



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 09:03 AM UTC

PDB ID : 7WLT / pdb_00007wlt
EMDB ID : EMD-32592
Title : the Curved Structure of mPIEZO1 in Lipid Bilayer
Authors : Yang, X.; Lin, C.; Chen, X.; Li, S.; Li, X.; Xiao, B.
Deposited on : 2022-01-13
Resolution : 3.46 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

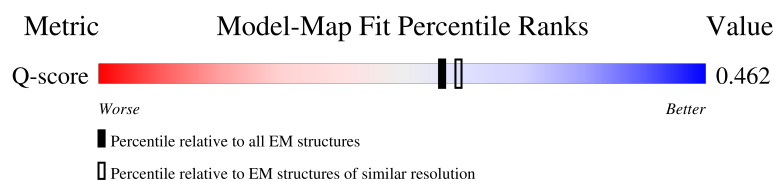
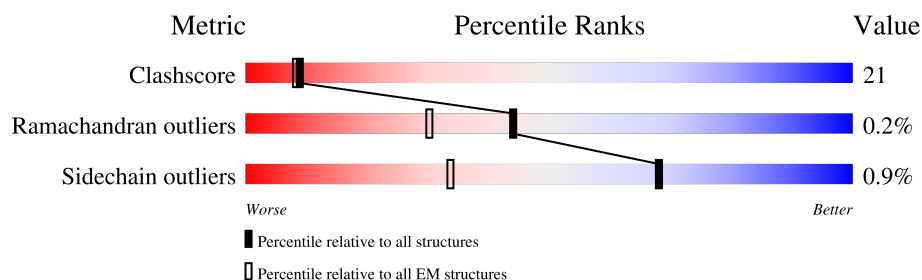
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.46 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2547	25% 35% 17% 47%
1	C	2547	25% 36% 17% 47%
1	E	2547	25% 35% 17% 47%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PLX	A	2608	-	-	X	-
2	PLX	C	2609	-	-	X	-
2	PLX	E	2601	-	-	X	-
3	PEE	A	2606	-	-	X	-
3	PEE	C	2607	-	-	X	-
3	PEE	E	2608	-	-	X	-

2 Entry composition (i)

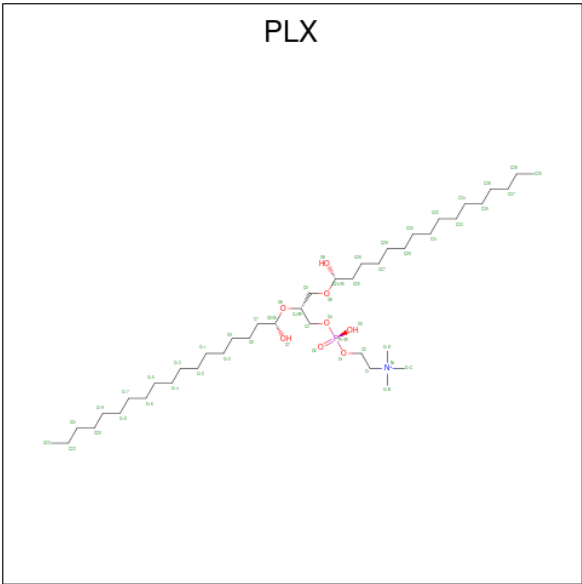
There are 4 unique types of molecules in this entry. The entry contains 33912 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Piezo-type mechanosensitive ion channel component 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1353	Total	C	N	O	S	0	0
			10835	7108	1813	1849	65		
1	C	1353	Total	C	N	O	S	0	0
			10835	7108	1813	1849	65		
1	E	1353	Total	C	N	O	S	0	0
			10835	7108	1813	1849	65		

- Molecule 2 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 (CCD ID: PLX) (formula: C₄₂H₈₉NO₈P) (labeled as "Ligand of Interest" by depositor).



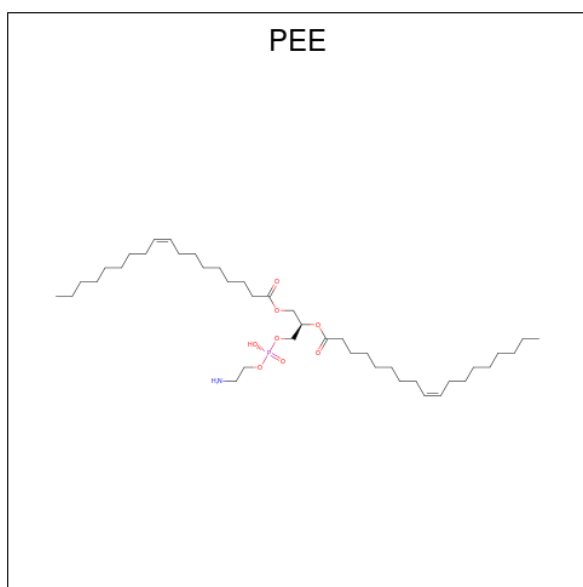
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	A	1	Total	C	N	O	P	0
			52	42	1	8	1	

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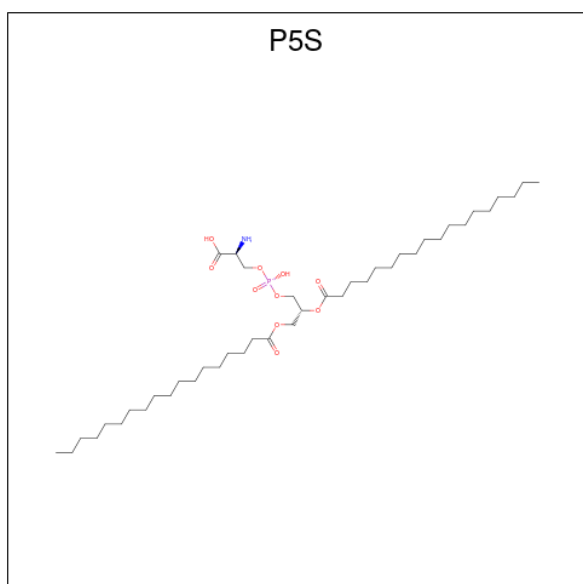
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	E	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 3 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$) (labeled as "Ligand of Interest" by depositor).



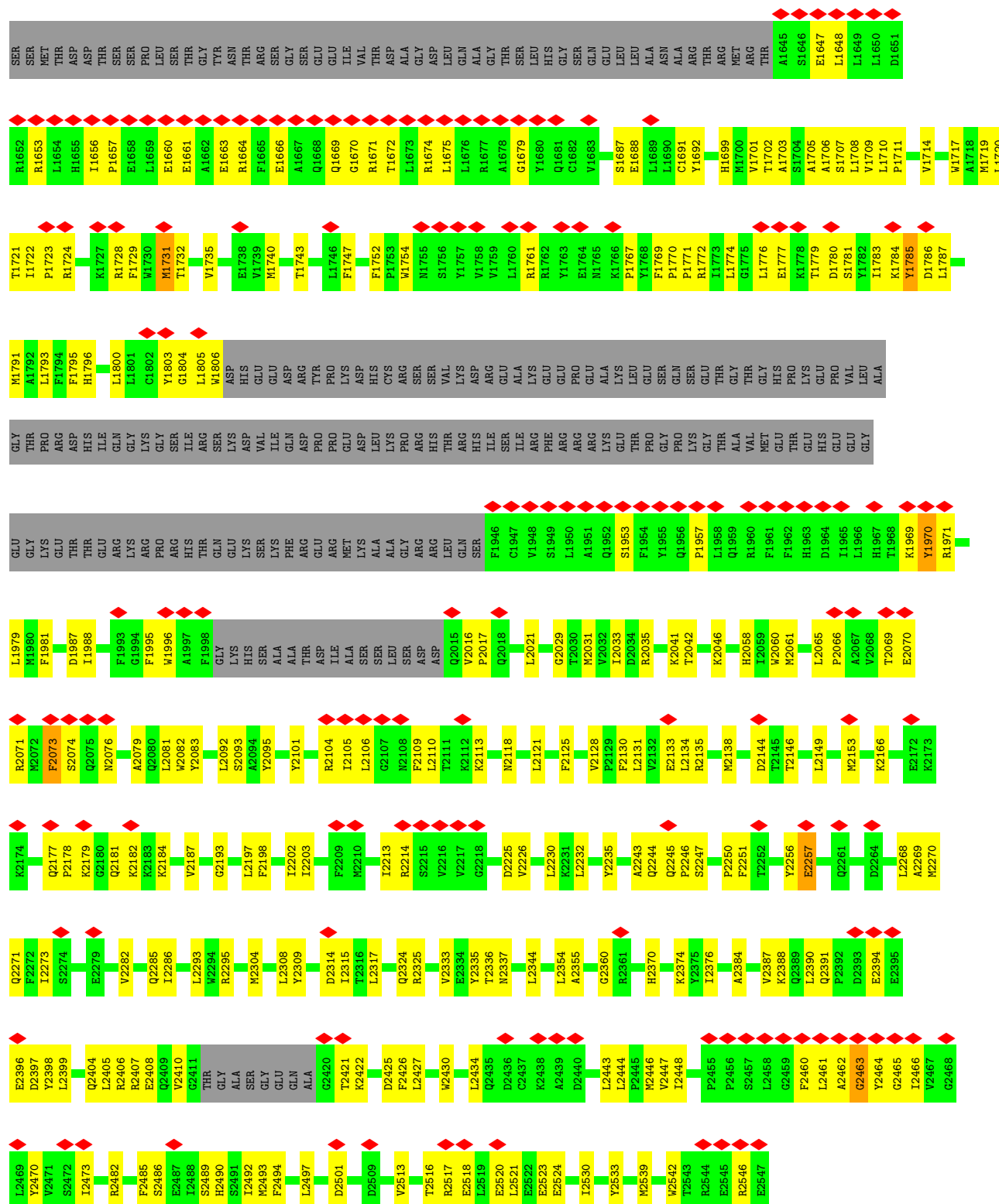
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
3	C	1	Total	C	N	O	P	0
			51	41	1	8	1	
3	E	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 4 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-serine (CCD ID: P5S) (formula: $C_{42}H_{82}NO_{10}P$) (labeled as "Ligand of Interest" by depositor).

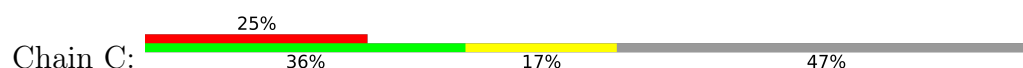


Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total 54	C 42	N 1	O 10	P 1	0
4	C	1	Total 54	C 42	N 1	O 10	P 1	0
4	E	1	Total 54	C 42	N 1	O 10	P 1	0

D1532	ASP	D1411	R1351	W1282	T1219	I1144	D1084	R1024	ALA	R903	P843
V1533	ASP	Y1412	I1352	L1283	V1220	H1145	F1085	R1025	ASP	G904	R844
L1534	ASN	F1413	R1353	S1284	I1221	C1146	F1086	R1026	GLY	P905	P845
C1535	PRO		A1354	I1285	I1222	R1147	R1087	E1027	THR	V906	R846
A1536	ASP	E1416	K1355	L1290	K1223	S1148	A1088	A1028		D907	R847
E1537	VAL	S1417	Q1356	L1291	S1224	Y1149	P1089	I1029		P908	M848
R1538	GLU	D1418	Q1357	L1292	N1225	D1150	N1090	A1030		A909	A849
Y1539	VAL	S1419	K1358	Q1293	M1226	L1151	S1091	A1031		N910	S850
L1540	ASP	E1420	R1359	R1294	L1229	D1152	T1092	I1032		W911	C851
L1541	VAL		Y1360	R1295	L1230	M1153	T1093	L1033		F912	L852
L1542	PRO	D1421	R1360	I1296	S1231	K1154	N1093	W1033		G913	S791
T1542	GLU		Q1361	F1297	S1232	V1155	L1094	P1034		C913	S853
Q1543	ASP	GLU	S1362	C1232	C1232	V1155	I1095	Y1036		Y914	T854
Q1543	GLU	ALA	Q1363	V1233	V1233	A1156	S1096	C1037		R915	V855
E1544	GLU	LEU	A1364	F1234	F1234	V1157	D1097	L1038		K916	W856
L1545	ALA	PRO	A1364	V1235	V1235	F1158	F1098	F1039		C917	W856
L1546	GLY	GLU	S1365	Y1301	E1236	R1159	L1099	L1040		K918	T857
ASP	ARG	ASP	ARG	F1302	Q1237	Y1160	L1100	Y1040		K919	C958
R1547	GLY	PRO	GLN	L1303	Q1238	L1161	L1101	T1041		N920	I859
V1548	SER	ARG	LEU	H1304	M1238	F1162	L1102	F981		N920	I860
H1493			GLN	H1304	Q1239	W1163	F1043	L921		N921	I861
M1494			GLN	S1240	F1240	F1163	C1103	G922		G922	F862
M1495			SER	S1241	F1241	L1164	A1104	Y923		Y923	V862
Q1496			LVS	N1241	F1242		S1105	Y923		I924	C863
R1497			ASP	A1307	C1243	F1170	Q1106	Q1047		I924	K864
R1553			PRO	D1308	G1243		Q1107	Y987		Q925	M865
G1554			GLN	L1309	I1246	R1176	Q1108	Q1049		N926	L866
L1499			ASP	K1310		I1177	W1108	L1050		H927	Y867
S1500			PRO	A1311	F1249	S1178	Q1109	C1051		N928	Q868
T1501			SER		S1250	I1179	Q1109	L1052		N929	L869
L1501			GLN	L1314	V1251	F1180	W1110	C1051		I930	K870
M1502			GLU	Q1315	V1252	G1181	F1111	L1052		L931	L870
Q1503			PRO	A1316			S1112	G1053		E932	I871
F1504			GLY	A1316	C1253	C1188	A1113	MET		L932	F810
VAL			PRO	S1317	T1254	F1189	E1114	PRO		L933	K811
L1505			ASP	V1318	C1254	Y1190	A1114	PRO		L933	W872
W1506			SER	L1318	V1255	L1191	R1115	ALA		L934	N873
V1507			PRO	Q1319	K1256	L1192	R1115	ALA		L934	N873
ASP			GLY	G1319	L1256	L1192	T1116	LEU		V935	P874
L1508			GLY	F1320	G1257	L1193	T1116	LEU		V935	P874
G1509			SER		Y1258	F1194	E1117	CYS		N997	H15
ALA			SER		G1258	G1195	E1118	ILE		N998	GLU
THR			SER	Y1323	Y1259	T1196	E1118	ILE		E937	TYR
LEU			PRO		D1260	T1197	W1119	ASP		N1000	L315
SER			PRO	N1327	F1261	T1197	Q1120	TRP		V939	SER
GLY			ARG	L1328	K1262	L1198	ARG	PRO		V939	TS17
PRO			ARG	K1329	E1263	L1199	MET	ARG		N880	
VAL			GLN	S1330	E1263	L1199	ALA	ARG		C881	V820
GLU			TRP	K1330	M1264	Q1200	ALA	TRP		V940	A821
GLU			TRP	I1331	M1265	K1201	GLY	SER		R942	L822
THR			ARG	N1332	M1265	D1202	ILE	LYS		R943	K823
ASP			PRO	F1333	T1266	T1203	THR	ALA		Q944	P884
GLY			TRP	F1333	R1267	R1204	ASP	PRO		P886	F885
GLY			LEU	H1334	D1268	R1204	HIS	GLN		E945	E824
PRO			H1403	R1335	R1269	A1205	LEU	Y1010		H946	ASN
SER			ALA	Q1336	R1269	Q1206	GLU	Y1011		Y947	ASN
ALA			ALA	I1337	D1270	L1207	PRO	T1012		R948	M828
SER			A1404	E1338	C1271		ALA	H1013		L830	N829
SER			T1405	I1337	L1272	D1211	GLU	A1075		R949	L831
GLY			V1406	E1339	L1272	C1212	LEU	L1076		R949	L831
LEU			H1408	I1340	F1274	L1213	R1134	G1014		Q950	L832
GLY			S1409	Q1344	Y1275	L1214	E1136	GLN		H951	V833
GLY			G1410	K1345	F1276	L1214	P1137	W1079		GLN	W834
GLY				L1345	E1276	L1215	Y1079	ALA		ALA	V834
GLY				K1346	E1277	L1216	N1138	L1080		L835	L835
GLU				R1347	E1278	N1217	A1019	Y1081		P900	P836
PRO				Q1347	A1278	V1218	P1139	L1082		LEU	N997
LEU				Q1348	G1279		T1140	L1082		PRO	Q898
				M1349	I1280		T1022	P1083		ALA	S899
				K1350	I1281		F1141			GLN	L900
							N1142			ALA	L901
							F1143			VAL	Y902
										CYS	

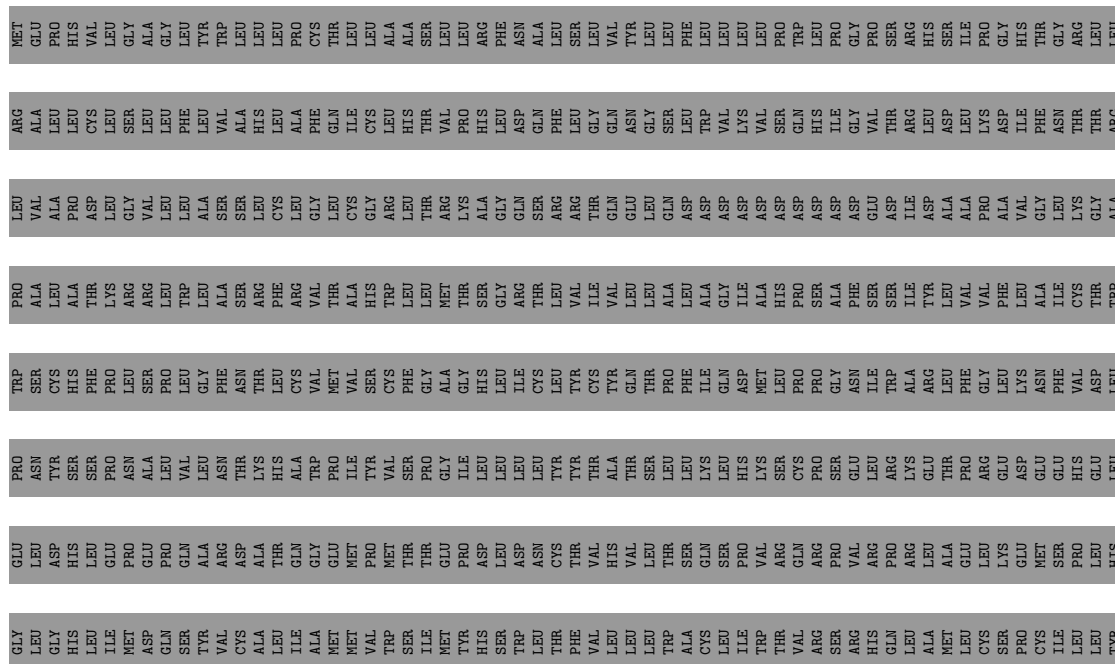


- Molecule 1: Piezo-type mechanosensitive ion channel component 1



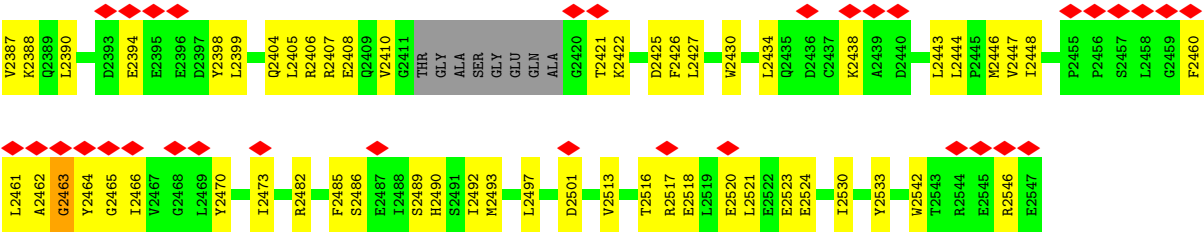












4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	209166	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.089	Depositor
Minimum map value	-0.045	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.018	Depositor
Map size ($\text{\AA}$)	395.28003, 395.28003, 395.28003	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.098, 1.098, 1.098	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: PEE, P5S, PLX

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	0.47	0/11108	0.62	3/15083 (0.0%)
1	C	0.47	0/11108	0.62	3/15083 (0.0%)
1	E	0.47	0/11108	0.62	3/15083 (0.0%)
All	All	0.47	0/33324	0.62	9/45249 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	2463	GLY	CA-C-N	6.09	133.16	121.54
1	E	2463	GLY	C-N-CA	6.09	133.16	121.54
1	A	2463	GLY	CA-C-N	6.07	133.14	121.54
1	A	2463	GLY	C-N-CA	6.07	133.14	121.54
1	C	2463	GLY	CA-C-N	6.06	133.12	121.54
1	C	2463	GLY	C-N-CA	6.06	133.12	121.54
1	E	1142	ASN	N-CA-C	5.47	119.18	110.70
1	A	1142	ASN	N-CA-C	5.46	119.16	110.70
1	C	1142	ASN	N-CA-C	5.45	119.15	110.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10835	0	10713	442	0
1	C	10835	0	10713	425	0
1	E	10835	0	10713	440	0
2	A	364	0	616	88	0
2	C	364	0	616	92	0
2	E	364	0	616	90	0
3	A	51	0	82	41	0
3	C	51	0	82	42	0
3	E	51	0	82	41	0
4	A	54	0	80	3	0
4	C	54	0	80	3	0
4	E	54	0	80	3	0
All	All	33912	0	34473	1425	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 21.

