Full wwPDB EM Validation Report ⓘ

Nov 7, 2023 – 10:15 AM JST

PDB ID	:	5GJV
EMDB ID	:	EMD-9513
Title	:	Structure of the mammalian voltage-gated calcium channel Cav1.1 complex at near atomic resolution
Authors	:	Wu, J.P.; Yan, Z.; Li, Z.Q.; Zhou, Q.; Yan, N.
Deposited on	:	2016-07-02
Resolution	:	3.60 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:

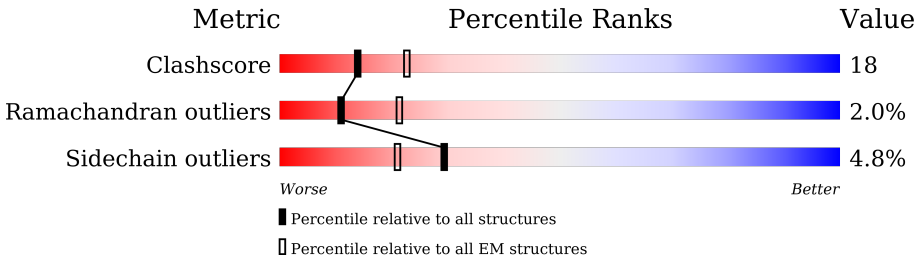
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	1873	27% 48% 17% • 32%
2	B	106	94% 88% 5% • 6%
3	C	199	89% 82% 7% 11%
4	E	222	52% 62% 9% • • 25%
5	F	1106	12% 55% 24% 6% • 15%
6	D	2	100% 50% 50%
6	G	2	100% 100%
6	J	2	50% 50% 50%

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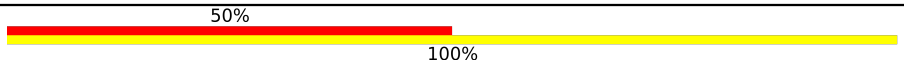
Mol	Chain	Length	Quality of chain
6	K	2	
7	H	3	
7	I	3	
8	L	3	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 21904 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 Voltage-dependent L-type calcium channel subunit alpha-1S.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1276	Total	C	N	O	S	4	0
			10183	6699	1673	1742	69		

- Molecule 2 is a protein called Voltage-dependent L-type calcium channel subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	100	Total	C	N	O	S	0	0
			710	455	125	129	1		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	69	SER	-	expression tag	UNP P19517
B	70	LEU	-	expression tag	UNP P19517
B	71	GLU	-	expression tag	UNP P19517
B	72	VAL	-	expression tag	UNP P19517
B	73	LEU	-	expression tag	UNP P19517
B	74	PHE	-	expression tag	UNP P19517
B	75	GLN	-	expression tag	UNP P19517
B	76	GLY	-	expression tag	UNP P19517
B	77	PRO	-	expression tag	UNP P19517
B	78	HIS	-	expression tag	UNP P19517
B	79	MET	-	expression tag	UNP P19517

- Molecule 3 is a protein called Voltage-dependent L-type calcium channel subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	178	Total	C	N	O	S	0	0
			1367	876	232	254	5		

- Molecule 4 is a protein called Voltage-dependent calcium channel gamma-1 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	166	Total	C	N	O	S	0	0
			1304	860	213	213	18		

- Molecule 5 is a protein called Voltage-dependent calcium channel subunit alpha-2/delta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	942	Total	C	N	O	S	1	0
			7567	4809	1277	1451	30		

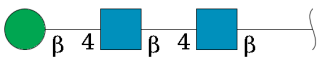
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	1075	ETA	GLY	conflict	UNP P13806

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	D	2	Total	C	N	O	0	0
			28	16	2	10		
6	G	2	Total	C	N	O	0	0
			28	16	2	10		
6	J	2	Total	C	N	O	0	0
			28	16	2	10		
6	K	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
7	H	3	Total	C	N	O	0	0
			39	22	2	15		

