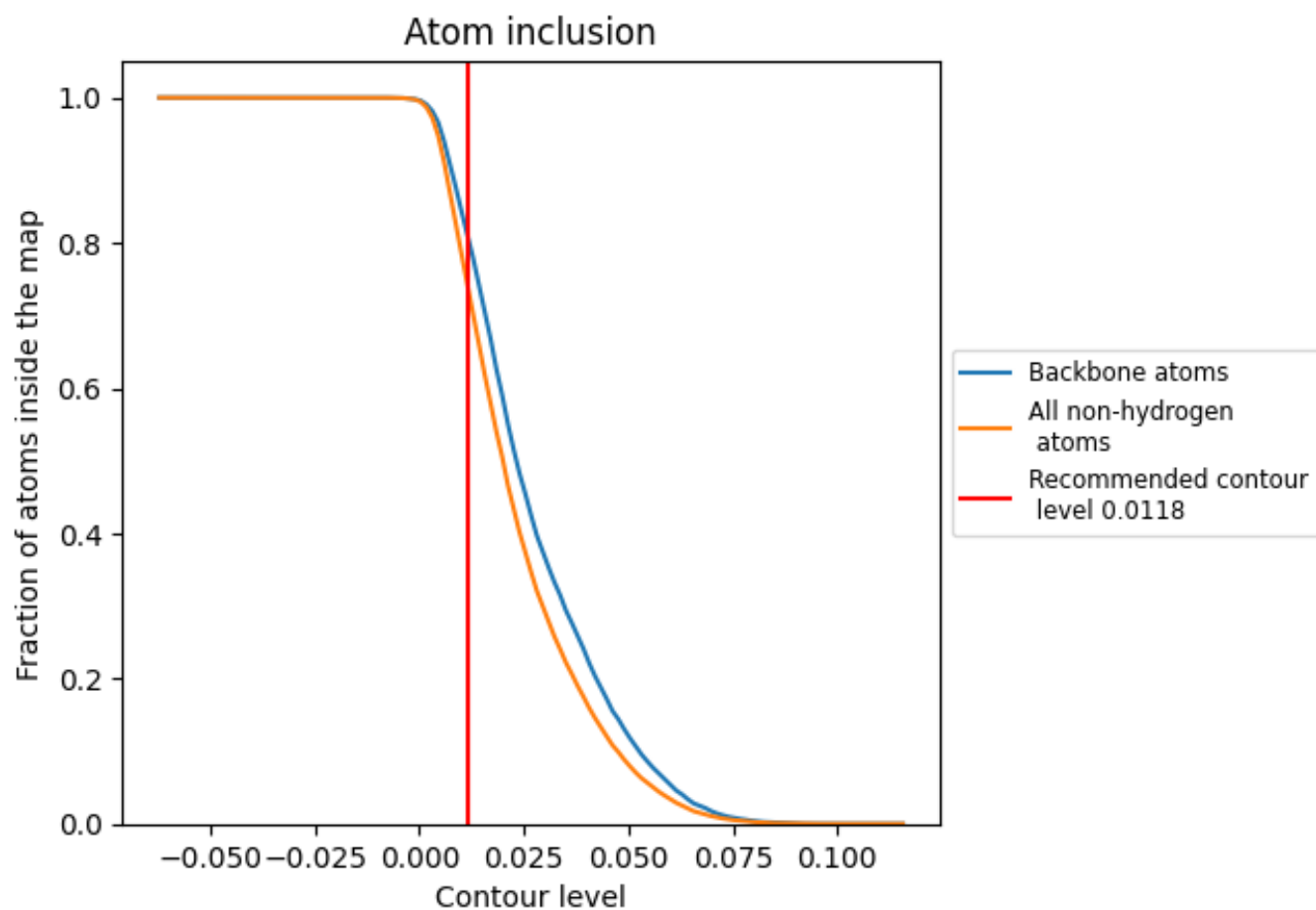
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0118).











9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.0118) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7335	 0.4030
A	 0.7330	 0.4030
B	 0.7338	 0.4030
C	 0.7336	 0.4030
D	 0.7335	 0.4030