All (1425) 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:C:2197:LEU:CD1	2:C:2609:PLX:H393	1.37	1.52
1:E:2197:LEU:CD1	2:E:2601:PLX:H393	1.37	1.49
1:A:2197:LEU:CD1	2:A:2608:PLX:H393	1.38	1.48
1:C:2197:LEU:HD13	2:C:2609:PLX:C39	1.49	1.41
1:E:2197:LEU:HD13	2:E:2601:PLX:C39	1.49	1.40
1:A:2197:LEU:HD13	2:A:2608:PLX:C39	1.50	1.40
1:A:2153:MET:HE1	1:E:2485:PHE:CD1	1.74	1.23
1:A:2485:PHE:CE1	1:C:2153:MET:HE1	1.74	1.23
1:C:2485:PHE:CD1	1:E:2153:MET:HE1	1.73	1.23
1:A:2153:MET:HE1	1:E:2485:PHE:CE1	1.74	1.22
1:A:2485:PHE:CD1	1:C:2153:MET:HE1	1.73	1.22
1:C:2485:PHE:CE1	1:E:2153:MET:HE1	1.74	1.22
1:E:1740:MET:HE1	2:E:2605:PLX:H233	1.25	1.15
1:C:2197:LEU:HD21	2:C:2609:PLX:C37	1.76	1.14
1:E:2197:LEU:HD21	2:E:2601:PLX:C37	1.76	1.14
1:A:2197:LEU:HD21	2:A:2608:PLX:C37	1.77	1.13
1:C:1735:VAL:CG1	2:C:2604:PLX:H131	1.79	1.13
1:E:2197:LEU:HD21	2:E:2601:PLX:H372	1.16	1.12
1:E:1735:VAL:CG1	2:E:2605:PLX:H131	1.79	1.12
1:E:1735:VAL:HG11	2:E:2605:PLX:H131	1.12	1.12
1:A:1735:VAL:CG1	2:A:2603:PLX:H131	1.79	1.11
1:A:2197:LEU:HD21	2:A:2608:PLX:H372	1.17	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1735:VAL:HG11	2:A:2603:PLX:H131	1.12	1.10
1:C:1740:MET:HE1	2:C:2604:PLX:H233	1.25	1.10
1:A:1740:MET:HE1	2:A:2603:PLX:H233	1.25	1.10
1:C:2197:LEU:CD2	2:C:2609:PLX:C37	2.29	1.10
1:E:2197:LEU:CD2	2:E:2601:PLX:C37	2.29	1.10
1:A:2197:LEU:CD2	2:A:2608:PLX:C37	2.30	1.09
1:C:2197:LEU:HD21	2:C:2609:PLX:H372	1.16	1.08
1:C:1735:VAL:HG11	2:C:2604:PLX:H131	1.12	1.07
2:C:2609:PLX:H1A3	1:E:2042:THR:HB	1.41	1.03
1:C:1502:MET:SD	1:C:1503:GLN:NE2	2.31	1.02
1:E:1502:MET:SD	1:E:1503:GLN:NE2	2.31	1.02
1:A:1502:MET:SD	1:A:1503:GLN:NE2	2.31	1.02
1:C:2197:LEU:CD2	2:C:2609:PLX:H371	1.90	1.02
1:A:2042:THR:HB	2:E:2601:PLX:H1A3	1.41	1.01
2:A:2608:PLX:H1A3	1:C:2042:THR:HB	1.41	1.00
1:E:2197:LEU:CD2	2:E:2601:PLX:H371	1.90	1.00
2:A:2608:PLX:H381	2:A:2608:PLX:H211	1.00	1.00
3:E:2608:PEE:H40	3:E:2608:PEE:H81	1.44	0.99
1:E:2193:GLY:O	1:E:2197:LEU:HD23	1.63	0.99
3:C:2607:PEE:H81	3:C:2607:PEE:H40	1.44	0.99
2:E:2601:PLX:H211	2:E:2601:PLX:C38	1.93	0.99
2:C:2609:PLX:H381	2:C:2609:PLX:H211	1.00	0.98
1:C:2193:GLY:O	1:C:2197:LEU:HD23	1.63	0.98
1:A:2197:LEU:CD2	2:A:2608:PLX:H371	1.91	0.98
2:C:2609:PLX:H211	2:C:2609:PLX:C38	1.93	0.98
2:E:2601:PLX:H211	2:E:2601:PLX:H381	1.00	0.98
2:A:2608:PLX:H211	2:A:2608:PLX:C38	1.93	0.97
2:E:2601:PLX:H381	2:E:2601:PLX:C21	1.94	0.97
2:A:2608:PLX:H381	2:A:2608:PLX:C21	1.94	0.97
1:A:1735:VAL:HG11	2:A:2603:PLX:C13	1.95	0.96
1:A:2193:GLY:O	1:A:2197:LEU:HD23	1.63	0.96
3:C:2607:PEE:C46	3:C:2607:PEE:H68	1.95	0.96
3:A:2606:PEE:H40	3:A:2606:PEE:H81	1.44	0.96
3:E:2608:PEE:C46	3:E:2608:PEE:H68	1.95	0.96
1:C:1735:VAL:HG11	2:C:2604:PLX:C13	1.95	0.96
3:C:2607:PEE:H68	3:C:2607:PEE:H82	1.48	0.96
2:C:2609:PLX:H381	2:C:2609:PLX:C21	1.94	0.96
1:E:1735:VAL:HG11	2:E:2605:PLX:C13	1.95	0.95
3:A:2606:PEE:C46	3:A:2606:PEE:H68	1.95	0.95
3:E:2608:PEE:H68	3:E:2608:PEE:H82	1.48	0.94
1:C:2485:PHE:CD1	1:E:2153:MET:CE	2.51	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2197:LEU:CD2	2:C:2609:PLX:H372	1.94	0.94
3:A:2606:PEE:H68	3:A:2606:PEE:H82	1.48	0.93
1:A:2153:MET:CE	1:E:2485:PHE:CD1	2.52	0.92
1:A:2485:PHE:CD1	1:C:2153:MET:CE	2.51	0.92
1:E:2197:LEU:CD2	2:E:2601:PLX:H372	1.94	0.92
1:A:2197:LEU:CD2	2:A:2608:PLX:H372	1.95	0.92
3:E:2608:PEE:H40	3:E:2608:PEE:C46	2.00	0.92
1:A:2295:ARG:HH21	1:C:2295:ARG:HD2	1.32	0.92
3:C:2607:PEE:H40	3:C:2607:PEE:C47	2.01	0.91
1:A:2295:ARG:HD2	1:E:2295:ARG:HH21	1.33	0.91
1:C:2295:ARG:HH21	1:E:2295:ARG:HD2	1.32	0.91
3:A:2606:PEE:H40	3:A:2606:PEE:C46	2.00	0.91
3:C:2607:PEE:H40	3:C:2607:PEE:C46	2.00	0.91
3:E:2608:PEE:H68	3:E:2608:PEE:C47	2.01	0.91
3:A:2606:PEE:H40	3:A:2606:PEE:C47	2.01	0.90
3:E:2608:PEE:H40	3:E:2608:PEE:C47	2.01	0.90
1:E:2197:LEU:HD22	2:E:2601:PLX:H371	1.52	0.90
2:A:2603:PLX:H222	2:A:2604:PLX:H211	1.53	0.90
2:E:2605:PLX:H222	2:E:2606:PLX:H211	1.53	0.90
3:A:2606:PEE:H68	3:A:2606:PEE:C47	2.01	0.89
3:C:2607:PEE:H68	3:C:2607:PEE:C47	2.01	0.89
1:C:863:CYS:SG	1:C:915:ARG:NH1	2.46	0.89
1:C:2197:LEU:HD22	2:C:2609:PLX:H371	1.52	0.88
2:E:2601:PLX:H192	2:E:2601:PLX:H361	1.55	0.88
1:A:2042:THR:HG22	2:E:2601:PLX:H1A2	1.55	0.88
1:E:863:CYS:SG	1:E:915:ARG:NH1	2.46	0.88
1:A:2153:MET:CE	1:E:2485:PHE:CE1	2.57	0.88
1:C:2485:PHE:CE1	1:E:2153:MET:CE	2.57	0.88
2:E:2601:PLX:H361	2:E:2601:PLX:H162	1.54	0.88
2:C:2604:PLX:H222	2:C:2605:PLX:H211	1.53	0.88
1:A:2197:LEU:HD22	2:A:2608:PLX:H371	1.53	0.88
1:A:2485:PHE:CE1	1:C:2153:MET:CE	2.57	0.87
1:A:863:CYS:SG	1:A:915:ARG:NH1	2.46	0.87
2:A:2608:PLX:H361	2:A:2608:PLX:H162	1.54	0.87
1:C:1246:ILE:HG13	1:C:1251:LEU:HB2	1.57	0.87
2:C:2609:PLX:H1A2	1:E:2042:THR:HG22	1.55	0.87
2:C:2609:PLX:H361	2:C:2609:PLX:H162	1.54	0.87
1:A:2197:LEU:HD22	2:A:2608:PLX:C37	2.06	0.86
1:C:1722:ILE:HG23	1:C:1723:PRO:HD2	1.57	0.86
2:A:2608:PLX:H361	2:A:2608:PLX:H192	1.55	0.86
2:A:2608:PLX:H1A2	1:C:2042:THR:HG22	1.55	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1246:ILE:HG13	1:E:1251:LEU:HB2	1.57	0.86
1:A:1246:ILE:HG13	1:A:1251:LEU:HB2	1.57	0.86
3:C:2607:PEE:H40	3:C:2607:PEE:C45	2.06	0.86
3:A:2606:PEE:H40	3:A:2606:PEE:C45	2.06	0.85
1:A:1722:ILE:HG23	1:A:1723:PRO:HD2	1.57	0.85
2:C:2609:PLX:H361	2:C:2609:PLX:H192	1.55	0.85
1:E:1722:ILE:HG23	1:E:1723:PRO:HD2	1.57	0.85
3:A:2606:PEE:H41	3:A:2606:PEE:H74	1.59	0.84
3:E:2608:PEE:H40	3:E:2608:PEE:C45	2.06	0.84
1:C:2197:LEU:CD1	2:C:2609:PLX:C39	2.29	0.84
1:E:2197:LEU:HD22	2:E:2601:PLX:C37	2.05	0.83
3:C:2607:PEE:H74	3:C:2607:PEE:H41	1.59	0.83
3:E:2608:PEE:H74	3:E:2608:PEE:H41	1.59	0.83
1:A:2042:THR:HB	2:E:2601:PLX:C1A	2.09	0.83
1:A:2179:LYS:HD3	1:C:1402:ASP:HB3	1.62	0.82
3:C:2607:PEE:H81	3:C:2607:PEE:C24	2.09	0.82
1:A:1702:THR:HB	1:A:1784:LYS:HD2	1.62	0.82
1:E:1002:ILE:HG23	1:E:1225:ASN:HD22	1.44	0.82
1:E:1702:THR:HB	1:E:1784:LYS:HD2	1.62	0.82
1:A:2042:THR:CB	2:E:2601:PLX:H1A3	2.10	0.82
3:A:2606:PEE:H81	3:A:2606:PEE:C24	2.09	0.82
3:E:2608:PEE:H81	3:E:2608:PEE:C24	2.09	0.81
2:C:2609:PLX:H1A3	1:E:2042:THR:CB	2.10	0.81
2:A:2608:PLX:H1A3	1:C:2042:THR:CB	2.10	0.81
2:A:2608:PLX:C1A	1:C:2042:THR:HB	2.09	0.81
1:C:1107:GLN:HE22	1:C:1111:PHE:HD1	1.26	0.81
1:E:2035:ARG:HD2	3:E:2608:PEE:O5	1.81	0.81
1:A:2042:THR:CG2	2:E:2601:PLX:C1A	2.59	0.81
1:C:1002:ILE:HG23	1:C:1225:ASN:HD22	1.44	0.81
1:C:1702:THR:HB	1:C:1784:LYS:HD2	1.62	0.81
2:C:2609:PLX:C1A	1:E:2042:THR:HB	2.09	0.81
1:E:1107:GLN:HE22	1:E:1111:PHE:HD1	1.27	0.81
1:A:2197:LEU:HD11	2:A:2608:PLX:H393	1.60	0.81
2:C:2609:PLX:C1A	1:E:2042:THR:CG2	2.59	0.81
1:E:2518:GLU:OE1	1:E:2518:GLU:N	2.14	0.80
1:A:1345:LEU:HB2	1:A:2104:ARG:HH11	1.47	0.80
1:A:2518:GLU:N	1:A:2518:GLU:OE1	2.14	0.80
2:C:2604:PLX:C22	2:C:2605:PLX:H211	2.12	0.80
1:A:1002:ILE:HG23	1:A:1225:ASN:HD22	1.44	0.80
1:C:2179:LYS:HD3	1:E:1402:ASP:HB3	1.63	0.80
1:C:2518:GLU:N	1:C:2518:GLU:OE1	2.14	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2197:LEU:HD11	2:E:2601:PLX:H393	1.59	0.80
2:A:2608:PLX:C1A	1:C:2042:THR:CG2	2.59	0.80
1:E:2197:LEU:HD22	2:E:2601:PLX:H392	1.64	0.80
1:E:2197:LEU:CD1	2:E:2601:PLX:C39	2.28	0.80
1:C:2035:ARG:HD2	3:C:2607:PEE:O5	1.81	0.79
2:E:2605:PLX:C22	2:E:2606:PLX:H211	2.12	0.79
1:A:1402:ASP:HB3	1:E:2179:LYS:HD3	1.62	0.79
1:A:2293:LEU:HD11	1:A:2427:LEU:HD23	1.64	0.79
2:A:2603:PLX:C22	2:A:2604:PLX:H211	2.12	0.79
1:A:2035:ARG:HD2	3:A:2606:PEE:O5	1.81	0.79
1:A:2197:LEU:HD22	2:A:2608:PLX:H392	1.65	0.78
1:C:2197:LEU:HD22	2:C:2609:PLX:C37	2.04	0.78
1:A:1107:GLN:HE22	1:A:1111:PHE:HD1	1.26	0.78
1:E:2293:LEU:HD11	1:E:2427:LEU:HD23	1.64	0.78
1:C:2197:LEU:HD22	2:C:2609:PLX:H392	1.64	0.78
1:C:2293:LEU:HD11	1:C:2427:LEU:HD23	1.64	0.78
1:E:1345:LEU:HB2	1:E:2104:ARG:HH11	1.47	0.78
1:C:1345:LEU:HB2	1:C:2104:ARG:HH11	1.47	0.77
1:E:2197:LEU:HA	2:E:2601:PLX:H392	1.67	0.77
1:A:2197:LEU:CD1	2:A:2608:PLX:C39	2.30	0.77
1:C:2387:VAL:HG11	1:C:2390:LEU:HD23	1.66	0.77
1:E:2387:VAL:HG11	1:E:2390:LEU:HD23	1.66	0.77
3:E:2608:PEE:H68	3:E:2608:PEE:C45	2.12	0.77
1:C:2197:LEU:HD11	2:C:2609:PLX:H393	1.60	0.76
1:A:2387:VAL:HG11	1:A:2390:LEU:HD23	1.66	0.76
1:C:907:ASP:CG	1:C:908:PRO:HD3	2.11	0.76
1:C:2197:LEU:HA	2:C:2609:PLX:H392	1.66	0.76
1:C:2243:ALA:HB1	1:C:2247:SER:HB2	1.68	0.76
1:E:907:ASP:CG	1:E:908:PRO:HD3	2.11	0.76
1:A:2243:ALA:HB1	1:A:2247:SER:HB2	1.68	0.76
1:A:2197:LEU:HA	2:A:2608:PLX:H392	1.67	0.75
1:E:2542:TRP:O	1:E:2546:ARG:NH2	2.20	0.75
1:E:2197:LEU:HD22	2:E:2601:PLX:C39	2.17	0.75
1:E:2243:ALA:HB1	1:E:2247:SER:HB2	1.68	0.74
1:A:907:ASP:CG	1:A:908:PRO:HD3	2.11	0.74
1:C:2295:ARG:NH2	1:E:2295:ARG:HD2	2.02	0.74
1:C:1743:THR:HG22	1:C:1776:LEU:HD11	1.69	0.74
1:A:2042:THR:HG22	2:E:2601:PLX:C1A	2.18	0.74
1:A:2197:LEU:HD22	2:A:2608:PLX:C39	2.18	0.74
1:A:2295:ARG:NH2	1:C:2295:ARG:HD2	2.02	0.74
2:C:2609:PLX:H1A3	1:E:2042:THR:CG2	2.18	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2608:PLX:H1A3	1:C:2042:THR:CG2	2.18	0.74
1:C:2542:TRP:O	1:C:2546:ARG:NH2	2.20	0.74
1:A:2042:THR:CG2	2:E:2601:PLX:H1A3	2.18	0.74
1:C:2197:LEU:HD22	2:C:2609:PLX:C39	2.17	0.73
3:C:2607:PEE:H68	3:C:2607:PEE:C45	2.12	0.73
2:C:2609:PLX:C1A	1:E:2042:THR:HG22	2.18	0.73
1:A:2542:TRP:O	1:A:2546:ARG:NH2	2.20	0.73
1:E:1743:THR:HG22	1:E:1776:LEU:HD11	1.69	0.73
1:A:1743:THR:HG22	1:A:1776:LEU:HD11	1.69	0.73
1:A:2029:GLY:O	1:A:2033:ILE:HD12	1.89	0.73
1:C:1234:PHE:HE1	1:C:1246:ILE:HD12	1.54	0.73
2:A:2608:PLX:C1A	1:C:2042:THR:HG22	2.18	0.73
1:E:2069:THR:HG22	1:E:2070:GLU:H	1.54	0.73
2:A:2608:PLX:H22	1:C:2042:THR:HG21	1.71	0.73
1:E:2235:TYR:CD2	1:E:2304:MET:HG3	2.24	0.73
2:A:2608:PLX:C16	2:A:2608:PLX:H341	2.19	0.73
2:E:2601:PLX:H162	2:E:2601:PLX:C36	2.19	0.73
1:A:2042:THR:HG21	2:E:2601:PLX:H22	1.71	0.72
1:A:2069:THR:HG22	1:A:2070:GLU:H	1.54	0.72
1:C:2235:TYR:CD2	1:C:2304:MET:HG3	2.24	0.72
1:A:2235:TYR:CD2	1:A:2304:MET:HG3	2.24	0.72
1:A:2388:LYS:HZ2	1:A:2394:GLU:CD	1.97	0.72
1:C:2325:ARG:NH1	1:C:2336:THR:OG1	2.22	0.72
1:E:1234:PHE:HE1	1:E:1246:ILE:HD12	1.54	0.72
1:E:2388:LYS:HZ2	1:E:2394:GLU:CD	1.98	0.72
1:C:2029:GLY:O	1:C:2033:ILE:HD12	1.89	0.72
1:E:2325:ARG:NH1	1:E:2336:THR:OG1	2.22	0.72
1:A:2295:ARG:HD2	1:E:2295:ARG:NH2	2.03	0.72
2:A:2608:PLX:H162	2:A:2608:PLX:C36	2.19	0.72
2:C:2609:PLX:H341	2:C:2609:PLX:C16	2.19	0.72
1:E:2029:GLY:O	1:E:2033:ILE:HD12	1.89	0.72
2:C:2609:PLX:H162	2:C:2609:PLX:C36	2.19	0.72
2:C:2609:PLX:H22	1:E:2042:THR:HG21	1.71	0.72
1:E:1724:ARG:HH12	1:E:1804:GLY:HA3	1.55	0.72
1:A:1703:ALA:H	1:A:2073:PHE:HD1	1.37	0.72
2:E:2601:PLX:H341	2:E:2601:PLX:C16	2.19	0.72
1:A:1234:PHE:HE1	1:A:1246:ILE:HD12	1.54	0.71
1:A:2325:ARG:NH1	1:A:2336:THR:OG1	2.22	0.71
1:A:1724:ARG:HH12	1:A:1804:GLY:HA3	1.55	0.71
1:C:1703:ALA:H	1:C:2073:PHE:HD1	1.37	0.71
1:C:2069:THR:HG22	1:C:2070:GLU:H	1.54	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1143:PHE:CD2	1:E:1154:LYS:HB3	2.27	0.70
1:C:1724:ARG:HH12	1:C:1804:GLY:HA3	1.55	0.70
1:E:2197:LEU:HD13	2:E:2601:PLX:H393	0.70	0.70
1:A:2109:PHE:CE1	3:A:2606:PEE:O4	2.45	0.70
1:C:1143:PHE:CD2	1:C:1154:LYS:HB3	2.27	0.70
1:C:1735:VAL:CG1	2:C:2604:PLX:C13	2.63	0.70
1:C:2109:PHE:CE1	3:C:2607:PEE:O4	2.45	0.70
1:E:2109:PHE:HE1	3:E:2608:PEE:O4	1.74	0.70
1:A:2109:PHE:HE1	3:A:2606:PEE:O4	1.75	0.70
1:C:2109:PHE:HE1	3:C:2607:PEE:O4	1.75	0.70
1:E:2109:PHE:CE1	3:E:2608:PEE:O4	2.44	0.70
1:E:2113:LYS:O	1:E:2118:ASN:ND2	2.24	0.70
1:E:1703:ALA:H	1:E:2073:PHE:HD1	1.37	0.70
1:C:1724:ARG:HH22	1:C:1805:LEU:H	1.39	0.69
2:E:2601:PLX:H232	2:E:2601:PLX:H391	1.74	0.69
3:A:2606:PEE:H68	3:A:2606:PEE:C45	2.12	0.69
1:E:1724:ARG:HH22	1:E:1805:LEU:H	1.39	0.69
1:E:2149:LEU:O	1:E:2153:MET:HG2	1.92	0.69
1:A:1143:PHE:CD2	1:A:1154:LYS:HB3	2.27	0.69
1:A:2197:LEU:HD13	2:A:2608:PLX:H393	0.71	0.69
1:A:1201:LYS:O	1:A:1206:GLN:NE2	2.26	0.69
2:C:2609:PLX:H1A2	1:E:2042:THR:CG2	2.22	0.69
1:A:2113:LYS:O	1:A:2118:ASN:ND2	2.24	0.69
1:A:2149:LEU:O	1:A:2153:MET:HG2	1.92	0.69
1:C:2149:LEU:O	1:C:2153:MET:HG2	1.92	0.69
3:C:2607:PEE:H82	3:C:2607:PEE:C41	2.22	0.69
1:E:1201:LYS:O	1:E:1206:GLN:NE2	2.26	0.69
2:C:2609:PLX:H232	2:C:2609:PLX:H391	1.74	0.68
1:A:1996:TRP:HE1	1:E:2463:GLY:HA2	1.59	0.68
1:C:1731:MET:HG2	2:C:2604:PLX:H4	1.76	0.68
1:A:1724:ARG:HH22	1:A:1805:LEU:H	1.39	0.68
1:C:1521:ARG:HE	1:C:1528:ARG:CZ	2.07	0.68
1:A:1521:ARG:HE	1:A:1528:ARG:CZ	2.07	0.68
1:A:1970:TYR:HD2	1:A:1970:TYR:O	1.77	0.68
2:A:2608:PLX:H232	2:A:2608:PLX:H391	1.74	0.68
1:C:2113:LYS:O	1:C:2118:ASN:ND2	2.24	0.68
1:A:1539:TYR:HE2	1:A:1656:ILE:HG21	1.58	0.68
3:A:2606:PEE:H82	3:A:2606:PEE:C41	2.22	0.68
1:E:1521:ARG:HE	1:E:1528:ARG:CZ	2.07	0.68
1:A:2144:ASP:HB2	1:E:2182:LYS:HE2	1.76	0.68
1:C:1201:LYS:O	1:C:1206:GLN:NE2	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2608:PLX:H1A2	1:C:2042:THR:CG2	2.22	0.68
1:C:1079:TRP:HE3	1:C:1080:LEU:HD12	1.58	0.68
1:C:1539:TYR:HE2	1:C:1656:ILE:HG21	1.58	0.68
1:C:2197:LEU:HD13	2:C:2609:PLX:H393	0.70	0.67
1:E:1970:TYR:HD2	1:E:1970:TYR:O	1.77	0.67
1:E:1539:TYR:HE2	1:E:1656:ILE:HG21	1.58	0.67
1:A:1731:MET:HG2	2:A:2603:PLX:H4	1.76	0.67
1:E:2125:PHE:CD1	3:E:2608:PEE:H19	2.30	0.67
1:A:1079:TRP:HE3	1:A:1080:LEU:HD12	1.58	0.67
1:C:1970:TYR:HD2	1:C:1970:TYR:O	1.77	0.67
1:C:2125:PHE:CD1	3:C:2607:PEE:H19	2.29	0.67
1:A:2182:LYS:HE2	1:C:2144:ASP:HB2	1.77	0.67
1:C:2463:GLY:HA2	1:E:1996:TRP:HE1	1.58	0.67
1:A:2125:PHE:CD1	3:A:2606:PEE:H19	2.30	0.67
1:E:1731:MET:HG2	2:E:2605:PLX:H4	1.76	0.66
1:E:1735:VAL:CG1	2:E:2605:PLX:C13	2.63	0.66
3:E:2608:PEE:H82	3:E:2608:PEE:C41	2.22	0.66
1:E:1221:ILE:HD11	1:E:1280:ILE:HG23	1.78	0.66
1:C:2071:ARG:CZ	1:C:2074:SER:HB2	2.26	0.66
1:C:2182:LYS:HE2	1:E:2144:ASP:HB2	1.77	0.66
1:E:1079:TRP:HE3	1:E:1080:LEU:HD12	1.58	0.66
1:E:2421:THR:O	1:E:2425:ASP:HB2	1.96	0.66
1:A:2071:ARG:CZ	1:A:2074:SER:HB2	2.26	0.66
1:A:2250:PRO:HA	1:A:2282:VAL:HG12	1.78	0.66
1:A:2463:GLY:HA2	1:C:1996:TRP:HE1	1.60	0.66
1:A:2421:THR:O	1:A:2425:ASP:HB2	1.96	0.65
1:C:1221:ILE:HD11	1:C:1280:ILE:HG23	1.78	0.65
1:E:2071:ARG:CZ	1:E:2074:SER:HB2	2.26	0.65
1:A:1510:GLN:HE22	1:A:1671:ARG:HH22	1.45	0.65
2:C:2609:PLX:H341	2:C:2609:PLX:H161	1.78	0.65
1:E:2128:VAL:HG11	1:E:2131:LEU:HD12	1.78	0.65
2:E:2601:PLX:H341	2:E:2601:PLX:H161	1.79	0.65
2:A:2608:PLX:H341	2:A:2608:PLX:H161	1.79	0.65
1:C:1157:VAL:HG21	4:C:2608:P5S:H46A	1.79	0.65
1:A:1157:VAL:HG21	4:A:2607:P5S:H46A	1.79	0.65
1:E:2135:ARG:CZ	3:E:2608:PEE:O1P	2.45	0.65
1:E:2250:PRO:HA	1:E:2282:VAL:HG12	1.78	0.65
1:C:2388:LYS:HZ2	1:C:2394:GLU:CD	2.05	0.65
1:A:1221:ILE:HD11	1:A:1280:ILE:HG23	1.78	0.64
3:A:2606:PEE:H74	3:A:2606:PEE:C25	2.26	0.64
1:A:2058:HIS:NE2	1:A:2083:TYR:OH	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2128:VAL:HG11	1:C:2131:LEU:HD12	1.78	0.64
1:C:2135:ARG:CZ	3:C:2607:PEE:O1P	2.45	0.64
1:C:2421:THR:O	1:C:2425:ASP:HB2	1.96	0.64
3:E:2608:PEE:H74	3:E:2608:PEE:C25	2.26	0.64
1:C:2250:PRO:HA	1:C:2282:VAL:HG12	1.78	0.64
1:A:2128:VAL:HG11	1:A:2131:LEU:HD12	1.78	0.64
1:C:1728:ARG:NH2	2:C:2605:PLX:O7	2.31	0.64
1:E:1539:TYR:CE2	1:E:1656:ILE:HG21	2.32	0.64
3:C:2607:PEE:H74	3:C:2607:PEE:C25	2.26	0.64
1:E:1728:ARG:NH2	2:E:2606:PLX:O7	2.31	0.64
1:A:2135:ARG:CZ	3:A:2606:PEE:O1P	2.45	0.64
1:C:822:LEU:HD12	1:C:1091:SER:HB3	1.80	0.64
1:A:1539:TYR:CE2	1:A:1656:ILE:HG21	2.32	0.64
1:C:1510:GLN:HE22	1:C:1671:ARG:HH22	1.45	0.64
1:A:1647:GLU:N	1:A:1647:GLU:OE1	2.31	0.64
1:A:1728:ARG:NH2	2:A:2604:PLX:O7	2.31	0.64
1:E:1510:GLN:HE22	1:E:1671:ARG:HH22	1.45	0.64
1:C:2058:HIS:NE2	1:C:2083:TYR:OH	2.28	0.63
1:C:2135:ARG:NH1	3:C:2607:PEE:O1P	2.31	0.63
2:C:2603:PLX:H82	2:C:2603:PLX:H291	1.80	0.63
2:A:2608:PLX:C39	2:A:2608:PLX:H232	2.29	0.63
2:E:2601:PLX:C39	2:E:2601:PLX:H232	2.29	0.63
1:A:2042:THR:CG2	2:E:2601:PLX:H1A2	2.22	0.63
1:C:1647:GLU:N	1:C:1647:GLU:OE1	2.31	0.63
1:E:1157:VAL:HG21	4:E:2609:P5S:H46A	1.79	0.63
1:E:2135:ARG:NH1	3:E:2608:PEE:O1P	2.31	0.63
1:E:2197:LEU:CD2	2:E:2601:PLX:C39	2.77	0.63
1:A:2135:ARG:NH1	3:A:2606:PEE:O1P	2.31	0.63
2:A:2609:PLX:H151	2:A:2609:PLX:H352	1.80	0.63
1:A:822:LEU:HD12	1:A:1091:SER:HB3	1.80	0.63
1:E:1647:GLU:OE1	1:E:1647:GLU:N	2.31	0.63
1:E:822:LEU:HD12	1:E:1091:SER:HB3	1.80	0.63
1:C:1539:TYR:CE2	1:C:1656:ILE:HG21	2.32	0.62
1:C:2197:LEU:HA	2:C:2609:PLX:C39	2.29	0.62
1:E:1262:LYS:HA	1:E:1265:MET:HE1	1.81	0.62
1:E:2058:HIS:NE2	1:E:2083:TYR:OH	2.29	0.62
1:E:1016:TRP:CD1	1:E:1036:TYR:HD2	2.18	0.62
1:A:1009:MET:HG3	1:A:1047:GLN:HE21	1.63	0.62
2:C:2609:PLX:C39	2:C:2609:PLX:H232	2.29	0.62
1:E:1009:MET:HG3	1:E:1047:GLN:HE21	1.63	0.62
1:A:2197:LEU:CD2	2:A:2608:PLX:C39	2.78	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1009:MET:HG3	1:C:1047:GLN:HE21	1.63	0.62
1:E:1005:ARG:NH1	1:E:1047:GLN:HE22	1.98	0.62
1:A:1735:VAL:CG1	2:A:2603:PLX:C13	2.63	0.62
1:C:2197:LEU:CD2	2:C:2609:PLX:C39	2.77	0.62
1:A:1016:TRP:CD1	1:A:1036:TYR:HD2	2.18	0.62
1:C:1005:ARG:NH1	1:C:1047:GLN:HE22	1.98	0.62
2:C:2601:PLX:H151	2:C:2601:PLX:H352	1.80	0.62
2:E:2604:PLX:H82	2:E:2604:PLX:H291	1.80	0.62
2:E:2601:PLX:H342	2:E:2601:PLX:C14	2.30	0.62
2:E:2602:PLX:H352	2:E:2602:PLX:H151	1.80	0.62
2:A:2602:PLX:H82	2:A:2602:PLX:H291	1.80	0.62
1:C:1016:TRP:CD1	1:C:1036:TYR:HD2	2.18	0.62
1:C:1722:ILE:CG2	1:C:1723:PRO:HD2	2.28	0.62
2:C:2609:PLX:C1A	1:E:2042:THR:CB	2.74	0.62
1:A:1005:ARG:NH1	1:A:1047:GLN:HE22	1.98	0.61
2:A:2608:PLX:H342	2:A:2608:PLX:C14	2.30	0.61
1:A:2197:LEU:HA	2:A:2608:PLX:C39	2.31	0.61
3:A:2606:PEE:H70	1:E:2203:ILE:HD13	1.81	0.61
1:E:2184:LYS:HB2	1:E:2187:VAL:HG12	1.81	0.61
1:A:2042:THR:CB	2:E:2601:PLX:C1A	2.74	0.61
1:C:2203:ILE:HD13	3:E:2608:PEE:H70	1.82	0.61
1:A:1262:LYS:HA	1:A:1265:MET:HE1	1.81	0.61
1:E:1033:TRP:HD1	1:E:1108:TRP:CD1	2.19	0.61
1:A:2325:ARG:HH22	1:A:2333:VAL:HG13	1.65	0.61
1:C:1033:TRP:HD1	1:C:1108:TRP:CD1	2.19	0.61
1:C:2325:ARG:HH22	1:C:2333:VAL:HG13	1.65	0.61
1:A:2184:LYS:HB2	1:A:2187:VAL:HG12	1.81	0.61
1:C:1262:LYS:HA	1:C:1265:MET:HE1	1.81	0.61
2:C:2609:PLX:C14	2:C:2609:PLX:H342	2.30	0.61
1:A:1033:TRP:HD1	1:A:1108:TRP:CD1	2.19	0.61
1:E:1722:ILE:CG2	1:E:1723:PRO:HD2	2.28	0.61
1:E:1969:LYS:HD3	1:E:1970:TYR:N	2.16	0.61
1:E:2325:ARG:HH22	1:E:2333:VAL:HG13	1.65	0.61
1:C:2235:TYR:HD2	1:C:2304:MET:HG3	1.66	0.61
1:A:1234:PHE:CE1	1:A:1246:ILE:HD12	2.36	0.60
1:A:2203:ILE:HD13	3:C:2607:PEE:H70	1.82	0.60
1:C:2184:LYS:HB2	1:C:2187:VAL:HG12	1.82	0.60
1:A:1969:LYS:HD3	1:A:1970:TYR:N	2.16	0.60
2:A:2608:PLX:H342	2:A:2608:PLX:H142	1.83	0.60
1:C:1234:PHE:CE1	1:C:1246:ILE:HD12	2.36	0.60
1:C:1559:LEU:HG	1:C:1653:ARG:HD2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1153:LEU:HD23	4:E:2609:P5S:H49	1.84	0.60
1:A:801:VAL:O	1:A:804:LEU:N	2.35	0.60
1:A:2513:VAL:HG23	1:A:2518:GLU:HG2	1.84	0.60
1:E:2197:LEU:HA	2:E:2601:PLX:C39	2.30	0.60
3:E:2608:PEE:H40	3:E:2608:PEE:C44	2.31	0.60
3:A:2606:PEE:H40	3:A:2606:PEE:C44	2.31	0.60
1:C:992:GLU:OE1	1:C:992:GLU:N	2.35	0.60
1:C:1081:TYR:CE1	1:C:1089:PRO:HB2	2.37	0.60
3:C:2607:PEE:H40	3:C:2607:PEE:C44	2.31	0.60
2:A:2608:PLX:C1A	1:C:2042:THR:CB	2.74	0.60
1:C:801:VAL:O	1:C:804:LEU:N	2.35	0.60
1:C:2513:VAL:HG23	1:C:2518:GLU:HG2	1.84	0.60
1:E:1081:TYR:CE1	1:E:1089:PRO:HB2	2.37	0.60
1:A:1559:LEU:HG	1:A:1653:ARG:HD2	1.84	0.60
2:C:2609:PLX:H342	2:C:2609:PLX:H142	1.83	0.59
2:E:2607:PLX:H342	2:E:2607:PLX:H302	1.83	0.59
1:A:2235:TYR:HD2	1:A:2304:MET:HG3	1.66	0.59
1:C:2324:GLN:HB2	1:C:2335:TYR:CE1	2.37	0.59
1:C:1969:LYS:HD3	1:C:1970:TYR:N	2.16	0.59
2:E:2601:PLX:H342	2:E:2601:PLX:H142	1.83	0.59
1:A:1081:TYR:CE1	1:A:1089:PRO:HB2	2.37	0.59
1:A:1722:ILE:CG2	1:A:1723:PRO:HD2	2.28	0.59
1:E:2235:TYR:HD2	1:E:2304:MET:HG3	1.66	0.59
2:A:2605:PLX:H342	2:A:2605:PLX:H302	1.83	0.59
1:E:1243:CYS:O	1:E:1246:ILE:HG22	2.03	0.59
1:C:1243:CYS:O	1:C:1246:ILE:HG22	2.03	0.59
1:E:1559:LEU:HG	1:E:1653:ARG:HD2	1.84	0.59
1:E:801:VAL:O	1:E:804:LEU:N	2.35	0.59
1:E:1234:PHE:CE1	1:E:1246:ILE:HD12	2.36	0.59
1:C:2179:LYS:CD	1:E:1402:ASP:HB3	2.33	0.59
2:C:2606:PLX:H342	2:C:2606:PLX:H302	1.83	0.58
1:E:2324:GLN:HB2	1:E:2335:TYR:CE1	2.37	0.58
1:C:1153:LEU:HD23	4:C:2608:P5S:H49	1.84	0.58
1:E:992:GLU:OE1	1:E:992:GLU:N	2.35	0.58
1:E:2513:VAL:HG23	1:E:2518:GLU:HG2	1.84	0.58
1:A:899:SER:OG	1:A:900:LEU:N	2.36	0.58
1:A:992:GLU:N	1:A:992:GLU:OE1	2.35	0.58
1:A:2182:LYS:CE	1:C:2144:ASP:HB2	2.33	0.58
1:A:2324:GLN:HB2	1:A:2335:TYR:CE1	2.37	0.58
1:C:2197:LEU:CA	2:C:2609:PLX:H392	2.32	0.58
1:A:2144:ASP:HB2	1:E:2182:LYS:CE	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2408:GLU:O	1:C:2426:PHE:HB2	2.04	0.58
1:E:899:SER:OG	1:E:900:LEU:N	2.36	0.58
1:A:1153:LEU:HD23	4:A:2607:P5S:H49	1.84	0.58
1:C:899:SER:OG	1:C:900:LEU:N	2.36	0.58
1:A:1243:CYS:O	1:A:1246:ILE:HG22	2.03	0.58
1:A:2408:GLU:O	1:A:2426:PHE:HB2	2.04	0.58
1:E:1547:ARG:HG3	1:E:1548:VAL:H	1.69	0.58
1:A:1402:ASP:HB3	1:E:2179:LYS:CD	2.33	0.58
1:A:2197:LEU:CA	2:A:2608:PLX:H392	2.33	0.58
1:C:2182:LYS:CE	1:E:2144:ASP:HB2	2.33	0.58
1:A:1213:LEU:HG	1:A:1290:LEU:HD21	1.86	0.58
1:A:2179:LYS:CD	1:C:1402:ASP:HB3	2.32	0.58
2:A:2608:PLX:H291	2:A:2608:PLX:H331	1.86	0.58
1:E:2197:LEU:CA	2:E:2601:PLX:H392	2.33	0.58
1:A:2461:LEU:O	1:A:2465:GLY:HA3	2.04	0.57
1:C:1213:LEU:HG	1:C:1290:LEU:HD21	1.86	0.57
2:C:2609:PLX:H291	2:C:2609:PLX:H331	1.86	0.57
1:E:842:TYR:HD1	1:E:844:ARG:HH21	1.52	0.57
1:E:1544:GLU:OE1	1:E:1550:GLU:N	2.30	0.57
1:E:1194:PHE:CZ	2:E:2605:PLX:H1B3	2.40	0.57
1:A:1194:PHE:CZ	2:A:2603:PLX:H1B3	2.39	0.57
1:A:1547:ARG:HG3	1:A:1548:VAL:H	1.69	0.57
1:E:1040:LEU:HG	1:E:1101:LEU:HD12	1.86	0.57
1:A:842:TYR:HD1	1:A:844:ARG:HH21	1.52	0.57
1:C:1194:PHE:CZ	2:C:2604:PLX:H1B3	2.39	0.57
1:C:1777:GLU:OE2	1:C:1779:THR:HG23	2.05	0.57
1:C:2461:LEU:O	1:C:2465:GLY:HA3	2.04	0.57
1:E:1106:GLN:O	1:E:1109:GLN:HG2	2.05	0.57
1:E:2463:GLY:O	1:E:2464:TYR:HD1	1.87	0.57
1:A:2463:GLY:O	1:A:2464:TYR:HD1	1.87	0.57
1:C:2463:GLY:O	1:C:2464:TYR:HD1	1.87	0.57
1:A:1106:GLN:O	1:A:1109:GLN:HG2	2.05	0.57
1:A:1777:GLU:OE2	1:A:1779:THR:HG23	2.05	0.57
1:C:1402:ASP:O	1:C:1405:THR:OG1	2.22	0.57
1:C:1547:ARG:HG3	1:C:1548:VAL:H	1.69	0.57
1:A:897:ASN:OD1	1:A:898:GLN:N	2.33	0.57
1:A:1040:LEU:HG	1:A:1101:LEU:HD12	1.86	0.57
1:E:1213:LEU:HG	1:E:1290:LEU:HD21	1.86	0.57
1:E:1402:ASP:O	1:E:1405:THR:OG1	2.22	0.57
1:E:2461:LEU:O	1:E:2465:GLY:HA3	2.04	0.57
3:E:2608:PEE:H68	3:E:2608:PEE:H78	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2608:PLX:C34	2:A:2608:PLX:H141	2.35	0.56
1:C:1202:ASP:OD1	1:C:1202:ASP:N	2.38	0.56
2:C:2609:PLX:H141	2:C:2609:PLX:C34	2.35	0.56
1:E:2125:PHE:O	1:E:2128:VAL:HG12	2.05	0.56
1:E:2408:GLU:O	1:E:2426:PHE:HB2	2.04	0.56
2:E:2601:PLX:H331	2:E:2601:PLX:H291	1.86	0.56
1:C:1051:CYS:SG	1:C:1091:SER:OG	2.63	0.56
1:C:1106:GLN:O	1:C:1109:GLN:HG2	2.05	0.56
1:A:2042:THR:CG2	2:E:2601:PLX:H22	2.34	0.56
1:C:1040:LEU:HG	1:C:1101:LEU:HD12	1.86	0.56
1:C:2492:ILE:HD11	1:E:2530:ILE:HD12	1.86	0.56
2:C:2609:PLX:O7	2:C:2609:PLX:O3	2.23	0.56
1:E:1687:SER:OG	1:E:1796:HIS:ND1	2.29	0.56
1:A:1783:ILE:HG23	1:A:1786:ASP:HB3	1.88	0.56
2:C:2609:PLX:H22	1:E:2042:THR:CG2	2.34	0.56
1:E:1777:GLU:OE2	1:E:1779:THR:HG23	2.05	0.56
1:A:2179:LYS:HE3	1:C:1402:ASP:C	2.30	0.56
1:C:1783:ILE:HG23	1:C:1786:ASP:HB3	1.88	0.56
1:E:2041:LYS:HA	1:E:2101:TYR:CD2	2.41	0.56
1:A:2041:LYS:HA	1:A:2101:TYR:CD2	2.41	0.56
1:A:2492:ILE:HD11	1:C:2530:ILE:HD12	1.87	0.56
1:A:1402:ASP:O	1:A:1405:THR:OG1	2.22	0.56
1:A:2530:ILE:HD12	1:E:2492:ILE:HD11	1.87	0.56
2:A:2608:PLX:H22	1:C:2042:THR:CG2	2.34	0.56
1:C:801:VAL:O	1:C:802:ARG:C	2.49	0.56
1:C:2394:GLU:OE1	1:C:2398:TYR:OH	2.20	0.56
1:C:2410:VAL:HG12	1:C:2426:PHE:HA	1.88	0.56
1:E:1315:GLN:HE22	1:E:1538:ARG:CB	2.19	0.56
2:E:2601:PLX:O7	2:E:2601:PLX:O3	2.23	0.56
1:C:2125:PHE:O	1:C:2128:VAL:HG12	2.05	0.56
1:A:1494:MET:HE1	1:A:1497:ARG:HH11	1.71	0.56
1:C:1315:GLN:HE22	1:C:1538:ARG:CB	2.19	0.56
1:C:2041:LYS:HA	1:C:2101:TYR:CD2	2.41	0.56
1:C:2125:PHE:CE1	3:C:2607:PEE:H19	2.41	0.56
2:E:2601:PLX:H141	2:E:2601:PLX:C34	2.35	0.56
1:A:1051:CYS:SG	1:A:1091:SER:OG	2.63	0.55
1:A:1687:SER:OG	1:A:1796:HIS:ND1	2.29	0.55
1:C:842:TYR:HD1	1:C:844:ARG:HH21	1.52	0.55
1:E:801:VAL:O	1:E:802:ARG:C	2.49	0.55
1:E:897:ASN:OD1	1:E:898:GLN:N	2.34	0.55
1:E:2134:LEU:HB3	1:E:2138:MET:HE2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1692:TYR:CE1	1:A:1714:VAL:HG13	2.41	0.55
2:A:2608:PLX:O7	2:A:2608:PLX:O3	2.23	0.55
1:E:1783:ILE:HG23	1:E:1786:ASP:HB3	1.88	0.55
1:E:1692:TYR:CE1	1:E:1714:VAL:HG13	2.42	0.55
1:E:2410:VAL:HG12	1:E:2426:PHE:HA	1.88	0.55
1:A:1402:ASP:C	1:E:2179:LYS:HE3	2.31	0.55
1:A:2125:PHE:O	1:A:2128:VAL:HG12	2.05	0.55
1:C:1494:MET:HE1	1:C:1497:ARG:HH11	1.71	0.55
3:A:2606:PEE:H68	3:A:2606:PEE:H78	1.87	0.55
1:E:1008:PHE:HD2	1:E:1009:MET:HE2	1.72	0.55
1:E:1494:MET:HE1	1:E:1497:ARG:HH11	1.71	0.55
1:A:1315:GLN:HE22	1:A:1538:ARG:CB	2.19	0.55
1:C:901:LEU:HG	1:C:1085:PHE:CG	2.42	0.55
1:A:2134:LEU:HB3	1:A:2138:MET:HE2	1.88	0.55
1:C:2134:LEU:HB3	1:C:2138:MET:HE2	1.88	0.55
1:A:2410:VAL:HG12	1:A:2426:PHE:HA	1.88	0.55
1:C:2138:MET:CE	3:C:2607:PEE:H49	2.37	0.54
1:C:2179:LYS:HE3	1:E:1402:ASP:C	2.32	0.54
1:E:901:LEU:HG	1:E:1085:PHE:CG	2.42	0.54
1:A:1403:HIS:O	1:A:1406:VAL:HG12	2.07	0.54
1:C:1403:HIS:O	1:C:1406:VAL:HG12	2.07	0.54
1:C:1544:GLU:OE1	1:C:1550:GLU:N	2.30	0.54
1:C:2308:LEU:HD21	1:C:2354:LEU:HB3	1.89	0.54
1:E:1403:HIS:O	1:E:1406:VAL:HG12	2.07	0.54
1:E:2138:MET:CE	3:E:2608:PEE:H49	2.37	0.54
1:A:2308:LEU:HD21	1:A:2354:LEU:HB3	1.90	0.54
1:C:1008:PHE:HD2	1:C:1009:MET:HE2	1.72	0.54
1:C:1687:SER:OG	1:C:1796:HIS:ND1	2.29	0.54
1:E:1051:CYS:SG	1:E:1091:SER:OG	2.63	0.54
1:A:901:LEU:HG	1:A:1085:PHE:CG	2.42	0.54
1:A:2138:MET:CE	3:A:2606:PEE:H49	2.37	0.54
1:A:2125:PHE:CE1	3:A:2606:PEE:H19	2.41	0.54
1:C:1163:TRP:CE2	2:C:2603:PLX:H51	2.43	0.54
1:C:2463:GLY:HA2	1:E:1996:TRP:NE1	2.23	0.54
1:A:801:VAL:O	1:A:802:ARG:C	2.49	0.54
3:A:2606:PEE:C45	3:A:2606:PEE:C41	2.85	0.54
1:C:1692:TYR:CE1	1:C:1714:VAL:HG13	2.42	0.54
1:E:1002:ILE:HG23	1:E:1225:ASN:ND2	2.20	0.54
1:E:1202:ASP:OD1	1:E:1202:ASP:N	2.38	0.54
1:E:2269:ALA:O	1:E:2273:ILE:HG13	2.08	0.54
1:A:1780:ASP:OD1	1:A:1781:SER:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1252:VAL:HG12	1:C:1278:ALA:HB3	1.90	0.54
1:C:2434:LEU:HD13	1:C:2444:LEU:HD22	1.89	0.54
3:C:2607:PEE:H68	3:C:2607:PEE:H78	1.87	0.54
1:E:2425:ASP:HB3	1:E:2426:PHE:HD1	1.73	0.54
1:E:2434:LEU:HD13	1:E:2444:LEU:HD22	1.89	0.54
1:A:2269:ALA:O	1:A:2273:ILE:HG13	2.08	0.54
1:E:1780:ASP:OD1	1:E:1781:SER:N	2.41	0.54
1:A:1008:PHE:HD2	1:A:1009:MET:HE2	1.72	0.53
1:A:1264:MET:HG3	1:A:1273:LEU:HD22	1.90	0.53
1:A:2434:LEU:HD13	1:A:2444:LEU:HD22	1.89	0.53
1:E:2125:PHE:CE1	3:E:2608:PEE:H19	2.41	0.53
1:A:1306:SER:O	1:A:1310:LYS:HG2	2.09	0.53
1:C:1780:ASP:OD1	1:C:1781:SER:N	2.41	0.53
1:E:897:ASN:O	1:E:903:ARG:NH2	2.42	0.53
1:E:1009:MET:HB3	1:E:1043:PHE:HZ	1.74	0.53
1:E:1264:MET:HG3	1:E:1273:LEU:HD22	1.91	0.53
1:E:2308:LEU:HD21	1:E:2354:LEU:HB3	1.89	0.53
1:A:2425:ASP:HB3	1:A:2426:PHE:HD1	1.73	0.53
1:C:2425:ASP:HB3	1:C:2426:PHE:HD1	1.73	0.53
1:E:1553:ARG:HH11	1:E:1556:LEU:HD12	1.74	0.53
1:E:1669:GLN:O	1:E:1674:ARG:HG3	2.08	0.53
1:C:1669:GLN:O	1:C:1674:ARG:HG3	2.08	0.53
1:E:1663:GLU:O	1:E:1666:GLU:HG3	2.09	0.53
1:A:1252:VAL:HG12	1:A:1278:ALA:HB3	1.90	0.53
1:A:1669:GLN:O	1:A:1674:ARG:HG3	2.08	0.53
1:A:1002:ILE:HG23	1:A:1225:ASN:ND2	2.20	0.53
1:A:1009:MET:HB3	1:A:1043:PHE:HZ	1.74	0.53
1:C:1306:SER:O	1:C:1310:LYS:HG2	2.09	0.53
1:E:1252:VAL:HG12	1:E:1278:ALA:HB3	1.90	0.53
1:E:1306:SER:O	1:E:1310:LYS:HG2	2.09	0.53
1:A:897:ASN:O	1:A:903:ARG:NH2	2.42	0.53
1:A:1163:TRP:CE2	2:A:2602:PLX:H51	2.43	0.53
1:A:1663:GLU:O	1:A:1666:GLU:HG3	2.09	0.53
1:C:1009:MET:HG3	1:C:1047:GLN:NE2	2.24	0.53
1:C:1264:MET:HG3	1:C:1273:LEU:HD22	1.91	0.53
1:C:1663:GLU:O	1:C:1666:GLU:HG3	2.09	0.53
1:C:2269:ALA:O	1:C:2273:ILE:HG13	2.08	0.53
1:A:2463:GLY:HA2	1:C:1996:TRP:NE1	2.24	0.52
1:C:1731:MET:CG	2:C:2604:PLX:H4	2.39	0.52
1:A:1553:ARG:HH11	1:A:1556:LEU:HD12	1.74	0.52
1:E:1731:MET:CG	2:E:2605:PLX:H4	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1987:ASP:OD2	1:C:2082:TRP:NE1	2.43	0.52
1:E:2244:GLN:HG2	1:E:2245:GLN:H	1.74	0.52
1:A:1232:CYS:SG	1:A:1233:VAL:N	2.83	0.52
1:C:2166:LYS:NZ	1:C:2501:ASP:OD1	2.41	0.52
1:C:2244:GLN:HG2	1:C:2245:GLN:H	1.74	0.52
1:A:1731:MET:CG	2:A:2603:PLX:H4	2.39	0.52
1:E:1163:TRP:CE2	2:E:2604:PLX:H51	2.43	0.52
1:E:1009:MET:HG3	1:E:1047:GLN:NE2	2.24	0.52
1:A:1009:MET:HG3	1:A:1047:GLN:NE2	2.24	0.52
1:A:1996:TRP:NE1	1:E:2463:GLY:HA2	2.23	0.52
1:A:2244:GLN:HG2	1:A:2245:GLN:H	1.74	0.52
1:C:1232:CYS:SG	1:C:1233:VAL:N	2.83	0.52
1:C:1553:ARG:HH11	1:C:1556:LEU:HD12	1.74	0.52
1:C:1752:PHE:HB3	1:C:1754:TRP:CE3	2.45	0.52
1:E:1752:PHE:HB3	1:E:1754:TRP:CE3	2.45	0.52
2:A:2608:PLX:H162	2:A:2608:PLX:H341	1.91	0.52
1:C:897:ASN:O	1:C:903:ARG:NH2	2.42	0.52
1:E:1232:CYS:SG	1:E:1233:VAL:N	2.83	0.52
3:E:2608:PEE:C45	3:E:2608:PEE:C24	2.85	0.52
1:A:1544:GLU:OE1	1:A:1550:GLU:N	2.29	0.52
1:A:2105:ILE:HG13	1:A:2106:LEU:HD12	1.92	0.52
1:C:897:ASN:OD1	1:C:898:GLN:N	2.33	0.51
1:C:1009:MET:HB3	1:C:1043:PHE:HZ	1.74	0.51
1:A:1265:MET:HE1	1:A:1275:VAL:HG11	1.92	0.51
1:A:2244:GLN:HG2	1:A:2245:GLN:N	2.25	0.51
1:C:2105:ILE:HG13	1:C:2106:LEU:HD12	1.92	0.51
1:E:2046:LYS:NZ	1:E:2093:SER:HB2	2.26	0.51
1:E:2128:VAL:HG21	3:E:2608:PEE:H79	1.92	0.51
1:E:2244:GLN:HG2	1:E:2245:GLN:N	2.25	0.51
1:A:1090:ASN:OD1	1:A:1092:THR:N	2.37	0.51
1:A:2128:VAL:HG21	3:A:2606:PEE:H79	1.92	0.51
1:E:1987:ASP:OD2	1:E:2082:TRP:NE1	2.43	0.51
1:E:2035:ARG:CD	3:E:2608:PEE:O5	2.57	0.51
1:A:1987:ASP:OD2	1:A:2082:TRP:NE1	2.43	0.51
1:A:2179:LYS:HD3	1:C:1402:ASP:CB	2.38	0.51
1:C:2128:VAL:HG21	3:C:2607:PEE:H79	1.92	0.51
1:C:2244:GLN:HG2	1:C:2245:GLN:N	2.25	0.51
1:C:2374:LYS:HD2	1:C:2399:LEU:HD11	1.93	0.51
1:A:1969:LYS:HB3	1:A:1971:ARG:HH11	1.76	0.51
1:C:1774:LEU:HD22	2:C:2605:PLX:H231	1.93	0.51
1:E:1774:LEU:HD22	2:E:2606:PLX:H231	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2105:ILE:HG13	1:E:2106:LEU:HD12	1.92	0.51
1:C:2404:GLN:CD	1:C:2406:ARG:HH12	2.19	0.51
3:E:2608:PEE:C45	3:E:2608:PEE:C41	2.85	0.51
1:A:1332:ASN:O	1:A:1336:GLN:HG2	2.11	0.51
1:A:1752:PHE:HB3	1:A:1754:TRP:CE3	2.45	0.51
1:E:1265:MET:HE1	1:E:1275:VAL:HG11	1.92	0.51
1:C:1661:GLU:HA	1:C:1664:ARG:NH2	2.26	0.51
3:C:2607:PEE:C45	3:C:2607:PEE:C24	2.85	0.51
2:C:2609:PLX:C14	2:C:2609:PLX:C34	2.89	0.51
1:E:1519:TRP:CE2	1:E:1523:PHE:HE2	2.29	0.51
2:E:2601:PLX:C14	2:E:2601:PLX:C34	2.89	0.51
1:A:1202:ASP:N	1:A:1202:ASP:OD1	2.38	0.50
1:A:2046:LYS:NZ	1:A:2093:SER:HB2	2.26	0.50
2:A:2608:PLX:C14	2:A:2608:PLX:C34	2.89	0.50
1:C:1519:TRP:CE2	1:C:1523:PHE:HE2	2.29	0.50
1:A:1005:ARG:HH12	1:A:1047:GLN:HE22	1.58	0.50
1:C:854:THR:HA	1:C:857:THR:HG22	1.93	0.50
1:C:2046:LYS:NZ	1:C:2093:SER:HB2	2.26	0.50
1:E:854:THR:HA	1:E:857:THR:HG22	1.93	0.50
1:E:1981:PHE:CE2	3:E:2608:PEE:H17	2.46	0.50
1:E:2404:GLN:CD	1:E:2406:ARG:HH12	2.19	0.50
1:C:1002:ILE:HG23	1:C:1225:ASN:ND2	2.20	0.50
2:C:2609:PLX:H162	2:C:2609:PLX:C34	2.41	0.50
1:A:1519:TRP:CE2	1:A:1523:PHE:HE2	2.30	0.50
2:A:2605:PLX:H182	2:A:2605:PLX:H281	1.94	0.50
1:E:1332:ASN:O	1:E:1336:GLN:HG2	2.11	0.50
1:E:1969:LYS:HB3	1:E:1971:ARG:HH11	1.76	0.50
1:E:2374:LYS:HD2	1:E:2399:LEU:HD11	1.93	0.50
2:E:2601:PLX:H162	2:E:2601:PLX:H341	1.91	0.50
1:A:1196:THR:O	1:A:1200:GLN:HG2	2.12	0.50
1:A:2404:GLN:CD	1:A:2406:ARG:HH12	2.19	0.50
1:A:2533:TYR:HB3	1:E:2492:ILE:HG21	1.94	0.50
1:E:2125:PHE:HD1	3:E:2608:PEE:H19	1.76	0.50
1:A:1774:LEU:HD22	2:A:2604:PLX:H231	1.93	0.50
1:C:907:ASP:OD2	1:C:908:PRO:HD3	2.11	0.50
1:C:1981:PHE:CE2	3:C:2607:PEE:H17	2.46	0.50
1:E:2314:ASP:OD1	1:E:2314:ASP:N	2.44	0.50
2:E:2601:PLX:H162	2:E:2601:PLX:C34	2.41	0.50
1:A:2374:LYS:HD2	1:A:2399:LEU:HD11	1.93	0.50
1:C:1196:THR:O	1:C:1200:GLN:HG2	2.12	0.50
1:C:1969:LYS:HB3	1:C:1971:ARG:HH11	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1332:ASN:O	1:C:1336:GLN:HG2	2.11	0.50
1:C:2492:ILE:HG21	1:E:2533:TYR:HB3	1.94	0.50
2:C:2609:PLX:H162	2:C:2609:PLX:H341	1.91	0.50
1:E:1161:LEU:HD13	2:E:2604:PLX:H392	1.94	0.50
1:A:2394:GLU:OE1	1:A:2398:TYR:OH	2.20	0.50
1:C:1981:PHE:HE1	3:C:2607:PEE:H53	1.77	0.50
2:E:2607:PLX:H281	2:E:2607:PLX:H182	1.94	0.50
1:A:1981:PHE:HE1	3:A:2606:PEE:H53	1.77	0.49
1:A:1981:PHE:CE2	3:A:2606:PEE:H17	2.46	0.49
3:A:2606:PEE:C45	3:A:2606:PEE:C24	2.85	0.49
2:A:2608:PLX:H162	2:A:2608:PLX:C34	2.41	0.49
1:C:1265:MET:HE1	1:C:1275:VAL:HG11	1.92	0.49
1:E:1092:THR:O	1:E:1095:ILE:HG22	2.12	0.49
1:E:1661:GLU:HA	1:E:1664:ARG:NH2	2.26	0.49
1:A:2073:PHE:C	1:A:2073:PHE:CD2	2.90	0.49
1:A:2198:PHE:CZ	1:A:2202:ILE:HD11	2.48	0.49
1:E:1143:PHE:CZ	1:E:1301:TYR:HD2	2.30	0.49
2:E:2604:PLX:H232	2:E:2604:PLX:H192	1.95	0.49
2:C:2606:PLX:H182	2:C:2606:PLX:H281	1.94	0.49
1:E:1196:THR:O	1:E:1200:GLN:HG2	2.12	0.49
1:E:2073:PHE:C	1:E:2073:PHE:CD2	2.90	0.49
1:A:1260:ASP:OD1	1:A:1263:GLU:HG2	2.13	0.49
1:A:2071:ARG:NH1	1:A:2073:PHE:HE2	2.11	0.49
1:C:2041:LYS:HA	1:C:2101:TYR:CE2	2.48	0.49
1:C:2073:PHE:C	1:C:2073:PHE:CD2	2.90	0.49
1:E:1981:PHE:HE1	3:E:2608:PEE:H53	1.77	0.49
1:A:907:ASP:OD2	1:A:908:PRO:HD3	2.11	0.49
1:A:2314:ASP:N	1:A:2314:ASP:OD1	2.44	0.49
1:A:2461:LEU:HD23	1:A:2462:ALA:N	2.28	0.49
1:C:1092:THR:O	1:C:1095:ILE:HG22	2.12	0.49
1:E:1218:VAL:O	1:E:1221:ILE:HG22	2.13	0.49
1:A:1214:ILE:HG12	1:A:1290:LEU:HD23	1.95	0.49
1:A:1661:GLU:HA	1:A:1664:ARG:NH2	2.26	0.49
1:A:2125:PHE:HD1	3:A:2606:PEE:H19	1.76	0.49
1:C:1115:ARG:NH2	1:C:1118:GLU:HG3	2.28	0.49
1:C:2071:ARG:NH1	1:C:2073:PHE:HE2	2.11	0.49
2:C:2603:PLX:H232	2:C:2603:PLX:H192	1.95	0.49
3:C:2607:PEE:C45	3:C:2607:PEE:C41	2.85	0.49
1:E:815:LEU:HD11	1:E:1095:ILE:HD11	1.95	0.49
1:E:907:ASP:OD2	1:E:908:PRO:HD3	2.11	0.49
1:E:1115:ARG:NH2	1:E:1118:GLU:HG3	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1161:LEU:HD13	2:A:2602:PLX:H392	1.94	0.49
1:C:1218:VAL:O	1:C:1221:ILE:HG22	2.13	0.49
1:E:1214:ILE:HG12	1:E:1290:LEU:HD23	1.95	0.49
1:E:2325:ARG:NH2	1:E:2333:VAL:HG13	2.27	0.49
1:A:815:LEU:HD11	1:A:1095:ILE:HD11	1.95	0.49
1:C:1005:ARG:HH12	1:C:1047:GLN:HE22	1.58	0.49
1:C:2198:PHE:CZ	1:C:2202:ILE:HD11	2.48	0.49
1:A:1117:GLU:CD	1:A:1118:GLU:HG2	2.38	0.49
1:C:1116:THR:HA	1:C:1119:TRP:CD1	2.48	0.49
1:C:1143:PHE:CZ	1:C:1301:TYR:HD2	2.30	0.49
1:C:1510:GLN:NE2	1:C:1671:ARG:HH22	2.10	0.49
1:A:1092:THR:O	1:A:1095:ILE:HG22	2.12	0.49
1:A:1143:PHE:CZ	1:A:1301:TYR:HD2	2.30	0.49
1:A:2041:LYS:HA	1:A:2101:TYR:CE2	2.48	0.49
1:A:2463:GLY:O	1:A:2464:TYR:CD1	2.65	0.49
1:C:1260:ASP:OD1	1:C:1263:GLU:HG2	2.13	0.49
1:E:1005:ARG:HH12	1:E:1047:GLN:HE22	1.58	0.49
1:A:854:THR:HA	1:A:857:THR:HG22	1.94	0.48
1:C:2179:LYS:HD3	1:E:1402:ASP:CB	2.40	0.48
1:C:2463:GLY:O	1:C:2464:TYR:CD1	2.66	0.48
1:E:1117:GLU:CD	1:E:1118:GLU:HG2	2.38	0.48
1:E:2071:ARG:NH1	1:E:2073:PHE:HE2	2.10	0.48
1:A:1010:VAL:CG2	1:A:1225:ASN:HD21	2.26	0.48
1:A:2460:PHE:HE2	1:A:2466:ILE:HD13	1.78	0.48
1:C:1161:LEU:HD13	2:C:2603:PLX:H392	1.94	0.48
1:C:1214:ILE:HG12	1:C:1290:LEU:HD23	1.95	0.48
1:C:1670:GLY:HA3	1:C:1674:ARG:HE	1.78	0.48
1:E:1090:ASN:OD1	1:E:1092:THR:N	2.37	0.48
1:A:1116:THR:HA	1:A:1119:TRP:CD1	2.48	0.48
1:A:2325:ARG:NH2	1:A:2333:VAL:HG13	2.27	0.48
2:A:2605:PLX:H181	2:A:2605:PLX:H142	1.95	0.48
1:C:815:LEU:HD11	1:C:1095:ILE:HD11	1.95	0.48
1:C:1010:VAL:CG2	1:C:1225:ASN:HD21	2.26	0.48
1:C:1970:TYR:O	1:C:1970:TYR:CD2	2.64	0.48
1:C:2461:LEU:HD23	1:C:2462:ALA:N	2.28	0.48
1:E:1969:LYS:HD3	1:E:1970:TYR:H	1.77	0.48
1:E:2460:PHE:HE2	1:E:2466:ILE:HD13	1.78	0.48
1:E:2461:LEU:HD23	1:E:2462:ALA:N	2.28	0.48
1:A:2492:ILE:HG21	1:C:2533:TYR:HB3	1.95	0.48
2:A:2608:PLX:H192	2:A:2608:PLX:C36	2.37	0.48
1:C:1200:GLN:HE22	1:C:1309:LEU:HB3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1260:ASP:OD1	1:E:1263:GLU:HG2	2.13	0.48
1:E:2041:LYS:HA	1:E:2101:TYR:CE2	2.48	0.48
1:A:1218:VAL:O	1:A:1221:ILE:HG22	2.13	0.48
1:A:1969:LYS:HD3	1:A:1970:TYR:H	1.77	0.48
1:C:1699:HIS:ND1	1:C:1707:SER:O	2.47	0.48
1:A:1200:GLN:HE22	1:A:1309:LEU:HB3	1.78	0.48
1:A:1515:GLY:O	1:A:1518:ARG:HG2	2.14	0.48
1:A:2033:ILE:HG13	2:E:2601:PLX:C15	2.44	0.48
1:C:908:PRO:HD2	1:C:914:VAL:HG12	1.96	0.48
1:C:1179:ILE:O	1:C:1179:ILE:HG23	2.14	0.48
1:C:2285:GLN:HB3	1:C:2443:LEU:HD11	1.96	0.48
1:E:2166:LYS:NZ	1:E:2501:ASP:OD1	2.41	0.48
1:E:2198:PHE:CZ	1:E:2202:ILE:HD11	2.48	0.48
2:A:2605:PLX:H292	2:A:2605:PLX:H261	1.68	0.48
1:E:1116:THR:HA	1:E:1119:TRP:CD1	2.48	0.48
1:E:1670:GLY:HA3	1:E:1674:ARG:HE	1.78	0.48
1:E:2130:PHE:O	1:E:2134:LEU:HD23	2.14	0.48
1:A:1402:ASP:CB	1:E:2179:LYS:HD3	2.39	0.48
1:A:1670:GLY:HA3	1:A:1674:ARG:HE	1.78	0.48
1:C:1969:LYS:HD3	1:C:1970:TYR:H	1.77	0.48
1:A:1115:ARG:NH2	1:A:1118:GLU:HG3	2.28	0.48
1:C:2071:ARG:HH11	1:C:2073:PHE:HE2	1.62	0.48
2:C:2606:PLX:H142	2:C:2606:PLX:H181	1.95	0.48
1:E:1515:GLY:O	1:E:1518:ARG:HG2	2.14	0.48
1:E:2376:ILE:HB	1:E:2448:ILE:HG22	1.96	0.48
2:E:2607:PLX:H181	2:E:2607:PLX:H142	1.95	0.48
1:A:908:PRO:HD2	1:A:914:VAL:HG12	1.96	0.48
1:A:1179:ILE:HG23	1:A:1179:ILE:O	2.14	0.48
1:A:2197:LEU:CG	2:A:2608:PLX:C39	2.92	0.48
2:A:2602:PLX:H192	2:A:2602:PLX:H232	1.95	0.48
1:C:1117:GLU:CD	1:C:1118:GLU:HG2	2.38	0.48
1:C:2460:PHE:HE2	1:C:2466:ILE:HD13	1.78	0.48
1:A:1510:GLN:NE2	1:A:1671:ARG:HH22	2.10	0.47
1:A:2285:GLN:HB3	1:A:2443:LEU:HD11	1.96	0.47
1:C:2130:PHE:O	1:C:2134:LEU:HD23	2.14	0.47
1:C:2182:LYS:CD	1:E:2144:ASP:HB2	2.44	0.47
1:C:2376:ILE:HB	1:C:2448:ILE:HG22	1.96	0.47
2:E:2601:PLX:H192	2:E:2601:PLX:C36	2.36	0.47
1:A:1143:PHE:CZ	1:A:1301:TYR:CD2	3.03	0.47
1:A:2130:PHE:O	1:A:2134:LEU:HD23	2.14	0.47
1:C:1331:ILE:O	1:C:1335:ARG:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2422:LYS:HA	1:C:2422:LYS:HE2	1.96	0.47
1:E:1200:GLN:HE22	1:E:1309:LEU:HB3	1.78	0.47
1:E:1699:HIS:ND1	1:E:1707:SER:O	2.47	0.47
1:E:1795:PHE:HA	2:E:2604:PLX:H251	1.96	0.47
1:E:2422:LYS:HA	1:E:2422:LYS:HE2	1.96	0.47
1:A:1040:LEU:HD21	1:A:1100:LEU:HG	1.96	0.47
1:A:1699:HIS:ND1	1:A:1707:SER:O	2.47	0.47
2:A:2608:PLX:H361	2:A:2608:PLX:C16	2.36	0.47
1:C:2314:ASP:OD1	1:C:2314:ASP:N	2.44	0.47
1:E:1179:ILE:HG23	1:E:1179:ILE:O	2.14	0.47
1:E:1331:ILE:O	1:E:1335:ARG:HG2	2.14	0.47
1:A:2035:ARG:CD	3:A:2606:PEE:O5	2.57	0.47
1:C:2325:ARG:NH2	1:C:2333:VAL:HG13	2.27	0.47
2:C:2609:PLX:C15	1:E:2033:ILE:HG13	2.44	0.47
1:E:1200:GLN:NE2	1:E:1309:LEU:HB3	2.30	0.47
1:A:1177:ILE:O	1:A:1177:ILE:HG22	2.15	0.47
1:A:1200:GLN:NE2	1:A:1309:LEU:HB3	2.30	0.47
1:E:897:ASN:CG	1:E:898:GLN:H	2.21	0.47
1:E:1311:ALA:O	1:E:1315:GLN:HG3	2.14	0.47
1:E:2197:LEU:CG	2:E:2601:PLX:C39	2.91	0.47
1:E:2463:GLY:O	1:E:2464:TYR:CD1	2.66	0.47
1:A:2144:ASP:HB2	1:E:2182:LYS:CD	2.44	0.47
1:C:1559:LEU:HD23	1:C:1559:LEU:H	1.79	0.47
1:E:1559:LEU:H	1:E:1559:LEU:HD23	1.80	0.47
1:A:1331:ILE:O	1:A:1335:ARG:HG2	2.14	0.47
1:A:1714:VAL:O	1:A:1719:MET:HG3	2.15	0.47
1:A:1795:PHE:HA	2:A:2602:PLX:H251	1.96	0.47
1:A:2422:LYS:HE2	1:A:2422:LYS:HA	1.96	0.47
1:C:1164:LEU:HD22	2:C:2603:PLX:H341	1.97	0.47
1:C:1200:GLN:NE2	1:C:1309:LEU:HB3	2.30	0.47
1:C:1221:ILE:CD1	1:C:1280:ILE:HD12	2.45	0.47
1:C:1345:LEU:HB2	1:C:2104:ARG:NH1	2.25	0.47
1:C:1515:GLY:O	1:C:1518:ARG:HG2	2.14	0.47
1:C:2489:SER:O	1:C:2492:ILE:HB	2.15	0.47
2:C:2609:PLX:H192	2:C:2609:PLX:C36	2.36	0.47
1:E:908:PRO:HD2	1:E:914:VAL:HG12	1.95	0.47
1:E:1010:VAL:CG2	1:E:1225:ASN:HD21	2.26	0.47
1:E:1040:LEU:HD21	1:E:1100:LEU:HG	1.96	0.47
1:E:1221:ILE:CD1	1:E:1280:ILE:HD12	2.45	0.47
1:E:1714:VAL:O	1:E:1719:MET:HG3	2.15	0.47
1:E:2285:GLN:HB3	1:E:2443:LEU:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2337:ASN:OD1	1:E:2337:ASN:N	2.47	0.47
1:A:1699:HIS:CE1	1:A:1708:LEU:HA	2.50	0.47
1:A:2376:ILE:HB	1:A:2448:ILE:HG22	1.96	0.47
1:E:1315:GLN:HE22	1:E:1538:ARG:CA	2.28	0.47
1:A:2182:LYS:CD	1:C:2144:ASP:HB2	2.45	0.47
1:C:946:HIS:O	1:C:950:GLN:N	2.47	0.47
1:E:2232:LEU:HD12	1:E:2317:LEU:HD12	1.97	0.47
1:A:1311:ALA:O	1:A:1315:GLN:HG3	2.14	0.47
1:A:2128:VAL:CG2	3:A:2606:PEE:H79	2.45	0.47
1:C:1010:VAL:HG23	1:C:1225:ASN:HD21	1.80	0.47
1:C:1170:PHE:HB2	1:C:1188:CYS:SG	2.55	0.47
1:C:1752:PHE:CD1	1:C:1754:TRP:HZ3	2.33	0.47
1:C:2138:MET:HE1	3:C:2607:PEE:C34	2.45	0.47
1:E:1143:PHE:CZ	1:E:1301:TYR:CD2	3.03	0.47
1:E:1177:ILE:HG22	1:E:1177:ILE:O	2.15	0.47
3:E:2608:PEE:H40	3:E:2608:PEE:H77	1.95	0.47
1:C:1090:ASN:OD1	1:C:1092:THR:N	2.37	0.46
1:C:1143:PHE:CZ	1:C:1301:TYR:CD2	3.03	0.46
1:C:1520:LEU:HD21	1:C:1679:GLY:HA2	1.97	0.46
1:C:2073:PHE:C	1:C:2073:PHE:HD2	2.23	0.46
1:E:1752:PHE:CD1	1:E:1754:TRP:HZ3	2.33	0.46
1:E:2073:PHE:C	1:E:2073:PHE:HD2	2.24	0.46
1:E:2360:GLY:HA2	1:E:2407:ARG:NH1	2.30	0.46
1:A:1010:VAL:HG23	1:A:1225:ASN:HD21	1.80	0.46
1:A:1559:LEU:HD23	1:A:1559:LEU:H	1.79	0.46
2:A:2608:PLX:C15	1:C:2033:ILE:HG13	2.44	0.46
1:C:897:ASN:CG	1:C:898:GLN:H	2.21	0.46
1:C:1200:GLN:O	1:C:1310:LYS:NZ	2.37	0.46
1:C:1311:ALA:O	1:C:1315:GLN:HG3	2.14	0.46
1:C:1795:PHE:HA	2:C:2603:PLX:H251	1.96	0.46
1:C:2360:GLY:HA2	1:C:2407:ARG:NH1	2.31	0.46
1:E:1170:PHE:HB2	1:E:1188:CYS:SG	2.56	0.46
1:E:2128:VAL:CG2	3:E:2608:PEE:H79	2.45	0.46
1:A:2166:LYS:NZ	1:A:2501:ASP:OD1	2.41	0.46
1:C:2128:VAL:CG2	3:C:2607:PEE:H79	2.45	0.46
3:C:2607:PEE:O2P	3:C:2607:PEE:H1	2.16	0.46
1:E:1164:LEU:HD22	2:E:2604:PLX:H341	1.97	0.46
1:A:1520:LEU:HD21	1:A:1679:GLY:HA2	1.97	0.46
1:A:2073:PHE:C	1:A:2073:PHE:HD2	2.23	0.46
1:A:2138:MET:HE1	3:A:2606:PEE:C34	2.45	0.46
1:C:1714:VAL:O	1:C:1719:MET:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1520:LEU:HD21	1:E:1679:GLY:HA2	1.97	0.46
1:E:2071:ARG:HH11	1:E:2073:PHE:HE2	1.62	0.46
1:C:1699:HIS:CE1	1:C:1708:LEU:HA	2.50	0.46
1:C:2197:LEU:CG	2:C:2609:PLX:H393	2.33	0.46
1:E:1699:HIS:CE1	1:E:1708:LEU:HA	2.50	0.46
1:E:2489:SER:O	1:E:2492:ILE:HB	2.15	0.46
1:A:1021:LEU:HA	1:A:1021:LEU:HD23	1.77	0.46
1:C:1177:ILE:HG22	1:C:1177:ILE:O	2.15	0.46
1:C:2065:LEU:HB3	1:C:2066:PRO:HD3	1.98	0.46
1:C:2197:LEU:CG	2:C:2609:PLX:C39	2.91	0.46
1:C:2337:ASN:OD1	1:C:2337:ASN:N	2.47	0.46
1:A:1315:GLN:HE22	1:A:1538:ARG:CA	2.28	0.46
1:A:1752:PHE:CD1	1:A:1754:TRP:HZ3	2.33	0.46
1:C:1315:GLN:HE22	1:C:1538:ARG:CA	2.28	0.46
1:C:1800:LEU:HD22	1:C:1806:TRP:HE3	1.81	0.46
1:A:2360:GLY:HA2	1:A:2407:ARG:NH1	2.31	0.46
1:C:1040:LEU:HD21	1:C:1100:LEU:HG	1.96	0.46
1:C:2125:PHE:HD1	3:C:2607:PEE:H19	1.76	0.46
2:C:2609:PLX:H361	2:C:2609:PLX:C16	2.36	0.46
1:A:897:ASN:CG	1:A:898:GLN:H	2.21	0.46
1:E:2138:MET:HE1	3:E:2608:PEE:C34	2.45	0.46
1:A:2489:SER:O	1:A:2492:ILE:HB	2.15	0.46
1:E:1010:VAL:HG23	1:E:1225:ASN:HD21	1.80	0.46
1:E:1303:LEU:O	1:E:1306:SER:OG	2.28	0.46
1:E:1800:LEU:HD22	1:E:1806:TRP:HE3	1.81	0.46
2:E:2607:PLX:H292	2:E:2607:PLX:H261	1.68	0.46
1:A:1170:PHE:CD2	1:A:1787:LEU:HD13	2.51	0.45
1:A:2244:GLN:N	1:A:2244:GLN:OE1	2.49	0.45
1:A:2513:VAL:CG2	1:A:2518:GLU:HG2	2.46	0.45
3:A:2606:PEE:H1	3:A:2606:PEE:O2P	2.15	0.45
1:E:2197:LEU:CD2	2:E:2601:PLX:H392	2.41	0.45
1:E:2244:GLN:N	1:E:2244:GLN:OE1	2.49	0.45
1:A:1345:LEU:HB2	1:A:2104:ARG:NH1	2.25	0.45
1:A:2232:LEU:HD12	1:A:2317:LEU:HD12	1.97	0.45
1:C:1221:ILE:HD11	1:C:1280:ILE:HD12	1.98	0.45
1:C:2513:VAL:CG2	1:C:2518:GLU:HG2	2.46	0.45
1:E:1995:PHE:CE1	1:E:2021:LEU:HD21	2.52	0.45
1:A:1221:ILE:CD1	1:A:1280:ILE:HD12	2.45	0.45
1:A:1502:MET:O	1:A:1505:LEU:HG	2.17	0.45
1:A:1995:PHE:CE1	1:A:2021:LEU:HD21	2.52	0.45
1:C:2244:GLN:N	1:C:2244:GLN:OE1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2434:LEU:HA	1:C:2434:LEU:HD12	1.64	0.45
1:A:1016:TRP:CD1	1:A:1036:TYR:CD2	3.02	0.45
1:A:1170:PHE:HB2	1:A:1188:CYS:SG	2.55	0.45
1:A:1800:LEU:HD22	1:A:1806:TRP:HE3	1.81	0.45
1:A:2225:ASP:OD2	1:A:2226:VAL:N	2.50	0.45
1:C:1292:LEU:HD11	4:C:2608:P5S:H23	1.98	0.45
1:C:1995:PHE:CE1	1:C:2021:LEU:HD21	2.51	0.45
1:C:2035:ARG:CD	3:C:2607:PEE:O5	2.57	0.45
1:E:1292:LEU:O	1:E:1296:ILE:HG12	2.17	0.45
3:E:2608:PEE:H1	3:E:2608:PEE:O2P	2.16	0.45
1:A:1299:SER:HB2	1:A:1301:TYR:HD1	1.81	0.45
1:A:1660:GLU:OE2	1:A:1660:GLU:N	2.47	0.45
1:A:2337:ASN:OD1	1:A:2337:ASN:N	2.47	0.45
1:C:2225:ASP:OD2	1:C:2226:VAL:N	2.50	0.45
1:C:2232:LEU:HD12	1:C:2317:LEU:HD12	1.97	0.45
1:E:1494:MET:HE1	1:E:1497:ARG:NH1	2.32	0.45
1:E:2434:LEU:HD12	1:E:2434:LEU:HA	1.64	0.45
1:A:1164:LEU:HD22	2:A:2602:PLX:H341	1.97	0.45
1:A:1761:ARG:HD2	1:A:1761:ARG:C	2.41	0.45
3:A:2606:PEE:C24	3:A:2606:PEE:C44	2.95	0.45
1:C:1016:TRP:CD1	1:C:1036:TYR:CD2	3.03	0.45
1:C:1117:GLU:OE2	1:C:1118:GLU:HG2	2.16	0.45
1:C:1292:LEU:O	1:C:1296:ILE:HG12	2.17	0.45
1:C:1660:GLU:OE2	1:C:1660:GLU:N	2.47	0.45
1:C:1761:ARG:C	1:C:1761:ARG:HD2	2.41	0.45
1:C:2407:ARG:NE	1:C:2426:PHE:CE2	2.84	0.45
1:E:1170:PHE:CD2	1:E:1787:LEU:HD13	2.51	0.45
1:E:1299:SER:HB2	1:E:1301:TYR:HD1	1.81	0.45
1:E:1701:VAL:HG12	1:E:1784:LYS:HD3	1.99	0.45
1:E:2086:LYS:HD2	1:E:2086:LYS:HA	1.81	0.45
1:E:2213:ILE:HG13	1:E:2214:ARG:N	2.32	0.45
1:A:1221:ILE:HD11	1:A:1280:ILE:HD12	1.98	0.45
1:A:1292:LEU:HD11	4:A:2607:P5S:H23	1.98	0.45
1:C:1299:SER:HB2	1:C:1301:TYR:HD1	1.81	0.45
1:C:2405:LEU:HD12	1:C:2430:TRP:CZ2	2.52	0.45
1:A:1117:GLU:OE2	1:A:1118:GLU:HG2	2.16	0.45
1:C:1192:LEU:HD11	1:C:1791:MET:HE1	1.99	0.45
1:C:1701:VAL:HG12	1:C:1784:LYS:HD3	1.98	0.45
1:E:1143:PHE:HD2	1:E:1154:LYS:HB3	1.81	0.45
1:E:1150:LEU:HG	1:E:1154:LYS:HD2	1.99	0.45
1:E:1970:TYR:O	1:E:1970:TYR:CD2	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1150:LEU:HG	1:A:1154:LYS:HD2	1.99	0.45
1:A:2387:VAL:HG12	1:A:2390:LEU:H	1.82	0.45
1:C:1150:LEU:HG	1:C:1154:LYS:HD2	1.99	0.45
1:C:1170:PHE:CD2	1:C:1787:LEU:HD13	2.51	0.45
3:C:2607:PEE:C24	3:C:2607:PEE:C44	2.95	0.45
1:E:1510:GLN:NE2	1:E:1671:ARG:HH22	2.10	0.45
1:A:1292:LEU:O	1:A:1296:ILE:HG12	2.17	0.45
1:A:1361:GLN:OE1	1:A:1361:GLN:HA	2.17	0.45
1:A:1769:PHE:CD1	1:A:1770:PRO:HD2	2.52	0.45
1:C:1494:MET:HE1	1:C:1497:ARG:NH1	2.32	0.45
2:C:2601:PLX:H131	2:C:2601:PLX:H161	1.89	0.45
1:E:1221:ILE:HD11	1:E:1280:ILE:HD12	1.98	0.45
1:E:1292:LEU:HD11	4:E:2609:P5S:H23	1.98	0.45
1:E:1660:GLU:HG2	1:E:1664:ARG:NH2	2.32	0.45
1:E:1660:GLU:OE2	1:E:1660:GLU:N	2.47	0.45
1:E:2225:ASP:OD2	1:E:2226:VAL:N	2.50	0.45
1:E:2387:VAL:HG12	1:E:2390:LEU:H	1.82	0.45
1:A:1970:TYR:O	1:A:1970:TYR:CD2	2.63	0.44
1:C:1403:HIS:ND1	1:C:2523:GLU:OE2	2.50	0.44
1:C:1769:PHE:CD1	1:C:1770:PRO:HD2	2.52	0.44
1:C:2387:VAL:HG12	1:C:2390:LEU:H	1.82	0.44
1:C:2513:VAL:HG21	1:C:2521:LEU:HB2	1.99	0.44
1:E:2065:LEU:HB3	1:E:2066:PRO:HD3	1.98	0.44
1:A:1660:GLU:HG2	1:A:1664:ARG:NH2	2.32	0.44
1:C:1235:VAL:HG13	1:C:1239:GLN:OE1	2.18	0.44
1:C:1361:GLN:OE1	1:C:1361:GLN:HA	2.17	0.44
1:C:2309:TYR:CE2	1:C:2355:ALA:HB1	2.53	0.44
1:E:1138:ASN:O	1:E:1141:PRO:HD3	2.18	0.44
1:E:1235:VAL:HG13	1:E:1239:GLN:OE1	2.18	0.44
1:E:1361:GLN:HA	1:E:1361:GLN:OE1	2.17	0.44
1:E:2109:PHE:CZ	1:E:2110:LEU:HD11	2.53	0.44
1:A:1701:VAL:HG12	1:A:1784:LYS:HD3	1.99	0.44
1:A:2065:LEU:HB3	1:A:2066:PRO:HD3	1.98	0.44
1:A:2071:ARG:HH11	1:A:2073:PHE:HE2	1.62	0.44
1:C:971:ASP:OD1	1:C:1154:LYS:NZ	2.50	0.44
1:C:1717:TRP:O	1:C:1721:THR:HG23	2.17	0.44
1:E:1301:TYR:CD1	1:E:1301:TYR:N	2.84	0.44
3:E:2608:PEE:H81	3:E:2608:PEE:C23	2.48	0.44
1:A:2309:TYR:CE2	1:A:2355:ALA:HB1	2.53	0.44
1:A:2407:ARG:NE	1:A:2426:PHE:CE2	2.84	0.44
1:C:1140:ILE:O	1:C:1143:PHE:CE1	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1502:MET:O	1:C:1505:LEU:HG	2.17	0.44
1:C:2162:ILE:HD13	1:C:2162:ILE:HA	1.83	0.44
2:C:2606:PLX:H172	2:C:2606:PLX:H212	2.00	0.44
1:E:1016:TRP:CD1	1:E:1036:TYR:CD2	3.02	0.44
1:E:1140:ILE:O	1:E:1143:PHE:CE1	2.71	0.44
1:E:1192:LEU:HD11	1:E:1791:MET:HE1	1.99	0.44
1:E:1769:PHE:CD1	1:E:1770:PRO:HD2	2.52	0.44
1:A:1176:ARG:NH1	1:A:1282:TRP:HD1	2.16	0.44
1:A:1717:TRP:O	1:A:1721:THR:HG23	2.17	0.44
3:A:2606:PEE:H40	3:A:2606:PEE:H77	1.95	0.44
1:C:1143:PHE:N	1:C:1143:PHE:CD1	2.86	0.44
1:E:1073:ASN:O	1:E:1077:ILE:HG12	2.18	0.44
2:E:2605:PLX:H202	2:E:2606:PLX:H191	2.00	0.44
1:A:822:LEU:HD11	1:A:1094:LEU:HD12	2.00	0.44
1:A:1084:ASP:OD2	1:A:1086:PHE:N	2.50	0.44
1:A:2046:LYS:HZ1	1:A:2093:SER:HB2	1.82	0.44
1:A:2513:VAL:HG21	1:A:2521:LEU:HB2	1.99	0.44
2:A:2603:PLX:H202	2:A:2604:PLX:H191	2.00	0.44
1:C:822:LEU:HD11	1:C:1094:LEU:HD12	2.00	0.44
1:C:2109:PHE:CZ	1:C:2110:LEU:HD11	2.53	0.44
1:E:1117:GLU:OE2	1:E:1118:GLU:HG2	2.16	0.44
1:E:1217:ASN:O	1:E:1220:VAL:HG22	2.18	0.44
1:E:1717:TRP:O	1:E:1721:THR:HG23	2.17	0.44
1:E:2309:TYR:CE2	1:E:2355:ALA:HB1	2.53	0.44
1:E:2405:LEU:HD12	1:E:2430:TRP:CZ2	2.52	0.44
1:E:2425:ASP:HB3	1:E:2426:PHE:CD1	2.52	0.44
1:E:2513:VAL:HG21	1:E:2521:LEU:HB2	1.99	0.44
2:E:2607:PLX:H172	2:E:2607:PLX:H212	2.00	0.44
1:A:1192:LEU:HD11	1:A:1791:MET:HE1	1.99	0.44
1:A:2095:TYR:CE1	2:A:2601:PLX:H31	2.53	0.44
2:A:2605:PLX:H212	2:A:2605:PLX:H172	2.00	0.44
1:C:2095:TYR:CE1	2:C:2602:PLX:H31	2.53	0.44
1:E:1761:ARG:C	1:E:1761:ARG:HD2	2.41	0.44
1:A:1138:ASN:O	1:A:1141:PRO:HD3	2.18	0.44
1:A:1494:MET:HE1	1:A:1497:ARG:NH1	2.32	0.44
1:A:2405:LEU:HD12	1:A:2430:TRP:CZ2	2.52	0.44
1:C:1005:ARG:HB2	1:C:1010:VAL:HG11	2.00	0.44
1:C:2425:ASP:HB3	1:C:2426:PHE:CD1	2.52	0.44
3:C:2607:PEE:C25	3:C:2607:PEE:C44	2.95	0.44
1:E:971:ASP:OD1	1:E:1154:LYS:NZ	2.50	0.44
1:E:1502:MET:O	1:E:1505:LEU:HG	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2130:PHE:HA	1:E:2133:GLU:HG2	1.99	0.44
1:E:2513:VAL:CG2	1:E:2518:GLU:HG2	2.46	0.44
1:A:1005:ARG:HB2	1:A:1010:VAL:HG11	2.00	0.44
1:A:1671:ARG:HG3	1:A:1672:THR:HG23	1.99	0.44
1:A:1710:LEU:HB3	1:A:1711:PRO:HD3	2.00	0.44
1:C:1050:LEU:HD12	1:C:1050:LEU:HA	1.90	0.44
1:C:1660:GLU:HG2	1:C:1664:ARG:NH2	2.32	0.44
1:C:1671:ARG:HG3	1:C:1672:THR:HG23	1.99	0.44
1:C:1740:MET:HE2	1:C:1740:MET:HA	2.00	0.44
1:E:2182:LYS:HB2	1:E:2182:LYS:HE3	1.70	0.44
3:E:2608:PEE:C24	3:E:2608:PEE:C44	2.95	0.44
1:A:1217:ASN:O	1:A:1220:VAL:HG22	2.18	0.43
1:A:1235:VAL:HG13	1:A:1239:GLN:OE1	2.18	0.43
1:C:1702:THR:HA	1:C:2073:PHE:CE1	2.53	0.43
1:C:1767:PRO:HB3	1:C:2071:ARG:HG2	2.00	0.43
1:C:2213:ILE:HG13	1:C:2214:ARG:N	2.32	0.43
1:E:1657:PRO:HA	1:E:1660:GLU:OE1	2.18	0.43
1:A:1657:PRO:HA	1:A:1660:GLU:OE1	2.18	0.43
1:A:1767:PRO:HB3	1:A:2071:ARG:HG2	2.00	0.43
1:A:2130:PHE:HA	1:A:2133:GLU:HG2	1.99	0.43
3:A:2606:PEE:H81	3:A:2606:PEE:C23	2.48	0.43
1:C:1143:PHE:N	1:C:1143:PHE:HD1	2.16	0.43
1:C:1671:ARG:HA	1:C:1671:ARG:NH2	2.34	0.43
1:C:2376:ILE:O	1:C:2448:ILE:HA	2.18	0.43
1:E:1005:ARG:HB2	1:E:1010:VAL:HG11	2.00	0.43
1:E:1176:ARG:NH1	1:E:1282:TRP:HD1	2.16	0.43
1:E:2178:PRO:HD2	1:E:2181:GLN:NE2	2.33	0.43
1:E:2482:ARG:HG3	1:E:2486:SER:HB2	2.00	0.43
1:A:901:LEU:HG	1:A:1085:PHE:CD1	2.53	0.43
1:A:1710:LEU:HD12	1:A:1710:LEU:HA	1.81	0.43
1:A:2109:PHE:CZ	1:A:2110:LEU:HD11	2.53	0.43
1:A:2213:ILE:HG13	1:A:2214:ARG:N	2.32	0.43
1:C:2076:ASN:HB3	1:C:2079:ALA:HB3	2.01	0.43
1:E:901:LEU:HG	1:E:1085:PHE:CD1	2.53	0.43
1:E:2394:GLU:OE1	1:E:2398:TYR:OH	2.20	0.43
1:A:1221:ILE:HD12	1:A:1221:ILE:HA	1.84	0.43
1:A:2482:ARG:HG3	1:A:2486:SER:HB2	2.00	0.43
1:C:1953:SER:O	1:C:1957:PRO:HG2	2.18	0.43
2:C:2604:PLX:H202	2:C:2605:PLX:H191	2.00	0.43
1:E:1709:VAL:HG21	2:E:2606:PLX:H162	2.01	0.43
1:E:2225:ASP:OD2	1:E:2225:ASP:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2256:TYR:OH	1:E:2273:ILE:O	2.31	0.43
1:A:1140:ILE:O	1:A:1143:PHE:CE1	2.71	0.43
1:A:1140:ILE:O	1:A:1143:PHE:HE1	2.00	0.43
1:A:1143:PHE:N	1:A:1143:PHE:HD1	2.16	0.43
1:A:1198:LEU:O	1:A:1206:GLN:NE2	2.52	0.43
1:A:1221:ILE:CD1	1:A:1280:ILE:HG23	2.47	0.43
1:A:2076:ASN:HB3	1:A:2079:ALA:HB3	2.00	0.43
1:A:2177:GLN:HG3	1:A:2181:GLN:NE2	2.34	0.43
2:A:2608:PLX:C16	2:A:2608:PLX:C34	2.94	0.43
1:C:1176:ARG:NH1	1:C:1282:TRP:HD1	2.16	0.43
1:C:2230:LEU:HD11	1:C:2317:LEU:HD21	2.00	0.43
3:C:2607:PEE:H81	3:C:2607:PEE:C23	2.48	0.43
1:E:1198:LEU:O	1:E:1206:GLN:NE2	2.52	0.43
1:E:2177:GLN:HG3	1:E:2181:GLN:NE2	2.34	0.43
1:A:908:PRO:HD2	1:A:914:VAL:CG1	2.49	0.43
1:A:1303:LEU:O	1:A:1306:SER:OG	2.28	0.43
1:A:1702:THR:HA	1:A:2073:PHE:CE1	2.53	0.43
1:A:1953:SER:O	1:A:1957:PRO:HG2	2.18	0.43
1:A:2376:ILE:O	1:A:2448:ILE:HA	2.19	0.43
1:A:2425:ASP:HB3	1:A:2426:PHE:CD1	2.52	0.43
3:A:2606:PEE:H43	3:A:2606:PEE:H38	1.83	0.43
1:C:1073:ASN:O	1:C:1077:ILE:HG12	2.18	0.43
1:C:1190:TYR:HD2	1:C:1191:LEU:HD22	1.83	0.43
1:C:1315:GLN:HE22	1:C:1538:ARG:HA	1.83	0.43
1:C:2016:VAL:HG12	1:C:2017:PRO:HD3	2.01	0.43
1:C:2178:PRO:HD2	1:C:2181:GLN:NE2	2.33	0.43
1:E:821:ALA:O	1:E:1048:TYR:OH	2.35	0.43
1:E:1315:GLN:HE22	1:E:1538:ARG:HA	1.83	0.43
1:E:1710:LEU:HB3	1:E:1711:PRO:HD3	2.01	0.43
1:E:1767:PRO:HB3	1:E:2071:ARG:HG2	2.00	0.43
3:E:2608:PEE:H38	3:E:2608:PEE:H43	1.83	0.43
1:A:971:ASP:OD1	1:A:1154:LYS:NZ	2.50	0.43
1:A:1194:PHE:CE1	2:A:2603:PLX:H1B3	2.54	0.43
1:A:1315:GLN:HE22	1:A:1538:ARG:HA	1.83	0.43
1:A:1403:HIS:ND1	1:A:2523:GLU:OE2	2.50	0.43
1:A:2121:LEU:HD23	1:A:2121:LEU:HA	1.82	0.43
1:A:2179:LYS:HA	1:A:2179:LYS:HE2	2.01	0.43
1:C:1710:LEU:HB3	1:C:1711:PRO:HD3	2.00	0.43
1:C:2130:PHE:HA	1:C:2133:GLU:HG2	1.99	0.43
1:C:2520:GLU:O	1:C:2524:GLU:HG3	2.19	0.43
1:E:822:LEU:HD11	1:E:1094:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:894:LEU:H	1:E:894:LEU:HD23	1.84	0.43
1:E:1143:PHE:HD1	1:E:1143:PHE:N	2.16	0.43
1:E:1953:SER:O	1:E:1957:PRO:HG2	2.18	0.43
1:E:2076:ASN:HB3	1:E:2079:ALA:HB3	2.01	0.43
1:A:1073:ASN:O	1:A:1077:ILE:HG12	2.18	0.43
1:A:1517:THR:HG22	1:A:1675:LEU:HD13	2.01	0.43
1:A:1740:MET:HE2	1:A:1740:MET:HA	2.00	0.43
1:C:1138:ASN:O	1:C:1141:PRO:HD3	2.18	0.43
1:C:1145:HIS:HB2	1:C:1147:ARG:HH12	1.84	0.43
1:C:1346:LYS:O	1:C:1346:LYS:HD3	2.19	0.43
1:C:1499:LEU:HA	1:C:1502:MET:HG3	2.01	0.43
1:C:1657:PRO:HA	1:C:1660:GLU:OE1	2.18	0.43
1:C:1772:ARG:HA	1:C:1777:GLU:HG2	2.00	0.43
2:C:2609:PLX:H261	2:C:2609:PLX:H292	1.78	0.43
1:E:1249:PHE:HB2	1:E:1251:LEU:CD2	2.49	0.43
1:E:1517:THR:HG22	1:E:1675:LEU:HD13	2.01	0.43
1:E:2095:TYR:CE1	2:E:2603:PLX:H31	2.53	0.43
1:A:1499:LEU:HA	1:A:1502:MET:HG3	2.01	0.43
1:A:2178:PRO:HD2	1:A:2181:GLN:NE2	2.33	0.43
3:A:2606:PEE:C25	3:A:2606:PEE:C44	2.95	0.43
1:C:901:LEU:HG	1:C:1085:PHE:CD1	2.53	0.43
1:C:908:PRO:HD2	1:C:914:VAL:CG1	2.49	0.43
1:C:1221:ILE:CD1	1:C:1280:ILE:HG23	2.47	0.43
1:C:2225:ASP:OD2	1:C:2225:ASP:C	2.62	0.43
1:E:996:LEU:HA	1:E:999:VAL:HG12	2.01	0.43
1:E:1140:ILE:O	1:E:1143:PHE:HE1	2.00	0.43
1:E:1143:PHE:N	1:E:1143:PHE:CD1	2.86	0.43
1:E:1702:THR:HA	1:E:2073:PHE:CE1	2.53	0.43
1:E:2162:ILE:HD13	1:E:2162:ILE:HA	1.83	0.43
1:E:2520:GLU:O	1:E:2524:GLU:HG3	2.19	0.43
1:A:1204:ARG:O	1:A:1207:LEU:HG	2.19	0.43
1:A:1671:ARG:NH2	1:A:1671:ARG:HA	2.34	0.43
1:A:2144:ASP:HB2	1:E:2182:LYS:HD2	2.01	0.43
1:A:2225:ASP:OD2	1:A:2225:ASP:C	2.62	0.43
1:C:1134:ARG:HG3	1:C:1137:PRO:HG3	2.00	0.43
1:C:1194:PHE:CE1	2:C:2604:PLX:H1B3	2.54	0.43
1:C:1262:LYS:HA	1:C:1265:MET:CE	2.49	0.43
1:C:1706:ALA:HB1	1:C:1740:MET:SD	2.59	0.43
1:C:1709:VAL:HG21	2:C:2605:PLX:H162	2.01	0.43
1:E:1134:ARG:HG3	1:E:1137:PRO:HG3	2.00	0.43
1:E:1706:ALA:HB1	1:E:1740:MET:SD	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2407:ARG:NE	1:E:2426:PHE:CE2	2.84	0.43
1:A:894:LEU:HD23	1:A:894:LEU:H	1.84	0.42
3:A:2606:PEE:C24	3:A:2606:PEE:H77	2.48	0.42
1:C:996:LEU:HA	1:C:999:VAL:HG12	2.01	0.42
1:C:1217:ASN:O	1:C:1220:VAL:HG22	2.18	0.42
2:C:2604:PLX:H1C3	2:C:2604:PLX:H21	1.79	0.42
1:E:1699:HIS:HE1	1:E:1708:LEU:HB2	1.84	0.42
1:E:2230:LEU:HD11	1:E:2317:LEU:HD21	2.01	0.42
3:E:2608:PEE:C24	3:E:2608:PEE:H77	2.48	0.42
1:A:1143:PHE:N	1:A:1143:PHE:CD1	2.86	0.42
1:C:808:HIS:O	1:C:809:VAL:C	2.62	0.42
1:C:1140:ILE:O	1:C:1143:PHE:HE1	2.00	0.42
1:C:1204:ARG:O	1:C:1207:LEU:HG	2.19	0.42
1:E:908:PRO:HD2	1:E:914:VAL:CG1	2.49	0.42
1:E:1190:TYR:HD2	1:E:1191:LEU:HD22	1.83	0.42
1:E:1222:ILE:HD13	1:E:1222:ILE:HA	1.85	0.42
1:E:1671:ARG:HA	1:E:1671:ARG:NH2	2.34	0.42
1:E:2016:VAL:HG12	1:E:2017:PRO:HD3	2.01	0.42
1:E:2376:ILE:O	1:E:2448:ILE:HA	2.18	0.42
1:E:2516:THR:C	1:E:2518:GLU:OE1	2.62	0.42
1:A:1772:ARG:HA	1:A:1777:GLU:HG2	2.01	0.42
1:A:2016:VAL:HG12	1:A:2017:PRO:HD3	2.01	0.42
1:C:1249:PHE:HB2	1:C:1251:LEU:CD2	2.49	0.42
1:E:848:MET:H	1:E:848:MET:HG2	1.54	0.42
1:E:1086:PHE:CD1	1:E:1087:ARG:HG3	2.54	0.42
1:E:1194:PHE:CE1	2:E:2605:PLX:H1B3	2.54	0.42
1:E:1346:LYS:O	1:E:1346:LYS:HD3	2.19	0.42
1:E:2092:LEU:HD11	2:E:2603:PLX:H121	2.02	0.42
1:E:2138:MET:HE1	3:E:2608:PEE:H49	2.01	0.42
1:E:2405:LEU:HD21	1:E:2407:ARG:HD3	2.02	0.42
1:A:1050:LEU:HD12	1:A:1050:LEU:HA	1.90	0.42
1:A:1706:ALA:HB1	1:A:1740:MET:SD	2.59	0.42
1:A:1979:LEU:HD13	2:A:2601:PLX:H102	2.01	0.42
1:A:2230:LEU:HD11	1:A:2317:LEU:HD21	2.00	0.42
1:A:2325:ARG:HE	1:A:2325:ARG:HB2	1.70	0.42
1:C:821:ALA:O	1:C:1048:TYR:OH	2.35	0.42
1:C:2177:GLN:HG3	1:C:2181:GLN:NE2	2.34	0.42
1:C:2268:LEU:O	1:C:2271:GLN:HG3	2.20	0.42
1:E:1671:ARG:HG3	1:E:1672:THR:HG23	1.99	0.42
1:A:821:ALA:O	1:A:1048:TYR:OH	2.35	0.42
1:A:1143:PHE:HD2	1:A:1154:LYS:HB3	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1249:PHE:HB2	1:A:1251:LEU:CD2	2.49	0.42
1:A:2286:ILE:HG13	1:A:2444:LEU:HB2	2.02	0.42
1:A:2405:LEU:HD21	1:A:2407:ARG:HD3	2.02	0.42
2:A:2602:PLX:H6	2:A:2602:PLX:H52	1.77	0.42
1:C:1517:THR:HG22	1:C:1675:LEU:HD13	2.01	0.42
1:C:2169:ARG:NH2	1:C:2497:LEU:O	2.46	0.42
1:E:2268:LEU:O	1:E:2271:GLN:HG3	2.20	0.42
2:E:2601:PLX:H361	2:E:2601:PLX:C16	2.36	0.42
1:A:1134:ARG:HG3	1:A:1137:PRO:HG3	2.00	0.42
1:A:1315:GLN:O	1:A:1316:ALA:C	2.63	0.42
1:A:1691:CYS:SG	1:A:1793:LEU:HD23	2.59	0.42
1:A:2516:THR:O	1:A:2517:ARG:HB2	2.19	0.42
1:C:1086:PHE:CD1	1:C:1087:ARG:HG3	2.54	0.42
1:C:1349:MET:HE1	1:C:2521:LEU:HD22	2.01	0.42
1:C:2179:LYS:HE2	1:C:2179:LYS:HA	2.01	0.42
1:C:2482:ARG:HG3	1:C:2486:SER:HB2	2.00	0.42
1:E:946:HIS:O	1:E:950:GLN:N	2.47	0.42
1:E:1204:ARG:O	1:E:1207:LEU:HG	2.19	0.42
1:A:1145:HIS:HB2	1:A:1147:ARG:HH12	1.84	0.42
1:A:1346:LYS:O	1:A:1346:LYS:HD3	2.19	0.42
1:A:2092:LEU:HD11	2:A:2601:PLX:H121	2.02	0.42
1:A:2146:THR:HG22	1:E:2181:GLN:O	2.20	0.42
1:C:1198:LEU:O	1:C:1206:GLN:NE2	2.52	0.42
1:C:1691:CYS:SG	1:C:1793:LEU:HD23	2.59	0.42
1:C:2197:LEU:HD22	2:C:2609:PLX:C38	2.49	0.42
1:E:1005:ARG:NH1	1:E:1047:GLN:NE2	2.67	0.42
1:E:1740:MET:HE2	1:E:1740:MET:HA	2.00	0.42
1:E:1784:LYS:O	1:E:1785:TYR:HB2	2.20	0.42
1:E:2438:LYS:HE2	1:E:2438:LYS:HB3	1.77	0.42
1:A:1709:VAL:HG21	2:A:2604:PLX:H162	2.01	0.42
1:A:1784:LYS:O	1:A:1785:TYR:HB2	2.20	0.42
1:A:2268:LEU:O	1:A:2271:GLN:HG3	2.20	0.42
1:A:2470:TYR:O	1:A:2473:ILE:HG22	2.20	0.42
1:C:894:LEU:H	1:C:894:LEU:HD23	1.84	0.42
1:C:1328:LEU:O	1:C:1331:ILE:HG22	2.20	0.42
1:C:2405:LEU:HD21	1:C:2407:ARG:HD3	2.02	0.42
1:E:1221:ILE:CD1	1:E:1280:ILE:HG23	2.47	0.42
1:E:1770:PRO:HB2	1:E:1771:PRO:HD3	2.01	0.42
1:E:1979:LEU:HD13	2:E:2603:PLX:H102	2.01	0.42
1:E:2354:LEU:HD23	1:E:2354:LEU:HA	1.92	0.42
2:E:2601:PLX:H92	2:E:2601:PLX:O6	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2605:PLX:H21	2:E:2605:PLX:H1C3	1.79	0.42
1:A:1190:TYR:HD2	1:A:1191:LEU:HD22	1.83	0.42
1:A:2197:LEU:HD22	2:A:2608:PLX:C38	2.50	0.42
1:C:1770:PRO:HB2	1:C:1771:PRO:HD3	2.01	0.42
1:C:1985:ILE:HD13	1:C:1985:ILE:HA	1.89	0.42
1:C:2092:LEU:HD11	2:C:2602:PLX:H121	2.01	0.42
1:E:808:HIS:O	1:E:809:VAL:C	2.62	0.42
1:E:1145:HIS:HB2	1:E:1147:ARG:HH12	1.84	0.42
1:E:2516:THR:O	1:E:2517:ARG:HB2	2.19	0.42
1:A:996:LEU:HA	1:A:999:VAL:HG12	2.01	0.42
1:A:1007:ASN:H	1:A:1010:VAL:CG2	2.33	0.42
1:A:1094:LEU:HD23	1:A:1094:LEU:HA	1.77	0.42
1:A:1705:ALA:HA	1:A:1708:LEU:HB3	2.02	0.42
1:C:1729:PHE:O	1:C:1732:THR:HG22	2.20	0.42
1:C:2182:LYS:HB2	1:C:2182:LYS:HE3	1.69	0.42
1:C:2516:THR:O	1:C:2517:ARG:HB2	2.19	0.42
2:C:2609:PLX:H92	2:C:2609:PLX:O6	2.20	0.42
1:E:1499:LEU:HA	1:E:1502:MET:HG3	2.01	0.42
1:E:2121:LEU:HD23	1:E:2121:LEU:HA	1.82	0.42
1:A:1328:LEU:O	1:A:1331:ILE:HG22	2.20	0.41
1:A:2110:LEU:HD23	1:A:2121:LEU:HB3	2.02	0.41
1:A:2256:TYR:OH	1:A:2273:ILE:O	2.31	0.41
1:C:1979:LEU:HD13	2:C:2602:PLX:H102	2.01	0.41
1:C:1981:PHE:CD2	3:C:2607:PEE:H13	2.55	0.41
1:C:2138:MET:HE1	3:C:2607:PEE:H49	2.01	0.41
1:C:2182:LYS:HD2	1:E:2144:ASP:HB2	2.01	0.41
1:A:946:HIS:O	1:A:950:GLN:N	2.47	0.41
1:A:1981:PHE:CD2	3:A:2606:PEE:H13	2.55	0.41
1:A:2520:GLU:O	1:A:2524:GLU:HG3	2.19	0.41
2:A:2608:PLX:H92	2:A:2608:PLX:O6	2.20	0.41
1:C:2286:ILE:HG13	1:C:2444:LEU:HB2	2.02	0.41
2:C:2609:PLX:C16	2:C:2609:PLX:C34	2.94	0.41
1:E:1328:LEU:O	1:E:1331:ILE:HG22	2.20	0.41
1:E:1530:MET:HE2	1:E:1530:MET:HB3	1.81	0.41
1:E:1649:LEU:HD13	1:E:1649:LEU:HA	1.91	0.41
1:E:1719:MET:O	1:E:1720:LEU:HD23	2.20	0.41
1:E:1729:PHE:O	1:E:1732:THR:HG22	2.20	0.41
1:E:2041:LYS:HA	1:E:2101:TYR:HD2	1.84	0.41
1:E:2060:TRP:HE3	1:E:2061:MET:HE2	1.86	0.41
2:E:2601:PLX:H292	2:E:2601:PLX:H261	1.78	0.41
3:E:2608:PEE:C25	3:E:2608:PEE:C44	2.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1086:PHE:CD1	1:A:1087:ARG:HG3	2.54	0.41
1:A:1315:GLN:NE2	1:A:1538:ARG:HA	2.35	0.41
1:A:2516:THR:C	1:A:2518:GLU:OE1	2.62	0.41
1:C:2131:LEU:HD23	1:C:2131:LEU:HA	1.70	0.41
1:E:1315:GLN:O	1:E:1316:ALA:C	2.63	0.41
1:E:1697:LEU:HD23	1:E:1697:LEU:HA	1.87	0.41
1:E:1705:ALA:HA	1:E:1708:LEU:HB3	2.02	0.41
1:E:1772:ARG:HA	1:E:1777:GLU:HG2	2.01	0.41
1:E:2071:ARG:NH1	1:E:2074:SER:HB2	2.35	0.41
1:E:2179:LYS:HE2	1:E:2179:LYS:HA	2.01	0.41
1:A:1222:ILE:HD13	1:A:1222:ILE:HA	1.85	0.41
1:A:1770:PRO:HB2	1:A:1771:PRO:HD3	2.01	0.41
2:A:2608:PLX:H151	1:C:2033:ILE:HG13	2.03	0.41
1:C:2438:LYS:HB3	1:C:2438:LYS:HE2	1.77	0.41
2:C:2606:PLX:H292	2:C:2606:PLX:H261	1.68	0.41
1:E:1007:ASN:H	1:E:1010:VAL:CG2	2.33	0.41
1:E:1016:TRP:O	1:E:1020:ILE:HG12	2.21	0.41
1:E:1194:PHE:CE1	2:E:2605:PLX:C1B	3.04	0.41
1:E:1403:HIS:ND1	1:E:2523:GLU:OE2	2.50	0.41
1:E:1691:CYS:SG	1:E:1793:LEU:HD23	2.59	0.41
1:A:1719:MET:O	1:A:1720:LEU:HD23	2.21	0.41
1:C:1194:PHE:CE1	2:C:2604:PLX:C1B	3.04	0.41
1:C:1699:HIS:HE1	1:C:1708:LEU:HB2	1.84	0.41
1:C:1747:PHE:CG	1:C:1776:LEU:HD12	2.56	0.41
1:C:2516:THR:C	1:C:2518:GLU:OE1	2.62	0.41
3:C:2607:PEE:H40	3:C:2607:PEE:H77	1.94	0.41
2:C:2609:PLX:H151	1:E:2033:ILE:HG13	2.03	0.41
1:E:1969:LYS:O	1:E:1971:ARG:NH1	2.53	0.41
1:A:1699:HIS:HE1	1:A:1708:LEU:HB2	1.84	0.41
1:A:2245:GLN:HB2	1:A:2246:PRO:HD3	2.03	0.41
1:C:1021:LEU:HD23	1:C:1021:LEU:HA	1.77	0.41
1:C:2071:ARG:NH1	1:C:2074:SER:HB2	2.35	0.41
3:C:2607:PEE:C24	3:C:2607:PEE:H77	2.48	0.41
1:E:2110:LEU:HD23	1:E:2121:LEU:HB3	2.02	0.41
1:E:2315:ILE:HG22	1:E:2344:LEU:HB2	2.03	0.41
1:A:2041:LYS:HA	1:A:2101:TYR:HD2	1.84	0.41
1:A:2181:GLN:O	1:C:2146:THR:HG22	2.21	0.41
1:A:2336:THR:HG22	1:A:2384:ALA:HB2	2.03	0.41
1:A:2546:ARG:HA	1:A:2546:ARG:HD3	1.85	0.41
1:C:1007:ASN:H	1:C:1010:VAL:CG2	2.33	0.41
1:C:1315:GLN:NE2	1:C:1538:ARG:HA	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1687:SER:HG	1:C:1796:HIS:CE1	2.31	0.41
3:C:2607:PEE:H43	3:C:2607:PEE:H38	1.83	0.41
1:E:1262:LYS:HA	1:E:1265:MET:CE	2.49	0.41
1:A:996:LEU:HA	1:A:996:LEU:HD23	1.86	0.41
1:A:2182:LYS:HD2	1:C:2144:ASP:HB2	2.02	0.41
1:A:2490:HIS:CD2	1:C:2494:PHE:CD2	3.09	0.41
1:C:1315:GLN:NE2	1:C:1538:ARG:HG3	2.36	0.41
1:C:1784:LYS:O	1:C:1785:TYR:HB2	2.20	0.41
1:A:808:HIS:O	1:A:809:VAL:C	2.62	0.41
1:A:1301:TYR:CD1	1:A:1301:TYR:N	2.84	0.41
1:A:1411:ASP:HB3	1:A:1413:PHE:CD2	2.56	0.41
1:A:1552:ARG:HG2	1:A:1553:ARG:NH1	2.36	0.41
1:A:1729:PHE:O	1:A:1732:THR:HG22	2.20	0.41
1:A:2081:LEU:HA	1:A:2081:LEU:HD12	1.87	0.41
1:A:2138:MET:HE1	3:A:2606:PEE:H49	2.01	0.41
1:A:2494:PHE:CD2	1:E:2490:HIS:CD2	3.09	0.41
1:C:813:VAL:HG13	1:C:836:TRP:CH2	2.56	0.41
1:C:1160:TYR:O	2:C:2603:PLX:H342	2.20	0.41
1:C:1530:MET:SD	1:C:1803:TYR:CZ	3.14	0.41
1:C:1688:GLU:HG2	1:C:1692:TYR:CE2	2.56	0.41
1:C:2024:LEU:HA	1:C:2024:LEU:HD12	1.90	0.41
1:C:2110:LEU:HD23	1:C:2121:LEU:HB3	2.02	0.41
1:C:2315:ILE:HG22	1:C:2344:LEU:HB2	2.03	0.41
1:E:915:ARG:O	1:E:915:ARG:HG3	2.21	0.41
1:E:1315:GLN:NE2	1:E:1538:ARG:HA	2.35	0.41
1:E:1349:MET:HE1	1:E:2521:LEU:HD22	2.01	0.41
1:E:2081:LEU:HA	1:E:2081:LEU:HD12	1.87	0.41
1:E:2376:ILE:HG13	1:E:2446:MET:CE	2.51	0.41
1:A:813:VAL:HG13	1:A:836:TRP:CH2	2.56	0.41
1:A:1194:PHE:CE1	2:A:2603:PLX:C1B	3.04	0.41
1:A:2060:TRP:HE3	1:A:2061:MET:HE2	1.85	0.41
1:A:2251:PHE:HE2	1:A:2447:VAL:HG13	1.86	0.41
1:A:2257:GLU:OE1	1:A:2257:GLU:HA	2.21	0.41
1:C:2376:ILE:HG13	1:C:2446:MET:CE	2.51	0.41
3:C:2607:PEE:H82	3:C:2607:PEE:C40	2.51	0.41
1:E:1084:ASP:OD2	1:E:1086:PHE:N	2.50	0.41
1:E:1160:TYR:O	2:E:2604:PLX:H342	2.20	0.41
1:E:1411:ASP:HB3	1:E:1413:PHE:CD2	2.56	0.41
3:E:2608:PEE:H82	3:E:2608:PEE:C40	2.51	0.41
1:A:1160:TYR:O	2:A:2602:PLX:H342	2.20	0.40
1:A:1349:MET:HE1	1:A:2521:LEU:HD22	2.01	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1530:MET:SD	1:A:1803:TYR:CZ	3.14	0.40
1:A:2071:ARG:NH1	1:A:2074:SER:HB2	2.35	0.40
1:A:2315:ILE:HG22	1:A:2344:LEU:HB2	2.03	0.40
1:C:1411:ASP:HB3	1:C:1413:PHE:CD2	2.56	0.40
1:E:813:VAL:HG13	1:E:836:TRP:CH2	2.56	0.40
1:E:1246:ILE:HD13	1:E:1246:ILE:HG21	1.86	0.40
1:E:1287:PHE:O	1:E:1291:LEU:HD23	2.21	0.40
1:A:1005:ARG:NH1	1:A:1047:GLN:NE2	2.67	0.40
1:A:1016:TRP:O	1:A:1020:ILE:HG12	2.21	0.40
1:A:1315:GLN:NE2	1:A:1538:ARG:HG3	2.36	0.40
1:A:1687:SER:HG	1:A:1796:HIS:CE1	2.31	0.40
1:A:1969:LYS:O	1:A:1971:ARG:NH1	2.53	0.40
1:A:2391:GLN:HB3	1:A:2397:ASP:HB2	2.03	0.40
1:C:1016:TRP:O	1:C:1020:ILE:HG12	2.21	0.40
1:C:2181:GLN:O	1:E:2146:THR:HG22	2.21	0.40
1:C:2257:GLU:HA	1:C:2257:GLU:OE1	2.21	0.40
1:C:2336:THR:HG22	1:C:2384:ALA:HB2	2.03	0.40
1:C:2470:TYR:O	1:C:2473:ILE:HG22	2.20	0.40
1:E:1294:ARG:O	1:E:1298:LEU:HD23	2.22	0.40
1:E:1315:GLN:NE2	1:E:1538:ARG:HG3	2.36	0.40
1:E:1530:MET:SD	1:E:1803:TYR:CZ	3.14	0.40
1:E:1552:ARG:HG2	1:E:1553:ARG:NH1	2.36	0.40
1:E:2197:LEU:HD22	2:E:2601:PLX:C38	2.49	0.40
1:E:2245:GLN:HB2	1:E:2246:PRO:HD3	2.03	0.40
1:E:2251:PHE:HE2	1:E:2447:VAL:HG13	1.86	0.40
1:A:915:ARG:HG3	1:A:915:ARG:O	2.21	0.40
1:A:1772:ARG:HD3	1:A:2071:ARG:HD3	2.03	0.40
1:A:1988:ILE:HD11	1:A:2031:MET:SD	2.61	0.40
1:A:2497:LEU:HD21	1:A:2539:MET:HE2	2.04	0.40
1:C:1719:MET:O	1:C:1720:LEU:HD23	2.21	0.40
1:C:1969:LYS:O	1:C:1971:ARG:NH1	2.53	0.40
1:C:2370:HIS:CE1	1:C:2396:GLU:HA	2.57	0.40
2:C:2604:PLX:H171	2:C:2604:PLX:H142	1.92	0.40
1:E:1688:GLU:HG2	1:E:1692:TYR:CE2	2.56	0.40
1:E:1988:ILE:HD11	1:E:2031:MET:SD	2.61	0.40
1:E:2257:GLU:HA	1:E:2257:GLU:OE1	2.21	0.40
1:A:1747:PHE:CG	1:A:1776:LEU:HD12	2.56	0.40
1:A:2033:ILE:HG13	2:E:2601:PLX:H151	2.03	0.40
1:E:1747:PHE:CG	1:E:1776:LEU:HD12	2.56	0.40
1:E:2046:LYS:HZ1	1:E:2093:SER:HB2	1.85	0.40
1:E:2169:ARG:NH2	1:E:2497:LEU:O	2.45	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2470:TYR:O	1:E:2473:ILE:HG22	2.20	0.40
2:E:2605:PLX:H171	2:E:2605:PLX:H142	1.92	0.40
1:A:1648:LEU:HD12	1:A:1648:LEU:HA	1.89	0.40
1:A:1688:GLU:HG2	1:A:1692:TYR:CE2	2.56	0.40
1:A:2370:HIS:CE1	1:A:2396:GLU:HA	2.57	0.40
1:A:2376:ILE:HG13	1:A:2446:MET:CE	2.51	0.40
1:C:1315:GLN:O	1:C:1316:ALA:C	2.63	0.40
1:C:2223:PRO:HG3	1:C:2448:ILE:HD11	2.04	0.40
1:E:2286:ILE:HG21	1:E:2286:ILE:HD13	1.87	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	1329/2547 (52%)	1248 (94%)	79 (6%)	2 (0%)	43	74
1	C	1329/2547 (52%)	1248 (94%)	79 (6%)	2 (0%)	43	74
1	E	1329/2547 (52%)	1248 (94%)	79 (6%)	2 (0%)	43	74
All	All	3987/7641 (52%)	3744 (94%)	237 (6%)	6 (0%)	44	74

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1785	TYR
1	C	1785	TYR
1	E	1785	TYR
1	A	1259	TYR
1	C	1259	TYR
1	E	1259	TYR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1128/2246 (50%)	1118 (99%)	10 (1%)	70	76
1	C	1128/2246 (50%)	1118 (99%)	10 (1%)	70	76
1	E	1128/2246 (50%)	1118 (99%)	10 (1%)	70	76
All	All	3384/6738 (50%)	3354 (99%)	30 (1%)	68	76

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	848	MET
1	A	1013	HIS
1	A	1143	PHE
1	A	1238	MET
1	A	1731	MET
1	A	1970	TYR
1	A	2073	PHE
1	A	2257	GLU
1	A	2270	MET
1	A	2493	MET
1	C	848	MET
1	C	1013	HIS
1	C	1143	PHE
1	C	1238	MET
1	C	1731	MET
1	C	1970	TYR
1	C	2073	PHE
1	C	2257	GLU
1	C	2270	MET
1	C	2493	MET
1	E	848	MET
1	E	1013	HIS
1	E	1143	PHE
1	E	1238	MET
1	E	1731	MET
1	E	1970	TYR

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Mol	Chain	Res	Type
1	E	2073	PHE
1	E	2257	GLU
1	E	2270	MET
1	E	2493	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1047	GLN
1	A	1107	GLN
1	A	1138	ASN
1	A	1225	ASN
1	A	1304	HIS
1	A	1315	GLN
1	A	1408	HIS
1	A	1755	ASN
1	C	1047	GLN
1	C	1107	GLN
1	C	1138	ASN
1	C	1200	GLN
1	C	1225	ASN
1	C	1304	HIS
1	C	1315	GLN
1	C	1408	HIS
1	C	1755	ASN
1	E	1047	GLN
1	E	1107	GLN
1	E	1138	ASN
1	E	1200	GLN
1	E	1225	ASN
1	E	1304	HIS
1	E	1315	GLN
1	E	1408	HIS
1	E	1755	ASN
1	E	2181	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

27 ligands are modelled in this entry.

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
3	PEE	A	2606	-	50,50,50	1.20	7 (14%)	53,55,55	1.27	6 (11%)
4	P5S	E	2609	-	52,53,53	0.81	3 (5%)	54,60,60	0.96	2 (3%)
2	PLX	A	2602	-	51,51,51	1.14	3 (5%)	53,59,59	0.96	2 (3%)
2	PLX	E	2606	-	51,51,51	1.18	3 (5%)	53,59,59	0.92	1 (1%)
2	PLX	A	2609	-	51,51,51	1.18	4 (7%)	53,59,59	0.90	1 (1%)
2	PLX	C	2605	-	51,51,51	1.17	3 (5%)	53,59,59	0.92	1 (1%)
2	PLX	C	2609	-	51,51,51	0.61	0	53,59,59	0.69	1 (1%)
2	PLX	C	2603	-	51,51,51	1.14	3 (5%)	53,59,59	0.96	2 (3%)
2	PLX	A	2605	-	51,51,51	1.19	4 (7%)	53,59,59	0.78	0
2	PLX	E	2601	-	51,51,51	0.61	0	53,59,59	0.69	1 (1%)
2	PLX	E	2602	-	51,51,51	1.18	4 (7%)	53,59,59	0.90	1 (1%)
2	PLX	A	2608	-	51,51,51	0.61	0	53,59,59	0.69	1 (1%)
4	P5S	C	2608	-	52,53,53	0.82	3 (5%)	54,60,60	0.96	2 (3%)
2	PLX	C	2602	-	51,51,51	1.15	4 (7%)	53,59,59	0.80	0
2	PLX	C	2601	-	51,51,51	1.18	4 (7%)	53,59,59	0.90	1 (1%)
3	PEE	E	2608	-	50,50,50	1.20	7 (14%)	53,55,55	1.27	6 (11%)
2	PLX	A	2601	-	51,51,51	1.15	4 (7%)	53,59,59	0.80	0
3	PEE	C	2607	-	50,50,50	1.20	7 (14%)	53,55,55	1.27	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PLX	E	2607	-	51,51,51	1.19	4 (7%)	53,59,59	0.78	0
4	P5S	A	2607	-	52,53,53	0.82	3 (5%)	54,60,60	0.96	2 (3%)
2	PLX	A	2604	-	51,51,51	1.18	3 (5%)	53,59,59	0.92	1 (1%)
2	PLX	A	2603	-	51,51,51	0.61	0	53,59,59	0.70	0
2	PLX	C	2606	-	51,51,51	1.19	4 (7%)	53,59,59	0.78	0
2	PLX	E	2604	-	51,51,51	1.14	3 (5%)	53,59,59	0.96	2 (3%)
2	PLX	E	2605	-	51,51,51	0.61	0	53,59,59	0.70	0
2	PLX	C	2604	-	51,51,51	0.61	0	53,59,59	0.70	0
2	PLX	E	2603	-	51,51,51	1.14	4 (7%)	53,59,59	0.80	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
3	PEE	A	2606	-	-	27/54/54/54	-
4	P5S	E	2609	-	-	7/59/59/59	-
2	PLX	A	2602	-	-	12/55/55/55	-
2	PLX	E	2606	-	-	7/55/55/55	-
2	PLX	A	2609	-	-	6/55/55/55	-
2	PLX	C	2605	-	-	7/55/55/55	-
2	PLX	C	2609	-	-	18/55/55/55	-
2	PLX	C	2603	-	-	12/55/55/55	-
2	PLX	A	2605	-	-	20/55/55/55	-
2	PLX	E	2601	-	-	18/55/55/55	-
2	PLX	E	2602	-	-	6/55/55/55	-
2	PLX	A	2608	-	-	18/55/55/55	-
4	P5S	C	2608	-	-	7/59/59/59	-
2	PLX	C	2602	-	-	30/55/55/55	-
2	PLX	C	2601	-	-	6/55/55/55	-
3	PEE	E	2608	-	-	26/54/54/54	-
2	PLX	A	2601	-	-	30/55/55/55	-
3	PEE	C	2607	-	-	26/54/54/54	-
2	PLX	E	2607	-	-	20/55/55/55	-
4	P5S	A	2607	-	-	7/59/59/59	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLX	A	2604	-	-	7/55/55/55	-
2	PLX	A	2603	-	-	13/55/55/55	-
2	PLX	C	2606	-	-	20/55/55/55	-
2	PLX	E	2604	-	-	12/55/55/55	-
2	PLX	E	2605	-	-	13/55/55/55	-
2	PLX	C	2604	-	-	13/55/55/55	-
2	PLX	E	2603	-	-	30/55/55/55	-

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2608	PEE	C39-C38	3.77	1.53	1.31
2	E	2606	PLX	O6-C4	-3.76	1.39	1.44
3	A	2606	PEE	C39-C38	3.75	1.53	1.31
3	C	2607	PEE	C39-C38	3.75	1.53	1.31
2	A	2604	PLX	O6-C4	-3.74	1.39	1.44
2	C	2605	PLX	O6-C4	-3.72	1.39	1.44
2	C	2601	PLX	O6-C4	-3.61	1.39	1.44
2	E	2602	PLX	O6-C4	-3.61	1.39	1.44
2	A	2609	PLX	O6-C4	-3.59	1.40	1.44
3	A	2606	PEE	C18-C19	3.57	1.52	1.31
3	E	2608	PEE	C18-C19	3.57	1.52	1.31
3	C	2607	PEE	C18-C19	3.57	1.52	1.31
2	A	2602	PLX	O6-C4	-3.47	1.40	1.44
2	E	2604	PLX	O6-C4	-3.46	1.40	1.44
2	C	2603	PLX	O6-C4	-3.46	1.40	1.44
3	E	2608	PEE	P-O4P	3.13	1.71	1.59
3	C	2607	PEE	P-O4P	3.12	1.71	1.59
3	A	2606	PEE	P-O4P	3.12	1.71	1.59
4	A	2607	P5S	P12-O16	3.00	1.71	1.59
4	C	2608	P5S	P12-O16	2.99	1.71	1.59
4	E	2609	P5S	P12-O16	2.98	1.71	1.59
2	A	2605	PLX	O6-C4	-2.96	1.40	1.44
2	C	2606	PLX	O6-C4	-2.95	1.40	1.44
2	E	2607	PLX	O6-C4	-2.92	1.40	1.44
2	A	2601	PLX	C7-C6	2.79	1.56	1.50
2	E	2603	PLX	C7-C6	2.78	1.56	1.50
2	C	2602	PLX	C7-C6	2.78	1.56	1.50
3	C	2607	PEE	O3-C3	-2.76	1.39	1.45
3	E	2608	PEE	O3-C3	-2.75	1.39	1.45
3	A	2606	PEE	O3-C3	-2.74	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2605	PLX	C7-C6	2.59	1.56	1.50
2	E	2607	PLX	C7-C6	2.59	1.56	1.50
2	C	2606	PLX	C7-C6	2.59	1.56	1.50
3	C	2607	PEE	O4P-C4	-2.45	1.35	1.44
2	C	2602	PLX	P1-O4	2.45	1.69	1.59
3	A	2606	PEE	O4P-C4	-2.44	1.35	1.44
2	A	2601	PLX	P1-O4	2.44	1.68	1.59
3	E	2608	PEE	O4P-C4	-2.44	1.35	1.44
2	E	2603	PLX	P1-O4	2.43	1.68	1.59
2	E	2607	PLX	P1-O4	2.43	1.68	1.59
2	A	2605	PLX	P1-O4	2.41	1.68	1.59
2	A	2609	PLX	C7-C6	2.40	1.55	1.50
2	C	2606	PLX	P1-O4	2.39	1.68	1.59
2	E	2602	PLX	C7-C6	2.39	1.55	1.50
2	C	2601	PLX	C7-C6	2.39	1.55	1.50
3	E	2608	PEE	O3-C30	2.38	1.40	1.33
3	C	2607	PEE	O3-C30	2.38	1.40	1.33
3	A	2606	PEE	O3-C30	2.38	1.40	1.33
2	E	2606	PLX	P1-O4	2.33	1.68	1.59
2	A	2604	PLX	P1-O4	2.32	1.68	1.59
2	C	2605	PLX	P1-O4	2.31	1.68	1.59
2	C	2601	PLX	P1-O4	2.31	1.68	1.59
2	A	2609	PLX	P1-O4	2.31	1.68	1.59
2	E	2602	PLX	P1-O4	2.31	1.68	1.59
2	C	2603	PLX	P1-O4	2.31	1.68	1.59
2	A	2602	PLX	P1-O4	2.30	1.68	1.59
2	E	2604	PLX	P1-O4	2.29	1.68	1.59
2	C	2602	PLX	O6-C4	-2.23	1.41	1.44
2	A	2601	PLX	O6-C4	-2.23	1.41	1.44
4	A	2607	P5S	O16-C3	-2.20	1.36	1.44
4	C	2608	P5S	O16-C3	-2.19	1.36	1.44
4	E	2609	P5S	O16-C3	-2.18	1.36	1.44
2	E	2606	PLX	C7-C6	2.16	1.55	1.50
2	E	2603	PLX	O6-C4	-2.15	1.41	1.44
4	C	2608	P5S	O19-C1	-2.15	1.40	1.45
2	C	2606	PLX	P1-O1	2.15	1.67	1.59
2	A	2604	PLX	C7-C6	2.15	1.55	1.50
2	E	2603	PLX	P1-O1	2.14	1.67	1.59
2	C	2602	PLX	P1-O1	2.14	1.67	1.59
2	E	2607	PLX	P1-O1	2.14	1.67	1.59
2	A	2605	PLX	P1-O1	2.14	1.67	1.59
4	A	2607	P5S	O19-C1	-2.14	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2605	PLX	C7-C6	2.13	1.55	1.50
2	A	2601	PLX	P1-O1	2.13	1.67	1.59
3	C	2607	PEE	O2-C2	-2.13	1.41	1.46
2	E	2602	PLX	P1-O1	2.13	1.67	1.59
2	C	2601	PLX	P1-O1	2.12	1.67	1.59
3	A	2606	PEE	O2-C2	-2.12	1.41	1.46
2	A	2609	PLX	P1-O1	2.11	1.67	1.59
3	E	2608	PEE	O2-C2	-2.11	1.41	1.46
4	E	2609	P5S	O19-C1	-2.10	1.40	1.45
2	A	2602	PLX	C7-C6	2.10	1.55	1.50
2	C	2603	PLX	C7-C6	2.09	1.55	1.50
2	E	2604	PLX	C7-C6	2.07	1.55	1.50

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2606	PEE	O2P-P-O1P	3.48	128.63	112.44
3	E	2608	PEE	O2P-P-O1P	3.47	128.59	112.44
3	C	2607	PEE	O2P-P-O1P	3.47	128.59	112.44
4	C	2608	P5S	O15-P12-O13	2.76	125.27	112.44
4	A	2607	P5S	O15-P12-O13	2.76	125.27	112.44
4	E	2609	P5S	O15-P12-O13	2.76	125.26	112.44
2	C	2603	PLX	C8-C7-C6	-2.61	107.32	113.38
2	A	2602	PLX	C8-C7-C6	-2.60	107.33	113.38
2	E	2606	PLX	C8-C7-C6	-2.60	107.34	113.38
2	A	2604	PLX	C8-C7-C6	-2.60	107.34	113.38
2	E	2604	PLX	C8-C7-C6	-2.59	107.35	113.38
2	C	2605	PLX	C8-C7-C6	-2.59	107.35	113.38
3	C	2607	PEE	C2-O2-C10	2.36	123.45	117.80
3	A	2606	PEE	C2-O2-C10	2.35	123.43	117.80
3	E	2608	PEE	C2-O2-C10	2.35	123.42	117.80
3	A	2606	PEE	O4P-P-O1P	-2.31	99.80	108.94
3	C	2607	PEE	O4P-P-O1P	-2.30	99.81	108.94
3	E	2608	PEE	O4P-P-O1P	-2.30	99.82	108.94
2	A	2609	PLX	C8-C7-C6	-2.27	108.11	113.38
2	E	2602	PLX	C8-C7-C6	-2.26	108.11	113.38
2	C	2601	PLX	C8-C7-C6	-2.26	108.13	113.38
3	C	2607	PEE	C3-O3-C30	-2.25	108.88	117.12
3	A	2606	PEE	C3-O3-C30	-2.25	108.89	117.12
3	E	2608	PEE	C3-O3-C30	-2.25	108.90	117.12
3	C	2607	PEE	C12-C11-C10	-2.21	105.61	113.69
3	A	2606	PEE	C12-C11-C10	-2.20	105.63	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	2608	PEE	C12-C11-C10	-2.19	105.66	113.69
2	C	2603	PLX	C6-O6-C4	-2.18	110.86	115.20
2	A	2602	PLX	C6-O6-C4	-2.17	110.87	115.20
2	E	2604	PLX	C6-O6-C4	-2.16	110.88	115.20
2	C	2609	PLX	C6-O6-C4	-2.14	110.92	115.20
2	A	2608	PLX	C6-O6-C4	-2.14	110.93	115.20
2	E	2601	PLX	C6-O6-C4	-2.13	110.94	115.20
4	C	2608	P5S	O37-C38-C39	2.10	116.03	111.48
4	A	2607	P5S	O37-C38-C39	2.10	116.03	111.48
4	E	2609	P5S	O37-C38-C39	2.10	116.02	111.48
3	E	2608	PEE	O2-C2-C1	2.08	115.81	108.34
3	A	2606	PEE	O2-C2-C1	2.07	115.77	108.34
3	C	2607	PEE	O2-C2-C1	2.07	115.76	108.34

There are no chirality outliers.

All (418) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2601	PLX	O7-C6-C7-C8
2	A	2601	PLX	O7-C6-O6-C4
2	A	2601	PLX	C4-C3-O4-P1
2	A	2601	PLX	C3-O4-P1-O1
2	A	2601	PLX	C3-O4-P1-O2
2	A	2601	PLX	N1-C1-C2-O1
2	A	2602	PLX	O9-C24-C25-C26
2	A	2603	PLX	N1-C1-C2-O1
2	A	2604	PLX	O6-C4-C5-O8
2	A	2604	PLX	C3-O4-P1-O1
2	A	2604	PLX	C3-O4-P1-O3
2	A	2604	PLX	O9-C24-C25-C26
2	A	2605	PLX	O7-C6-O6-C4
2	A	2605	PLX	C2-O1-P1-O4
2	A	2605	PLX	C2-O1-P1-O2
2	A	2605	PLX	C2-O1-P1-O3
2	A	2605	PLX	O9-C24-O8-C5
2	A	2605	PLX	O9-C24-C25-C26
2	A	2608	PLX	O7-C6-O6-C4
2	A	2608	PLX	C3-O4-P1-O1
2	A	2608	PLX	C2-O1-P1-O4
2	A	2608	PLX	O9-C24-C25-C26
2	C	2602	PLX	O7-C6-C7-C8
2	C	2602	PLX	O7-C6-O6-C4

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Mol	Chain	Res	Type	Atoms
2	C	2602	PLX	C4-C3-O4-P1
2	C	2602	PLX	C3-O4-P1-O1
2	C	2602	PLX	C3-O4-P1-O2
2	C	2602	PLX	N1-C1-C2-O1
2	C	2603	PLX	O9-C24-C25-C26
2	C	2604	PLX	N1-C1-C2-O1
2	C	2605	PLX	O6-C4-C5-O8
2	C	2605	PLX	C3-O4-P1-O1
2	C	2605	PLX	C3-O4-P1-O3
2	C	2605	PLX	O9-C24-C25-C26
2	C	2606	PLX	O7-C6-O6-C4
2	C	2606	PLX	C2-O1-P1-O4
2	C	2606	PLX	C2-O1-P1-O2
2	C	2606	PLX	C2-O1-P1-O3
2	C	2606	PLX	O9-C24-O8-C5
2	C	2606	PLX	O9-C24-C25-C26
2	C	2609	PLX	O7-C6-O6-C4
2	C	2609	PLX	C3-O4-P1-O1
2	C	2609	PLX	C2-O1-P1-O4
2	C	2609	PLX	O9-C24-C25-C26
2	E	2601	PLX	O7-C6-O6-C4
2	E	2601	PLX	C3-O4-P1-O1
2	E	2601	PLX	C2-O1-P1-O4
2	E	2601	PLX	O9-C24-C25-C26
2	E	2603	PLX	O7-C6-C7-C8
2	E	2603	PLX	O7-C6-O6-C4
2	E	2603	PLX	C4-C3-O4-P1
2	E	2603	PLX	C3-O4-P1-O1
2	E	2603	PLX	C3-O4-P1-O2
2	E	2603	PLX	N1-C1-C2-O1
2	E	2604	PLX	O9-C24-C25-C26
2	E	2605	PLX	N1-C1-C2-O1
2	E	2606	PLX	O6-C4-C5-O8
2	E	2606	PLX	C3-O4-P1-O1
2	E	2606	PLX	C3-O4-P1-O3
2	E	2606	PLX	O9-C24-C25-C26
2	E	2607	PLX	O7-C6-O6-C4
2	E	2607	PLX	C2-O1-P1-O4
2	E	2607	PLX	C2-O1-P1-O2
2	E	2607	PLX	C2-O1-P1-O3
2	E	2607	PLX	O9-C24-O8-C5
2	E	2607	PLX	O9-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
3	A	2606	PEE	C2-C1-O3P-P
3	A	2606	PEE	C1-O3P-P-O4P
3	A	2606	PEE	C4-O4P-P-O3P
3	A	2606	PEE	C4-O4P-P-O1P
3	C	2607	PEE	C2-C1-O3P-P
3	C	2607	PEE	C1-O3P-P-O4P
3	C	2607	PEE	C4-O4P-P-O3P
3	C	2607	PEE	C4-O4P-P-O1P
3	E	2608	PEE	C2-C1-O3P-P
3	E	2608	PEE	C1-O3P-P-O4P
3	E	2608	PEE	C4-O4P-P-O3P
3	E	2608	PEE	C4-O4P-P-O1P
4	A	2607	P5S	CB-OG-P12-O13
4	C	2608	P5S	CB-OG-P12-O13
4	E	2609	P5S	CB-OG-P12-O13
2	A	2601	PLX	O6-C4-C5-O8
2	C	2602	PLX	O6-C4-C5-O8
2	E	2603	PLX	O6-C4-C5-O8
4	A	2607	P5S	O19-C1-C2-O37
4	C	2608	P5S	O19-C1-C2-O37
4	E	2609	P5S	O19-C1-C2-O37
3	A	2606	PEE	C31-C30-O3-C3
3	C	2607	PEE	C31-C30-O3-C3
3	E	2608	PEE	C31-C30-O3-C3
3	A	2606	PEE	C41-C42-C43-C44
3	C	2607	PEE	C41-C42-C43-C44
3	E	2608	PEE	C41-C42-C43-C44
2	A	2601	PLX	O6-C6-C7-C8
2	C	2602	PLX	O6-C6-C7-C8
2	E	2603	PLX	O6-C6-C7-C8
3	A	2606	PEE	C11-C10-O2-C2
3	C	2607	PEE	C11-C10-O2-C2
3	E	2608	PEE	C11-C10-O2-C2
3	A	2606	PEE	O5-C30-O3-C3
3	C	2607	PEE	O5-C30-O3-C3
3	E	2608	PEE	O5-C30-O3-C3
3	A	2606	PEE	C1-C2-O2-C10
3	C	2607	PEE	C1-C2-O2-C10
3	E	2608	PEE	C1-C2-O2-C10
2	A	2605	PLX	C17-C18-C19-C20
2	C	2606	PLX	C17-C18-C19-C20
2	E	2607	PLX	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
2	A	2604	PLX	O7-C6-C7-C8
2	A	2608	PLX	O7-C6-C7-C8
2	C	2605	PLX	O7-C6-C7-C8
2	C	2609	PLX	O7-C6-C7-C8
2	E	2601	PLX	O7-C6-C7-C8
2	E	2606	PLX	O7-C6-C7-C8
2	A	2605	PLX	C15-C16-C17-C18
2	E	2607	PLX	C15-C16-C17-C18
2	C	2606	PLX	C15-C16-C17-C18
3	C	2607	PEE	C31-C32-C33-C34
3	E	2608	PEE	C31-C32-C33-C34
3	A	2606	PEE	C31-C32-C33-C34
2	A	2603	PLX	C11-C12-C13-C14
2	C	2604	PLX	C11-C12-C13-C14
2	E	2605	PLX	C11-C12-C13-C14
2	A	2608	PLX	C17-C18-C19-C20
2	C	2609	PLX	C17-C18-C19-C20
2	E	2601	PLX	C17-C18-C19-C20
3	A	2606	PEE	C17-C18-C19-C20
3	C	2607	PEE	C17-C18-C19-C20
3	E	2608	PEE	C17-C18-C19-C20
3	A	2606	PEE	C43-C44-C45-C46
3	C	2607	PEE	C43-C44-C45-C46
3	E	2608	PEE	C43-C44-C45-C46
3	A	2606	PEE	O4-C10-O2-C2
3	C	2607	PEE	O4-C10-O2-C2
3	E	2608	PEE	O4-C10-O2-C2
3	A	2606	PEE	C44-C45-C46-C47
3	C	2607	PEE	C44-C45-C46-C47
3	E	2608	PEE	C44-C45-C46-C47
2	A	2601	PLX	C7-C8-C9-C10
2	C	2602	PLX	C7-C8-C9-C10
2	E	2603	PLX	C7-C8-C9-C10
2	A	2608	PLX	C6-C7-C8-C9
2	C	2609	PLX	C6-C7-C8-C9
2	E	2601	PLX	C6-C7-C8-C9
2	A	2602	PLX	C4-C3-O4-P1
2	C	2603	PLX	C4-C3-O4-P1
2	E	2604	PLX	C4-C3-O4-P1
3	A	2606	PEE	C14-C15-C16-C17
3	E	2608	PEE	C14-C15-C16-C17
3	C	2607	PEE	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
3	E	2608	PEE	C12-C13-C14-C15
3	A	2606	PEE	C12-C13-C14-C15
3	C	2607	PEE	C12-C13-C14-C15
2	A	2608	PLX	C27-C28-C29-C30
2	C	2609	PLX	C27-C28-C29-C30
2	E	2601	PLX	C27-C28-C29-C30
2	A	2603	PLX	C13-C14-C15-C16
2	C	2604	PLX	C13-C14-C15-C16
2	E	2605	PLX	C13-C14-C15-C16
2	A	2609	PLX	C14-C15-C16-C17
2	E	2602	PLX	C14-C15-C16-C17
4	A	2607	P5S	O19-C1-C2-C3
4	C	2608	P5S	O19-C1-C2-C3
4	E	2609	P5S	O19-C1-C2-C3
2	C	2601	PLX	C14-C15-C16-C17
2	A	2605	PLX	O6-C4-C5-O8
2	C	2606	PLX	O6-C4-C5-O8
2	E	2607	PLX	O6-C4-C5-O8
3	A	2606	PEE	O2-C2-C3-O3
3	C	2607	PEE	O2-C2-C3-O3
3	E	2608	PEE	O2-C2-C3-O3
2	A	2608	PLX	C29-C30-C31-C32
2	C	2609	PLX	C29-C30-C31-C32
2	E	2601	PLX	C29-C30-C31-C32
2	A	2603	PLX	C12-C13-C14-C15
2	C	2604	PLX	C12-C13-C14-C15
2	E	2605	PLX	C12-C13-C14-C15
2	A	2605	PLX	O7-C6-C7-C8
2	C	2606	PLX	O7-C6-C7-C8
2	E	2607	PLX	O7-C6-C7-C8
2	A	2601	PLX	O4-C3-C4-C5
2	A	2605	PLX	O4-C3-C4-C5
2	C	2602	PLX	O4-C3-C4-C5
2	C	2606	PLX	O4-C3-C4-C5
2	E	2603	PLX	O4-C3-C4-C5
2	E	2607	PLX	O4-C3-C4-C5
2	A	2601	PLX	C3-C4-C5-O8
2	A	2604	PLX	C3-C4-C5-O8
2	C	2602	PLX	C3-C4-C5-O8
2	C	2605	PLX	C3-C4-C5-O8
2	E	2603	PLX	C3-C4-C5-O8
2	E	2606	PLX	C3-C4-C5-O8

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Mol	Chain	Res	Type	Atoms
2	A	2601	PLX	O4-C3-C4-O6
2	C	2602	PLX	O4-C3-C4-O6
2	E	2603	PLX	O4-C3-C4-O6
2	A	2601	PLX	C12-C13-C14-C15
2	C	2602	PLX	C12-C13-C14-C15
2	E	2603	PLX	C12-C13-C14-C15
2	A	2601	PLX	C29-C30-C31-C32
2	C	2602	PLX	C29-C30-C31-C32
2	E	2603	PLX	C29-C30-C31-C32
3	C	2607	PEE	C42-C43-C44-C45
2	C	2604	PLX	C16-C17-C18-C19
2	E	2605	PLX	C16-C17-C18-C19
3	A	2606	PEE	C42-C43-C44-C45
3	E	2608	PEE	C42-C43-C44-C45
2	A	2603	PLX	C16-C17-C18-C19
2	A	2601	PLX	C17-C18-C19-C20
2	C	2602	PLX	C17-C18-C19-C20
2	E	2603	PLX	C17-C18-C19-C20
2	A	2605	PLX	C25-C26-C27-C28
2	C	2606	PLX	C25-C26-C27-C28
2	E	2607	PLX	C25-C26-C27-C28
2	A	2608	PLX	O4-C3-C4-C5
2	C	2609	PLX	O4-C3-C4-C5
2	E	2601	PLX	O4-C3-C4-C5
2	A	2609	PLX	C28-C29-C30-C31
2	E	2602	PLX	C28-C29-C30-C31
2	A	2601	PLX	C24-C25-C26-C27
2	C	2602	PLX	C24-C25-C26-C27
2	E	2603	PLX	C24-C25-C26-C27
2	C	2601	PLX	C28-C29-C30-C31
3	A	2606	PEE	C15-C16-C17-C18
3	C	2607	PEE	C15-C16-C17-C18
3	E	2608	PEE	C15-C16-C17-C18
2	A	2601	PLX	C13-C14-C15-C16
2	C	2602	PLX	C13-C14-C15-C16
2	E	2603	PLX	C13-C14-C15-C16
2	A	2605	PLX	O4-C3-C4-O6
2	A	2608	PLX	O4-C3-C4-O6
2	C	2606	PLX	O4-C3-C4-O6
2	C	2609	PLX	O4-C3-C4-O6
2	E	2601	PLX	O4-C3-C4-O6
2	E	2607	PLX	O4-C3-C4-O6

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Mol	Chain	Res	Type	Atoms
2	E	2603	PLX	C25-C26-C27-C28
2	A	2601	PLX	C25-C26-C27-C28
2	C	2602	PLX	C25-C26-C27-C28
4	A	2607	P5S	C2-C3-O16-P12
4	C	2608	P5S	C2-C3-O16-P12
4	E	2609	P5S	C2-C3-O16-P12
2	A	2605	PLX	N1-C1-C2-O1
2	A	2608	PLX	N1-C1-C2-O1
2	C	2606	PLX	N1-C1-C2-O1
2	C	2609	PLX	N1-C1-C2-O1
2	E	2601	PLX	N1-C1-C2-O1
2	E	2607	PLX	N1-C1-C2-O1
4	A	2607	P5S	N-CA-CB-OG
4	C	2608	P5S	N-CA-CB-OG
4	E	2609	P5S	N-CA-CB-OG
4	A	2607	P5S	CA-CB-OG-P12
4	C	2608	P5S	CA-CB-OG-P12
4	E	2609	P5S	CA-CB-OG-P12
2	A	2601	PLX	C25-C24-O8-C5
2	A	2602	PLX	C25-C24-O8-C5
2	A	2609	PLX	C25-C24-O8-C5
2	C	2601	PLX	C25-C24-O8-C5
2	C	2602	PLX	C25-C24-O8-C5
2	C	2603	PLX	C25-C24-O8-C5
2	E	2602	PLX	C25-C24-O8-C5
2	E	2603	PLX	C25-C24-O8-C5
2	E	2604	PLX	C25-C24-O8-C5
2	A	2603	PLX	C9-C10-C11-C12
2	C	2604	PLX	C9-C10-C11-C12
2	E	2605	PLX	C9-C10-C11-C12
2	A	2605	PLX	C26-C27-C28-C29
2	C	2606	PLX	C26-C27-C28-C29
2	A	2602	PLX	O8-C24-C25-C26
2	A	2605	PLX	O8-C24-C25-C26
2	C	2603	PLX	O8-C24-C25-C26
2	C	2606	PLX	O8-C24-C25-C26
2	E	2604	PLX	O8-C24-C25-C26
2	E	2607	PLX	O8-C24-C25-C26
2	E	2607	PLX	C26-C27-C28-C29
2	E	2605	PLX	C14-C15-C16-C17
2	C	2604	PLX	C14-C15-C16-C17
2	A	2603	PLX	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
3	A	2606	PEE	C38-C39-C40-C41
3	C	2607	PEE	C38-C39-C40-C41
3	E	2608	PEE	C38-C39-C40-C41
2	A	2605	PLX	C3-C4-C5-O8
2	C	2606	PLX	C3-C4-C5-O8
2	E	2607	PLX	C3-C4-C5-O8
2	C	2606	PLX	C14-C15-C16-C17
2	E	2607	PLX	C14-C15-C16-C17
2	A	2605	PLX	C14-C15-C16-C17
2	A	2601	PLX	C3-C4-O6-C6
2	A	2601	PLX	C5-C4-O6-C6
2	A	2601	PLX	C2-O1-P1-O4
2	A	2601	PLX	C2-O1-P1-O2
2	A	2601	PLX	C2-O1-P1-O3
2	A	2602	PLX	C3-C4-O6-C6
2	A	2602	PLX	C5-C4-O6-C6
2	A	2602	PLX	C3-O4-P1-O2
2	A	2602	PLX	C2-O1-P1-O4
2	A	2602	PLX	C2-O1-P1-O2
2	A	2602	PLX	C2-O1-P1-O3
2	A	2603	PLX	C3-O4-P1-O1
2	A	2603	PLX	C3-O4-P1-O3
2	A	2608	PLX	C3-O4-P1-O2
2	A	2608	PLX	C2-O1-P1-O2
2	A	2609	PLX	C3-O4-P1-O2
2	C	2601	PLX	C3-O4-P1-O2
2	C	2602	PLX	C3-C4-O6-C6
2	C	2602	PLX	C5-C4-O6-C6
2	C	2602	PLX	C2-O1-P1-O4
2	C	2602	PLX	C2-O1-P1-O2
2	C	2602	PLX	C2-O1-P1-O3
2	C	2603	PLX	C3-C4-O6-C6
2	C	2603	PLX	C5-C4-O6-C6
2	C	2603	PLX	C3-O4-P1-O2
2	C	2603	PLX	C2-O1-P1-O4
2	C	2603	PLX	C2-O1-P1-O2
2	C	2603	PLX	C2-O1-P1-O3
2	C	2604	PLX	C3-O4-P1-O1
2	C	2604	PLX	C3-O4-P1-O3
2	C	2609	PLX	C3-O4-P1-O2
2	C	2609	PLX	C2-O1-P1-O2
2	E	2601	PLX	C3-O4-P1-O2

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Mol	Chain	Res	Type	Atoms
2	E	2601	PLX	C2-O1-P1-O2
2	E	2602	PLX	C3-O4-P1-O2
2	E	2603	PLX	C3-C4-O6-C6
2	E	2603	PLX	C5-C4-O6-C6
2	E	2603	PLX	C2-O1-P1-O4
2	E	2603	PLX	C2-O1-P1-O2
2	E	2603	PLX	C2-O1-P1-O3
2	E	2604	PLX	C3-C4-O6-C6
2	E	2604	PLX	C5-C4-O6-C6
2	E	2604	PLX	C3-O4-P1-O2
2	E	2604	PLX	C2-O1-P1-O4
2	E	2604	PLX	C2-O1-P1-O2
2	E	2604	PLX	C2-O1-P1-O3
2	E	2605	PLX	C3-O4-P1-O1
2	E	2605	PLX	C3-O4-P1-O3
3	A	2606	PEE	C1-O3P-P-O1P
3	C	2607	PEE	C1-O3P-P-O1P
3	E	2608	PEE	C1-O3P-P-O1P
2	E	2607	PLX	C9-C10-C11-C12
2	A	2605	PLX	C9-C10-C11-C12
2	C	2606	PLX	C9-C10-C11-C12
2	A	2602	PLX	C25-C26-C27-C28
2	E	2604	PLX	C25-C26-C27-C28
2	A	2609	PLX	C4-C3-O4-P1
2	C	2601	PLX	C4-C3-O4-P1
2	E	2602	PLX	C4-C3-O4-P1
2	C	2603	PLX	C25-C26-C27-C28
2	A	2608	PLX	C15-C16-C17-C18
2	C	2609	PLX	C15-C16-C17-C18
2	E	2601	PLX	C15-C16-C17-C18
3	C	2607	PEE	C13-C14-C15-C16
3	A	2606	PEE	C13-C14-C15-C16
3	E	2608	PEE	C13-C14-C15-C16
3	A	2606	PEE	C1-C2-C3-O3
3	C	2607	PEE	C1-C2-C3-O3
3	E	2608	PEE	C1-C2-C3-O3
2	A	2601	PLX	O8-C24-C25-C26
2	C	2602	PLX	O8-C24-C25-C26
2	E	2603	PLX	O8-C24-C25-C26
3	A	2606	PEE	C40-C41-C42-C43
2	E	2603	PLX	C19-C20-C21-C22
3	E	2608	PEE	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
2	A	2601	PLX	C19-C20-C21-C22
2	C	2602	PLX	C19-C20-C21-C22
3	C	2607	PEE	C40-C41-C42-C43
2	A	2605	PLX	C18-C19-C20-C21
2	E	2607	PLX	C18-C19-C20-C21
2	C	2606	PLX	C18-C19-C20-C21
3	A	2606	PEE	C33-C34-C35-C36
3	E	2608	PEE	C33-C34-C35-C36
3	C	2607	PEE	C33-C34-C35-C36
2	A	2603	PLX	C3-C4-C5-O8
2	C	2604	PLX	C3-C4-C5-O8
2	E	2605	PLX	C3-C4-C5-O8
2	A	2603	PLX	C7-C8-C9-C10
2	C	2604	PLX	C7-C8-C9-C10
2	E	2605	PLX	C7-C8-C9-C10
4	A	2607	P5S	C1-C2-O37-C38
4	C	2608	P5S	C1-C2-O37-C38
4	E	2609	P5S	C1-C2-O37-C38
2	A	2604	PLX	O8-C24-C25-C26
2	C	2605	PLX	O8-C24-C25-C26
2	E	2606	PLX	O8-C24-C25-C26
2	A	2601	PLX	O9-C24-C25-C26
2	A	2603	PLX	O9-C24-C25-C26
2	A	2609	PLX	O7-C6-C7-C8
2	C	2601	PLX	O7-C6-C7-C8
2	C	2602	PLX	O9-C24-C25-C26
2	C	2604	PLX	O9-C24-C25-C26
2	E	2602	PLX	O7-C6-C7-C8
2	E	2603	PLX	O9-C24-C25-C26
2	E	2605	PLX	O9-C24-C25-C26
2	C	2609	PLX	C30-C31-C32-C33
2	E	2601	PLX	C30-C31-C32-C33
2	A	2608	PLX	C30-C31-C32-C33
2	A	2601	PLX	C20-C21-C22-C23
2	C	2602	PLX	C20-C21-C22-C23
2	E	2603	PLX	C20-C21-C22-C23
2	C	2602	PLX	C27-C28-C29-C30
2	C	2609	PLX	C31-C32-C33-C34
2	E	2603	PLX	C27-C28-C29-C30
2	E	2601	PLX	C31-C32-C33-C34
2	A	2608	PLX	C31-C32-C33-C34
2	A	2601	PLX	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
2	A	2603	PLX	O9-C24-O8-C5
2	C	2604	PLX	O9-C24-O8-C5
2	E	2605	PLX	O9-C24-O8-C5
2	A	2601	PLX	C18-C19-C20-C21
2	A	2608	PLX	C4-C3-O4-P1
2	C	2609	PLX	C4-C3-O4-P1
2	E	2601	PLX	C4-C3-O4-P1
2	A	2602	PLX	C17-C18-C19-C20
2	C	2603	PLX	C17-C18-C19-C20
2	E	2604	PLX	C17-C18-C19-C20
2	C	2602	PLX	C18-C19-C20-C21
2	E	2603	PLX	C18-C19-C20-C21
3	A	2606	PEE	O2-C10-C11-C12
3	A	2606	PEE	O4-C10-C11-C12
3	C	2607	PEE	O4-C10-C11-C12
3	E	2608	PEE	O4-C10-C11-C12

There are no ring outliers.

27 monomers are involved in 403 short contacts:

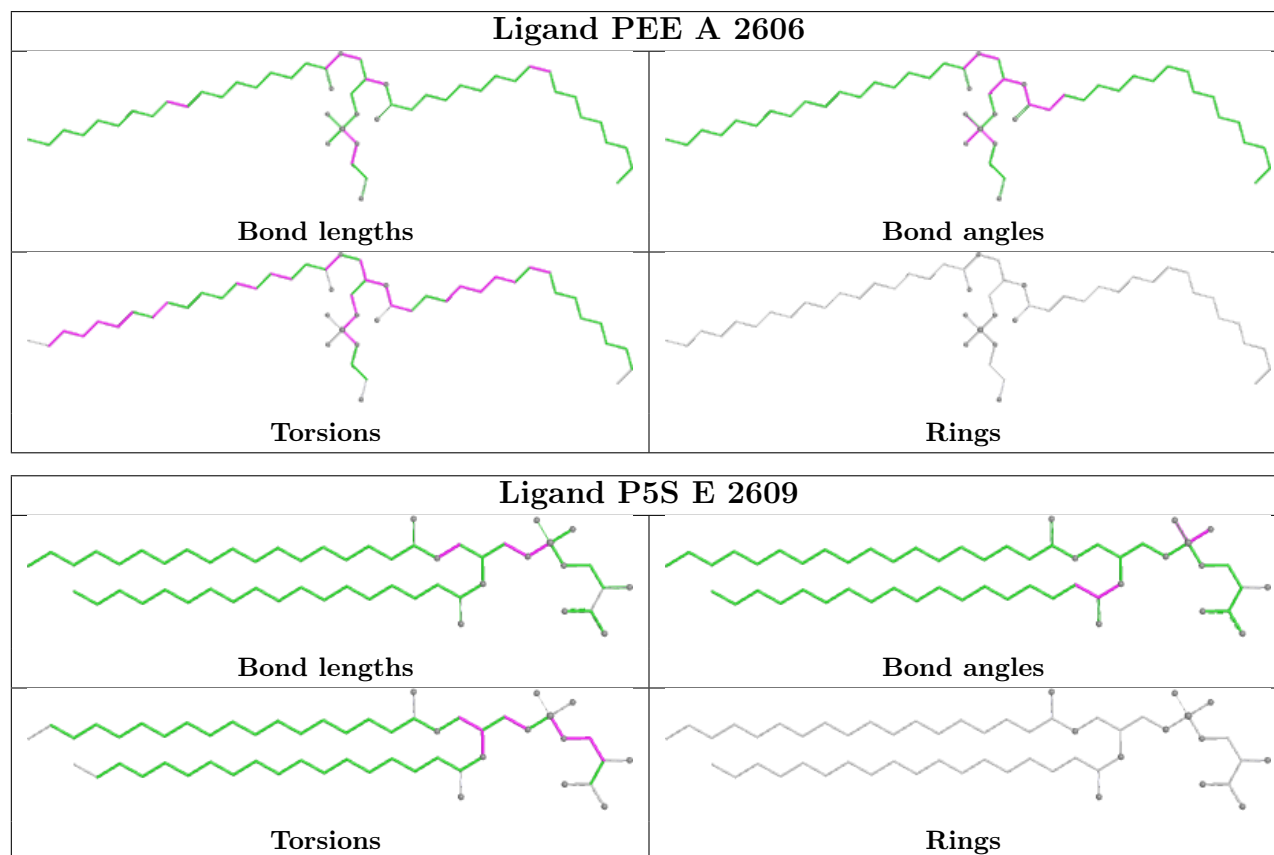
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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4	E	2609	P5S	3	0
2	A	2602	PLX	8	0
2	E	2606	PLX	6	0
2	A	2609	PLX	1	0
2	C	2605	PLX	6	0
2	C	2609	PLX	57	0
2	C	2603	PLX	7	0
2	A	2605	PLX	5	0
2	E	2601	PLX	56	0
2	E	2602	PLX	1	0
2	A	2608	PLX	55	0
4	C	2608	P5S	3	0
2	C	2602	PLX	3	0
2	C	2601	PLX	2	0
3	E	2608	PEE	41	0
2	A	2601	PLX	3	0
3	C	2607	PEE	42	0
2	E	2607	PLX	5	0
4	A	2607	P5S	3	0
2	A	2604	PLX	6	0

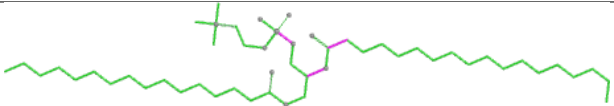
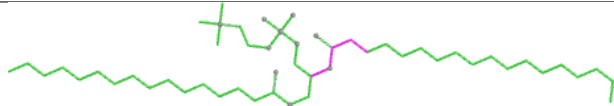
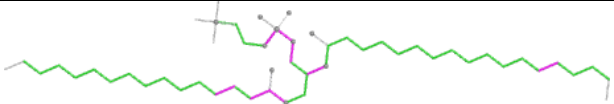
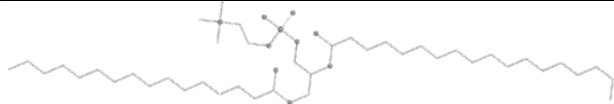
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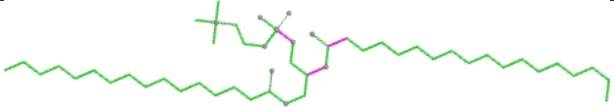
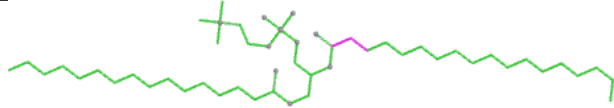
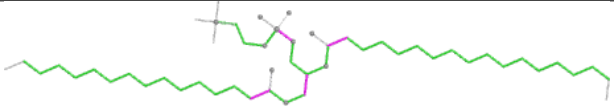
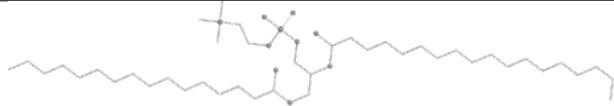
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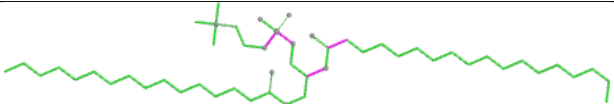
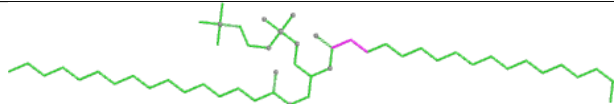
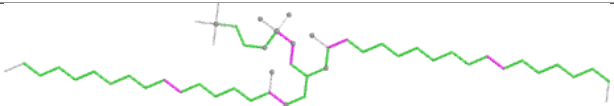
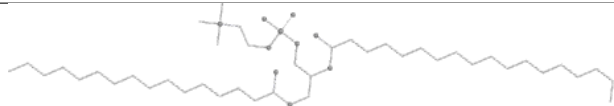
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2603	PLX	13	0
2	C	2606	PLX	5	0
2	E	2604	PLX	7	0
2	E	2605	PLX	15	0
2	C	2604	PLX	15	0
2	E	2603	PLX	3	0

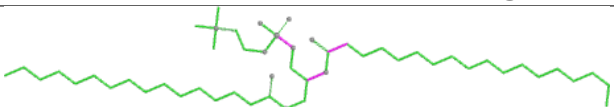
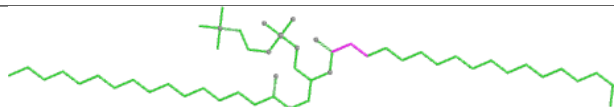
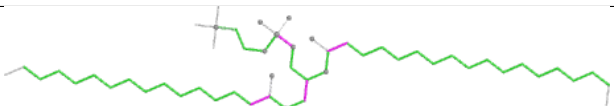
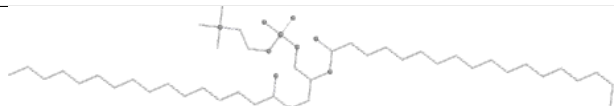
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

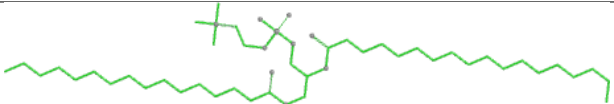
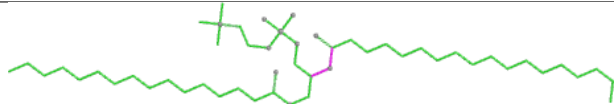
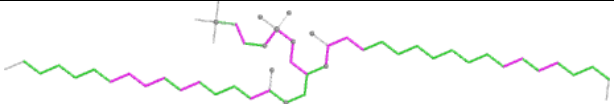
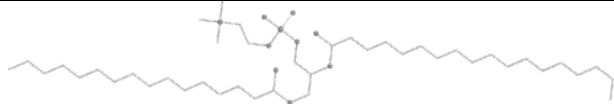


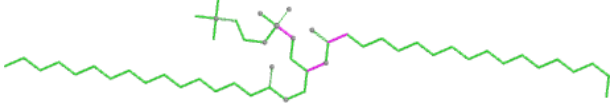
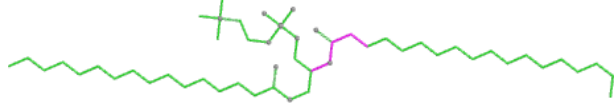
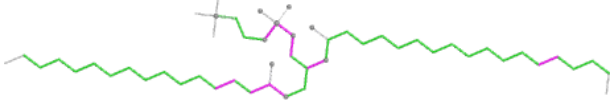
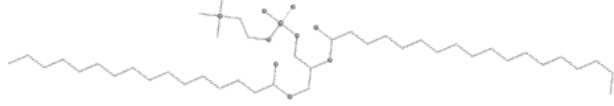
Ligand PLX A 2602	
	
Bond lengths	Bond angles
	
Torsions	Rings

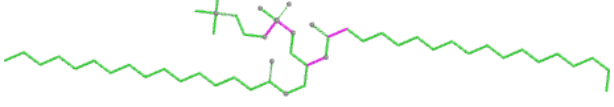
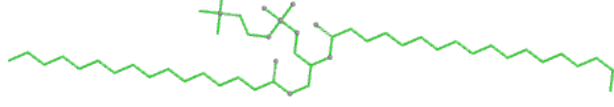
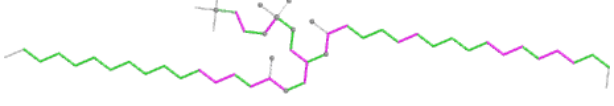
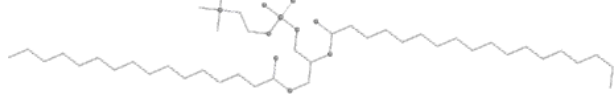
Ligand PLX E 2606	
	
Bond lengths	Bond angles
	
Torsions	Rings

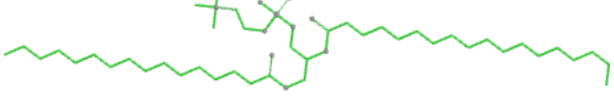
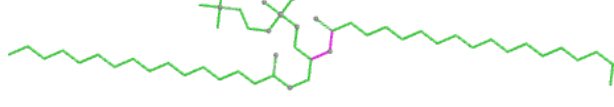
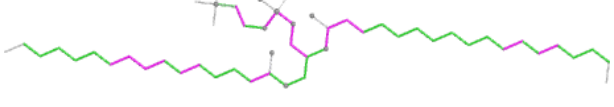
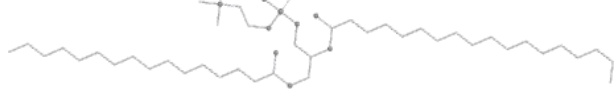
Ligand PLX A 2609	
	
Bond lengths	Bond angles
	
Torsions	Rings

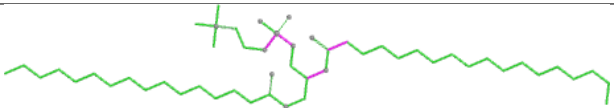
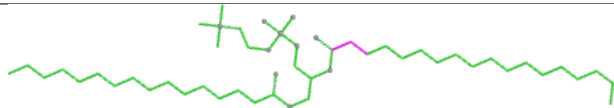
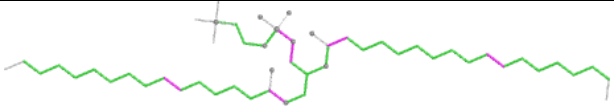
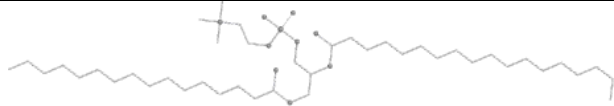
Ligand PLX C 2605	
	
Bond lengths	Bond angles
	
Torsions	Rings

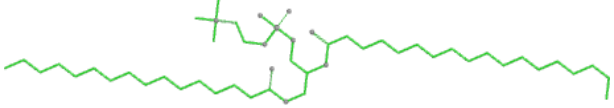
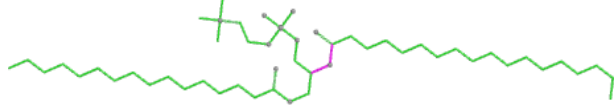
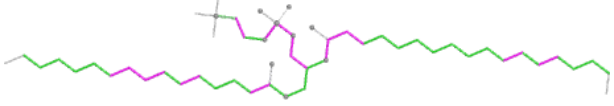
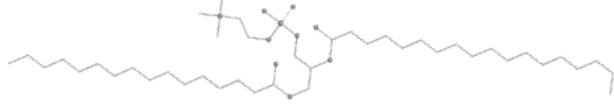
Ligand PLX C 2609	
	
Bond lengths	Bond angles
	
Torsions	Rings

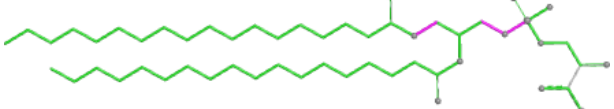
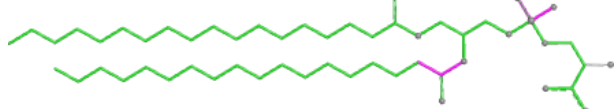
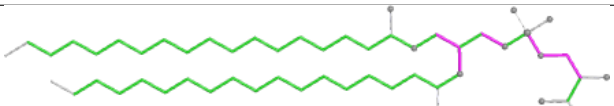
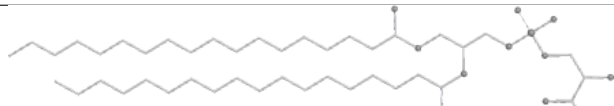
Ligand PLX C 2603	
	
Bond lengths	Bond angles
	
Torsions	Rings

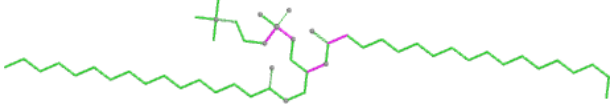
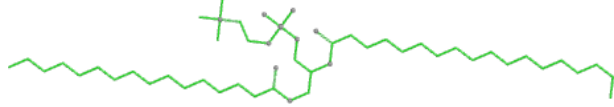
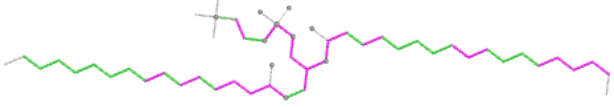
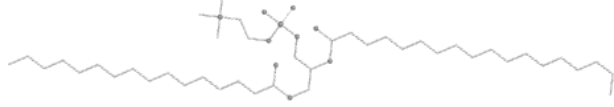
Ligand PLX A 2605	
	
Bond lengths	Bond angles
	
Torsions	Rings

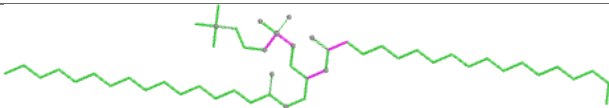
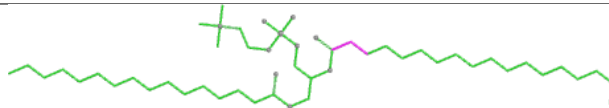
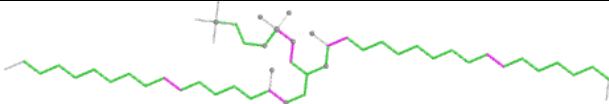
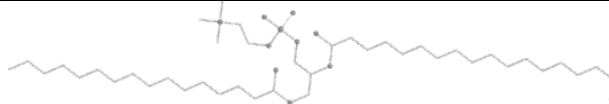
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Bond lengths	Bond angles
	
Torsions	Rings

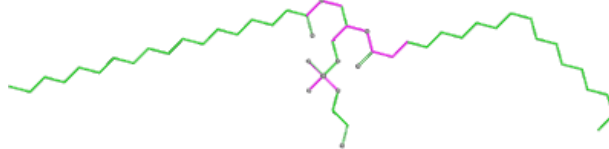
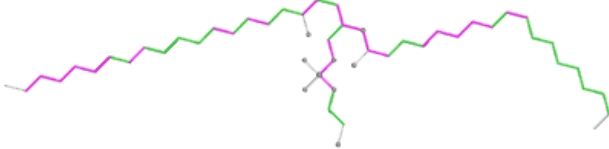
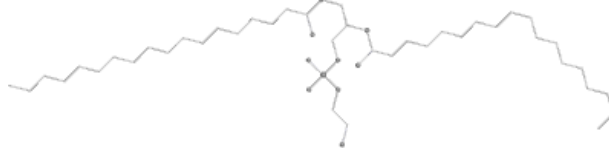
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Bond lengths	Bond angles
	
Torsions	Rings

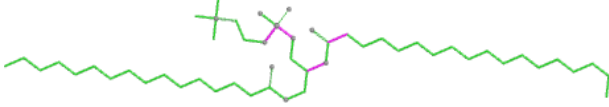
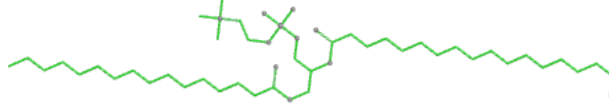
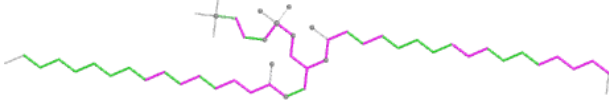
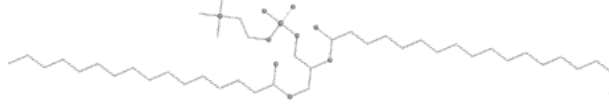
Ligand PLX A 2608	
	
Bond lengths	Bond angles
	
Torsions	Rings

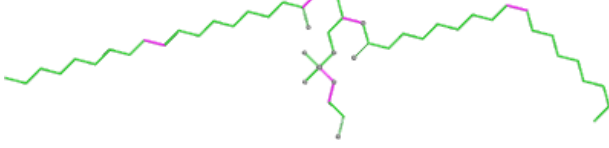
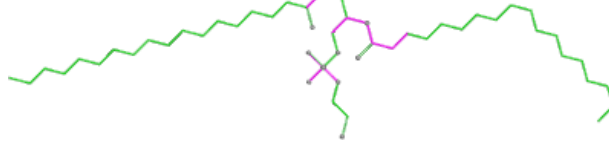
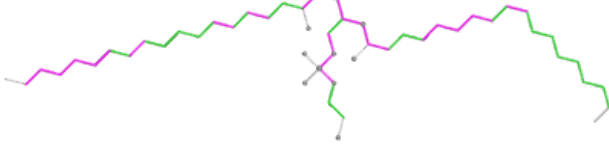
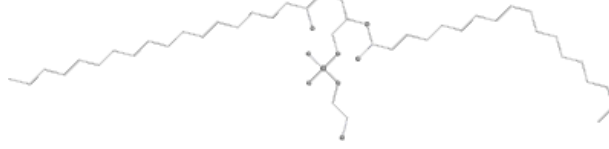
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Bond lengths	Bond angles
	
Torsions	Rings

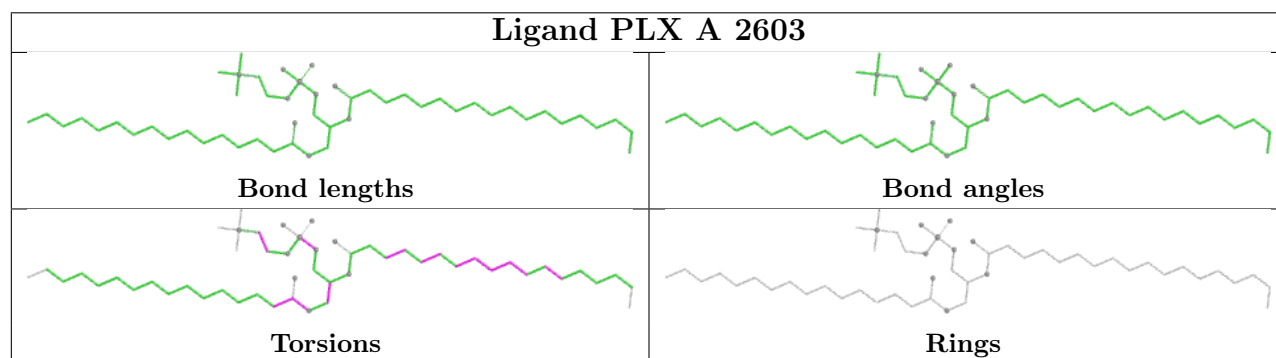
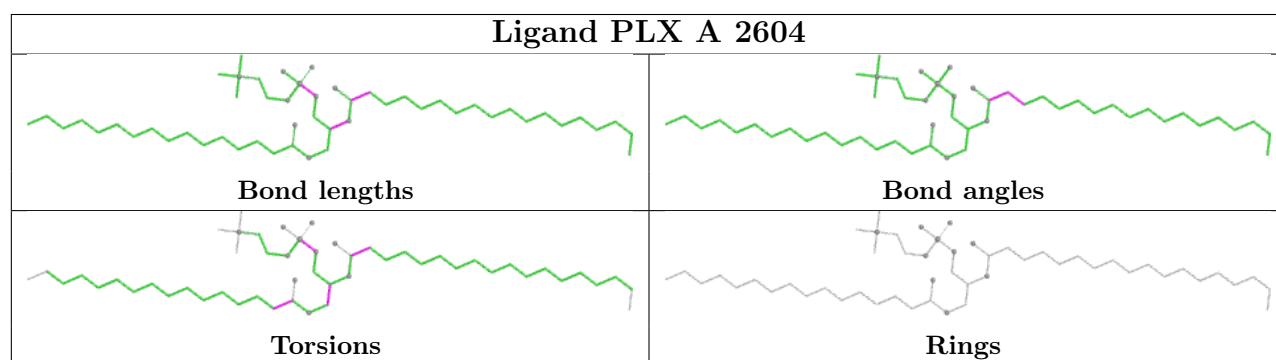
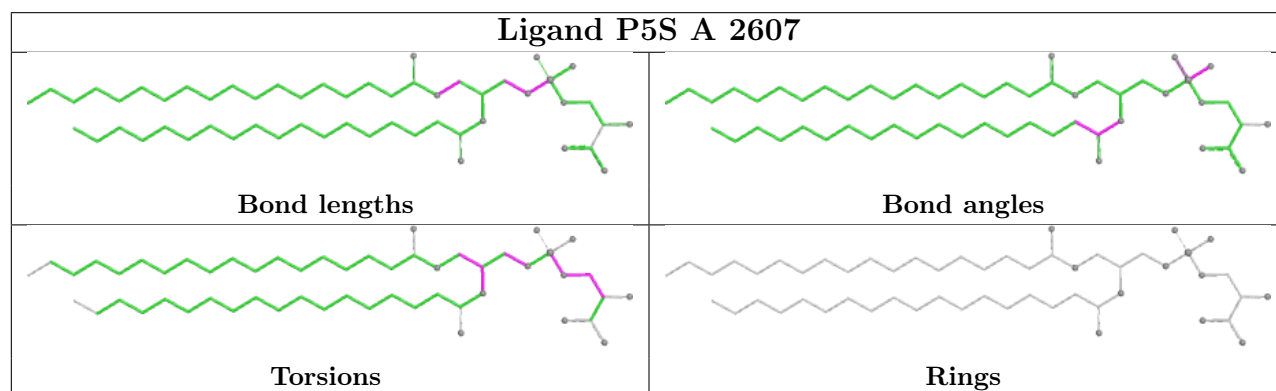
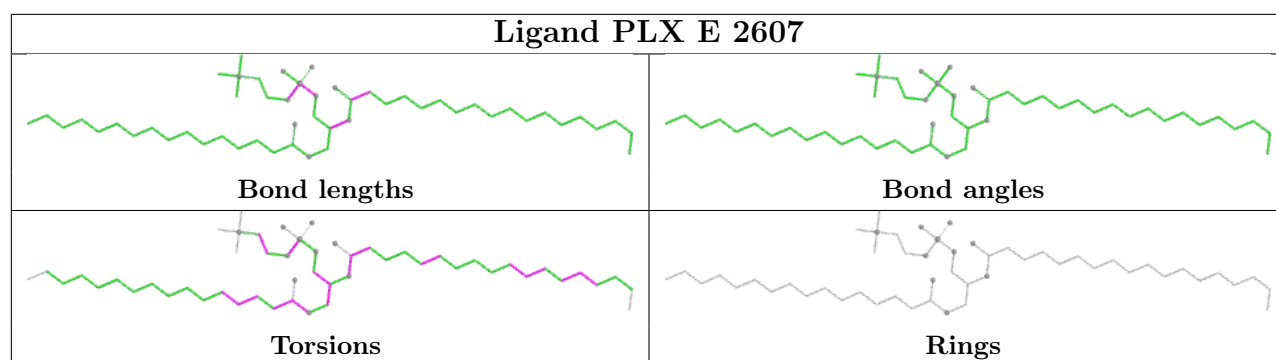
Ligand PLX C 2602	
	
Bond lengths	Bond angles
	
Torsions	Rings

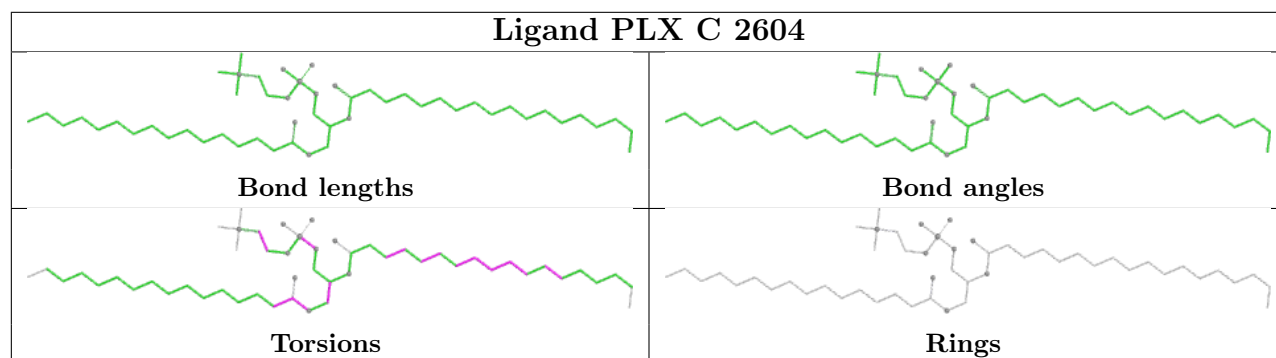
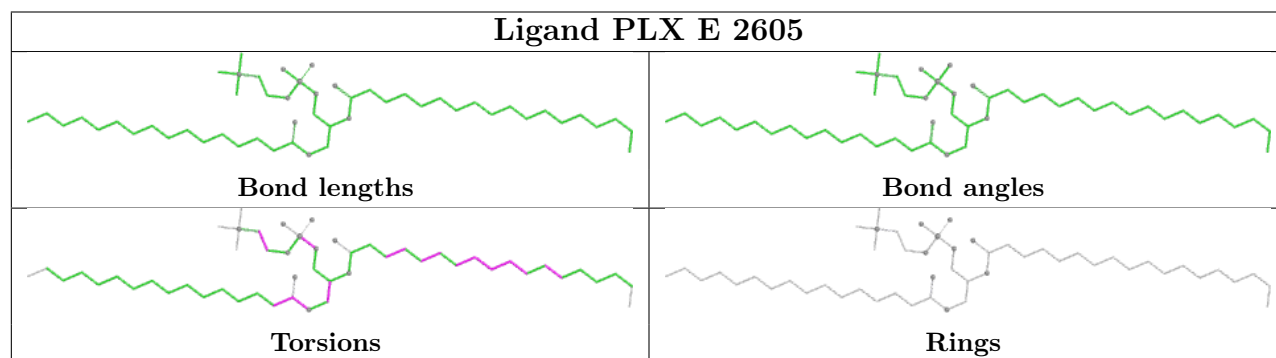
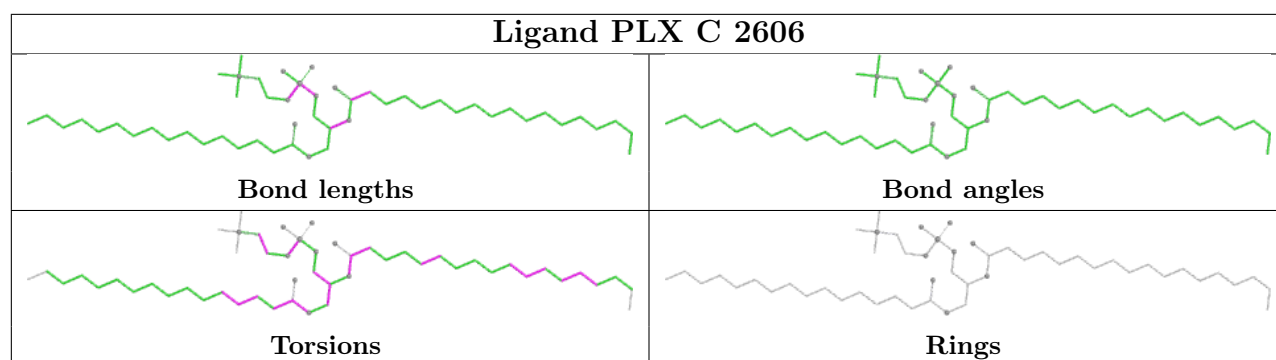
Ligand PLX C 2601	
 Bond lengths	 Bond angles
 Torsions	 Rings

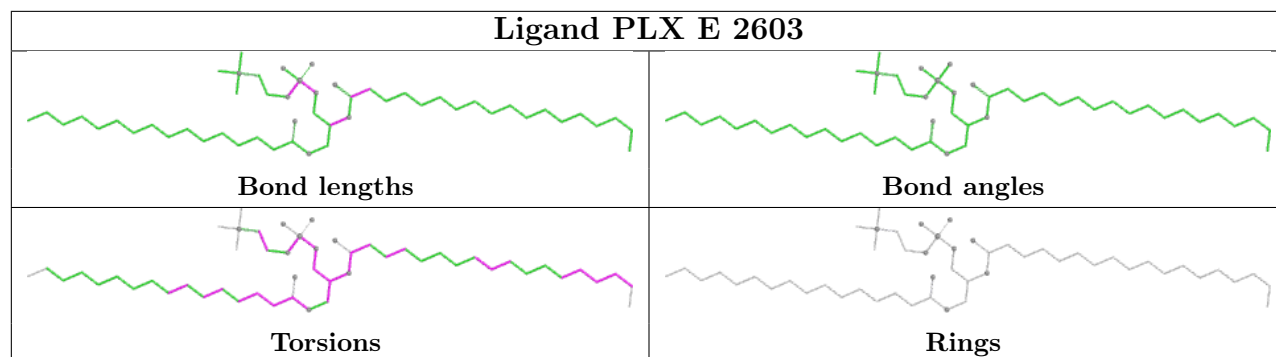
Ligand PEE E 2608	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PLX A 2601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PEE C 2607	
 Bond lengths	 Bond angles
 Torsions	 Rings







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.

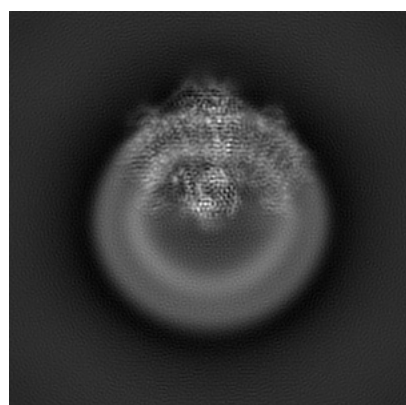
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32592. These allow visual inspection of the internal detail of the map and identification of artifacts.

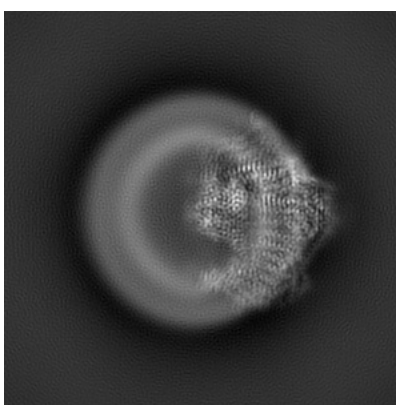
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

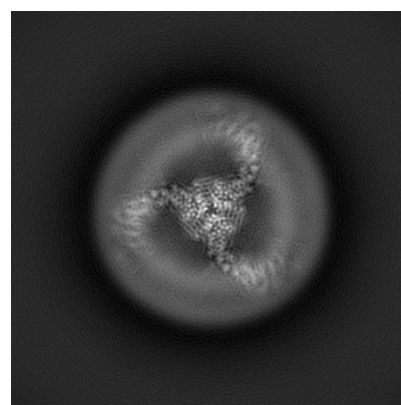
6.1.1 Primary map



X



Y

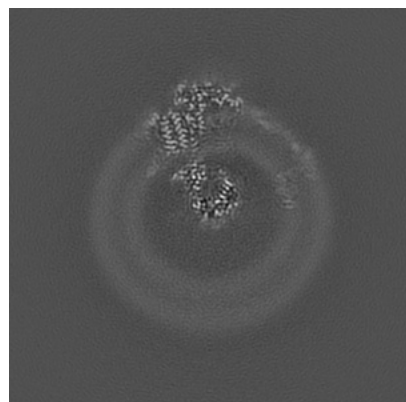


Z

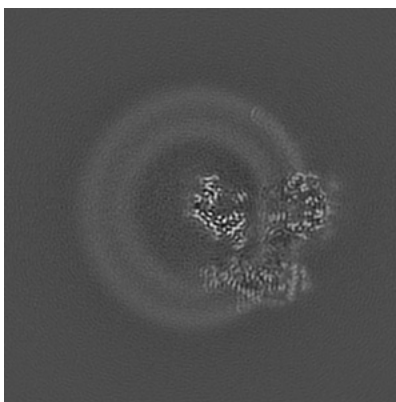
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

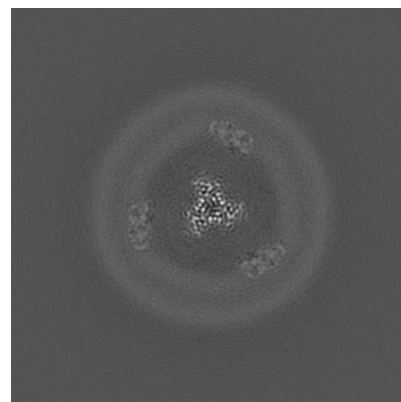
6.2.1 Primary map



X Index: 180



Y Index: 180

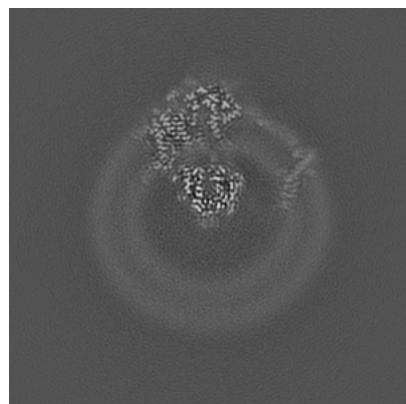


Z Index: 180

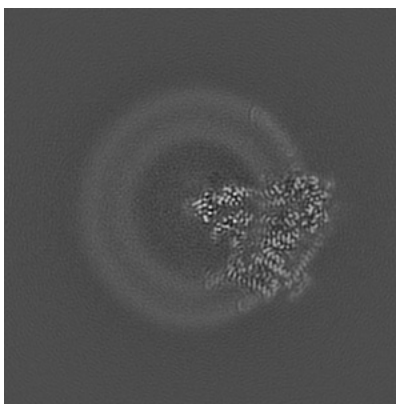
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

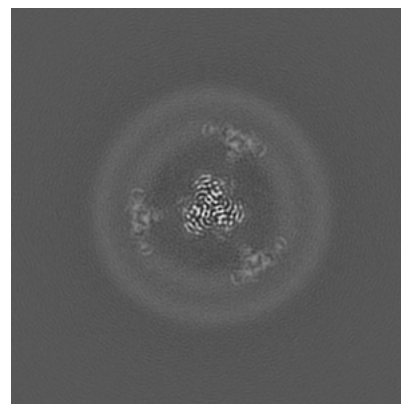
6.3.1 Primary map



X Index: 187



Y Index: 187

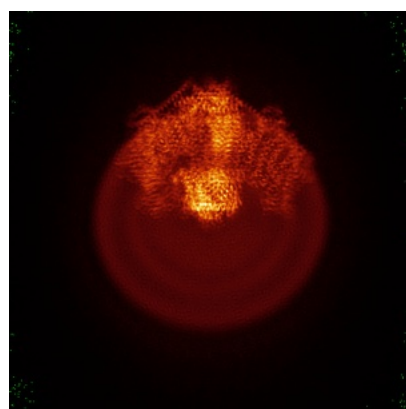


Z Index: 186

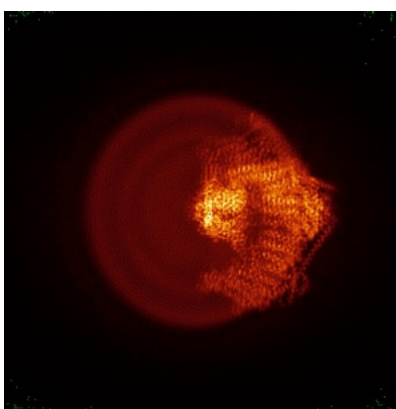
The images above show the largest variance slices of the map in three orthogonal directions.

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

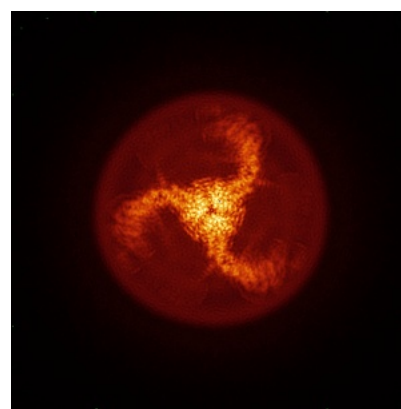
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

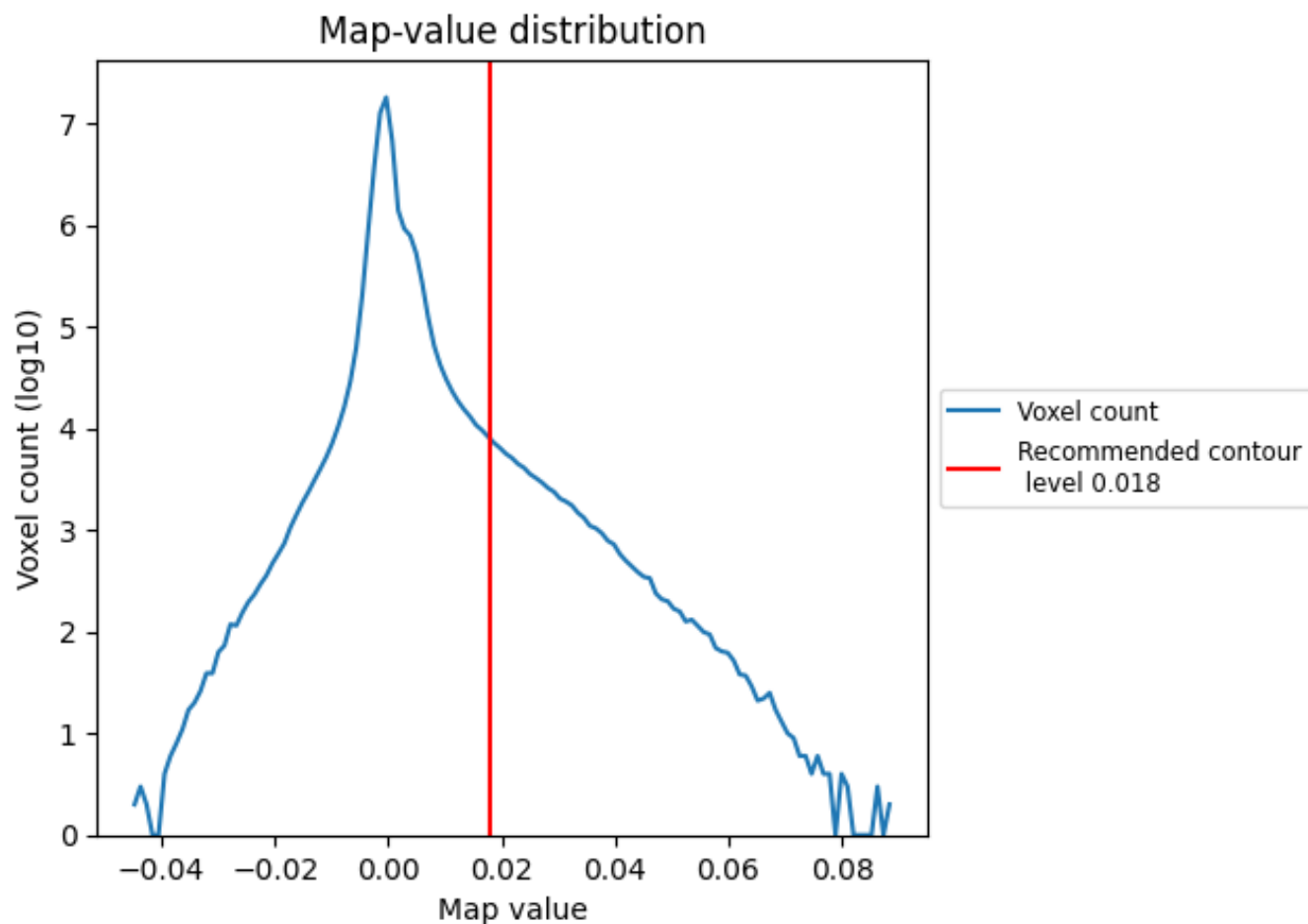
6.6 Mask visualisation

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

7 Map analysis [i](#)

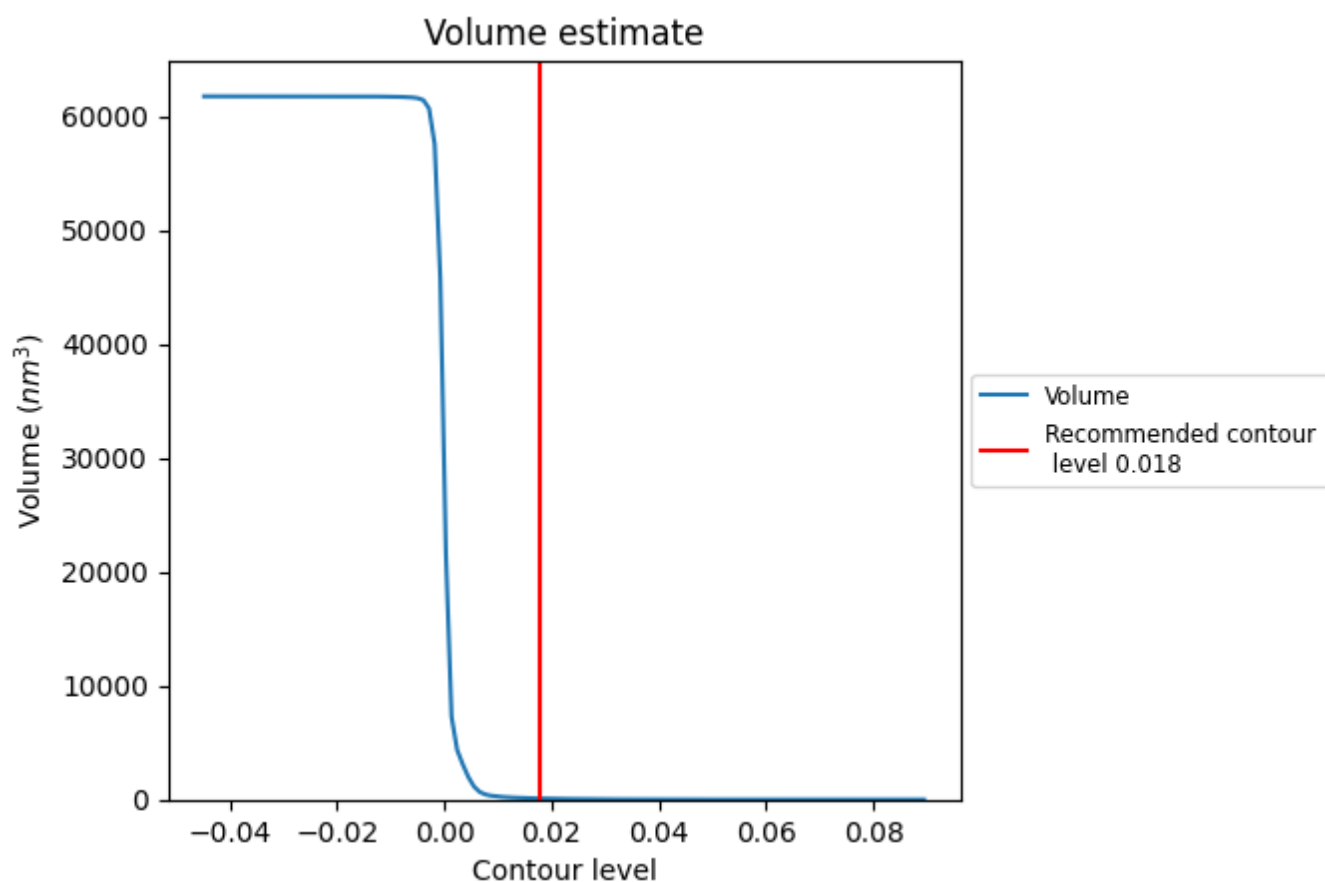
This section contains the results of statistical analysis of the map.

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.

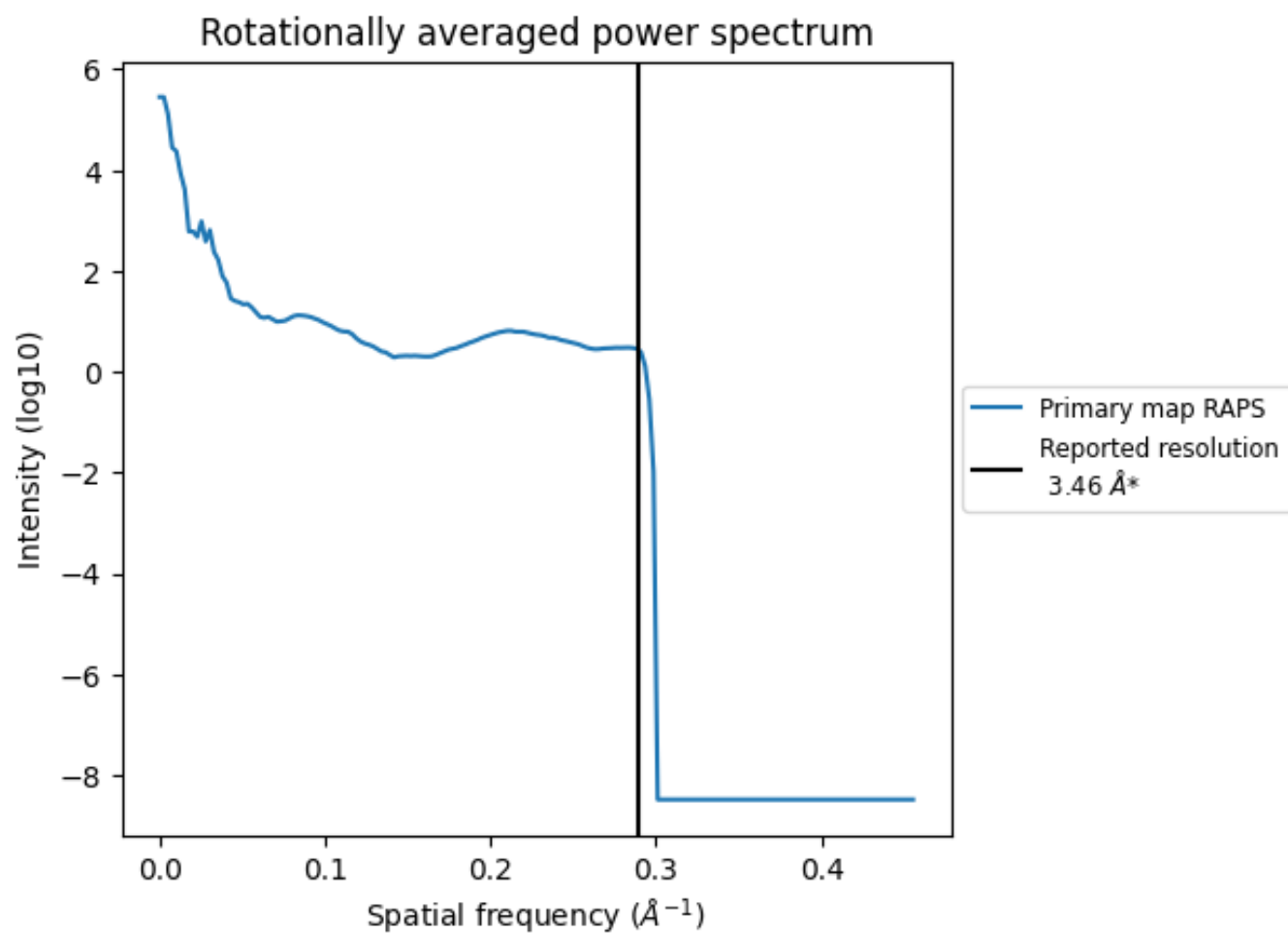
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 93 nm³; this corresponds to an approximate mass of 84 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



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

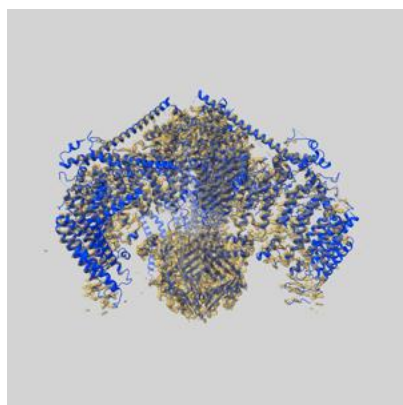
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

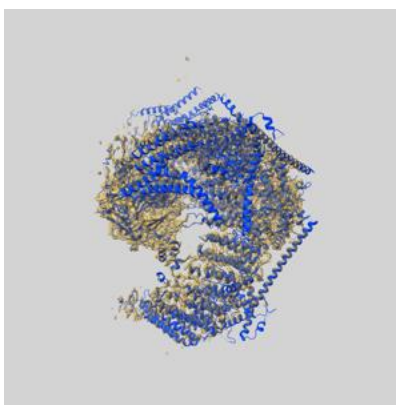
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32592 and PDB model 7WLT. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

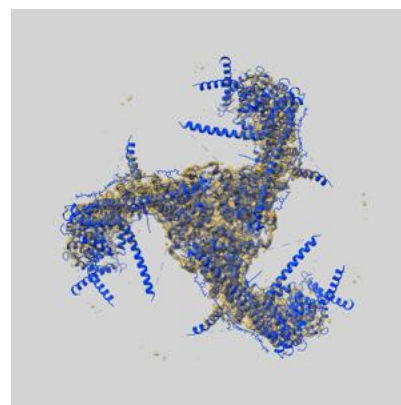
9.1 Map-model overlay [i](#)



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.018 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](#)

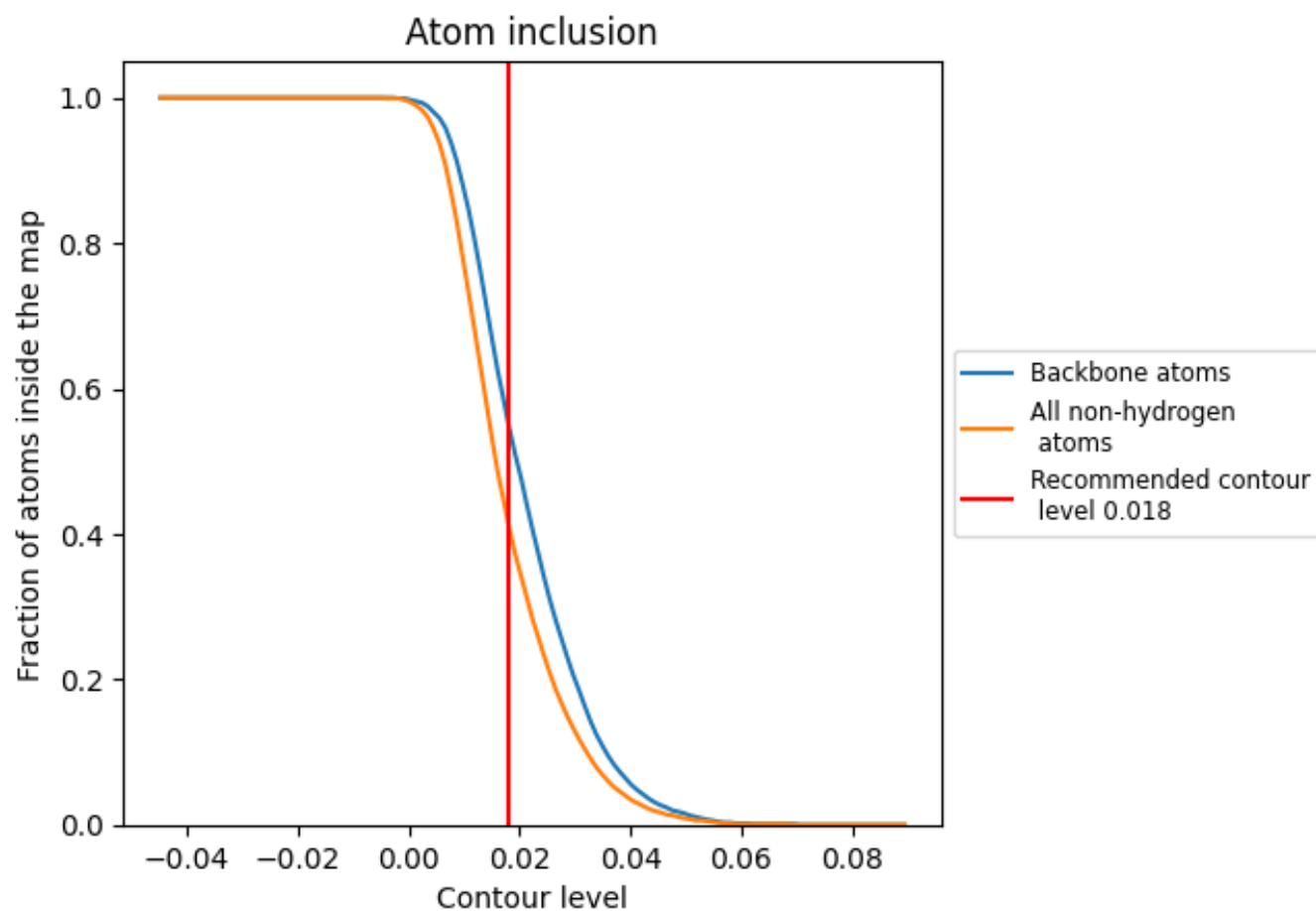


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 55% of all backbone atoms, 41% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4130	0.4620
A	0.4130	0.4620
C	0.4130	0.4620
E	0.4150	0.4620