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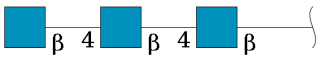
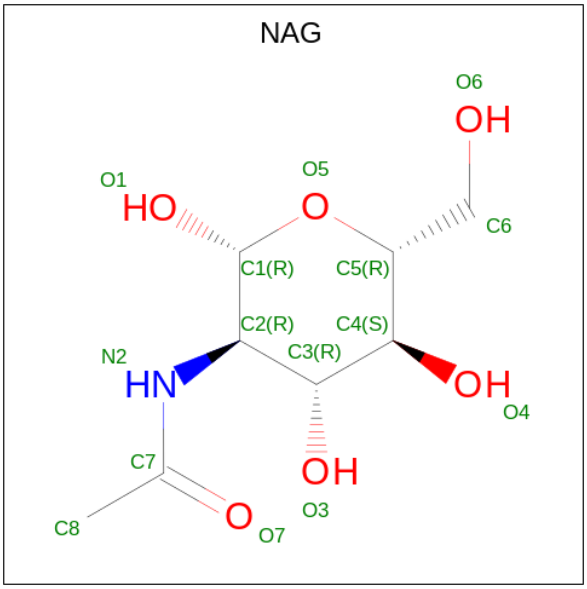
Mol	Chain	Residues	Atoms				AltConf	Trace
7	I	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 8 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
8	L	3	Total	C	N	O	0	0
			42	24	3	15		

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
9	A	1	Total	C	N	O	0
			14	8	1	5	
9	F	1	Total	C	N	O	0
			14	8	1	5	
9	F	1	Total	C	N	O	0
			14	8	1	5	
9	F	1	Total	C	N	O	0
			14	8	1	5	

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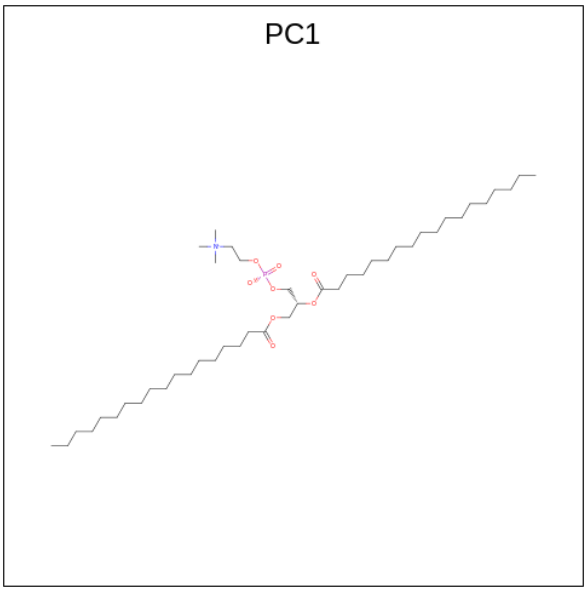
Mol	Chain	Residues	Atoms	AltConf
9	F	1	Total C N O 14 8 1 5	0
9	F	1	Total C N O 14 8 1 5	0
9	F	1	Total C N O 14 8 1 5	0
9	F	1	Total C N O 14 8 1 5	0

- Molecule 10 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms	AltConf
10	A	1	Total C N O P 44 34 1 8 1	0
10	A	1	Total C N O P 54 44 1 8 1	0
10	A	1	Total C N O P 42 32 1 8 1	0
10	A	1	Total C N O P 38 28 1 8 1	0
10	A	1	Total C 18 18	0
10	A	1	Total C 12 12	0
10	A	1	Total C 12 12	0

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Mol	Chain	Residues	Atoms	AltConf
10	A	1	Total C 15 15	0
10	A	1	Total C 18 18	0
10	A	1	Total C N O P 48 38 1 8 1	0
10	A	1	Total C N O P 45 35 1 8 1	0
10	A	1	Total C 18 18	0
10	A	1	Total C 14 14	0
10	A	1	Total C N O P 48 38 1 8 1	0

- Molecule 11 is CALCIUM ION (three-letter code: CA) (formula: Ca).

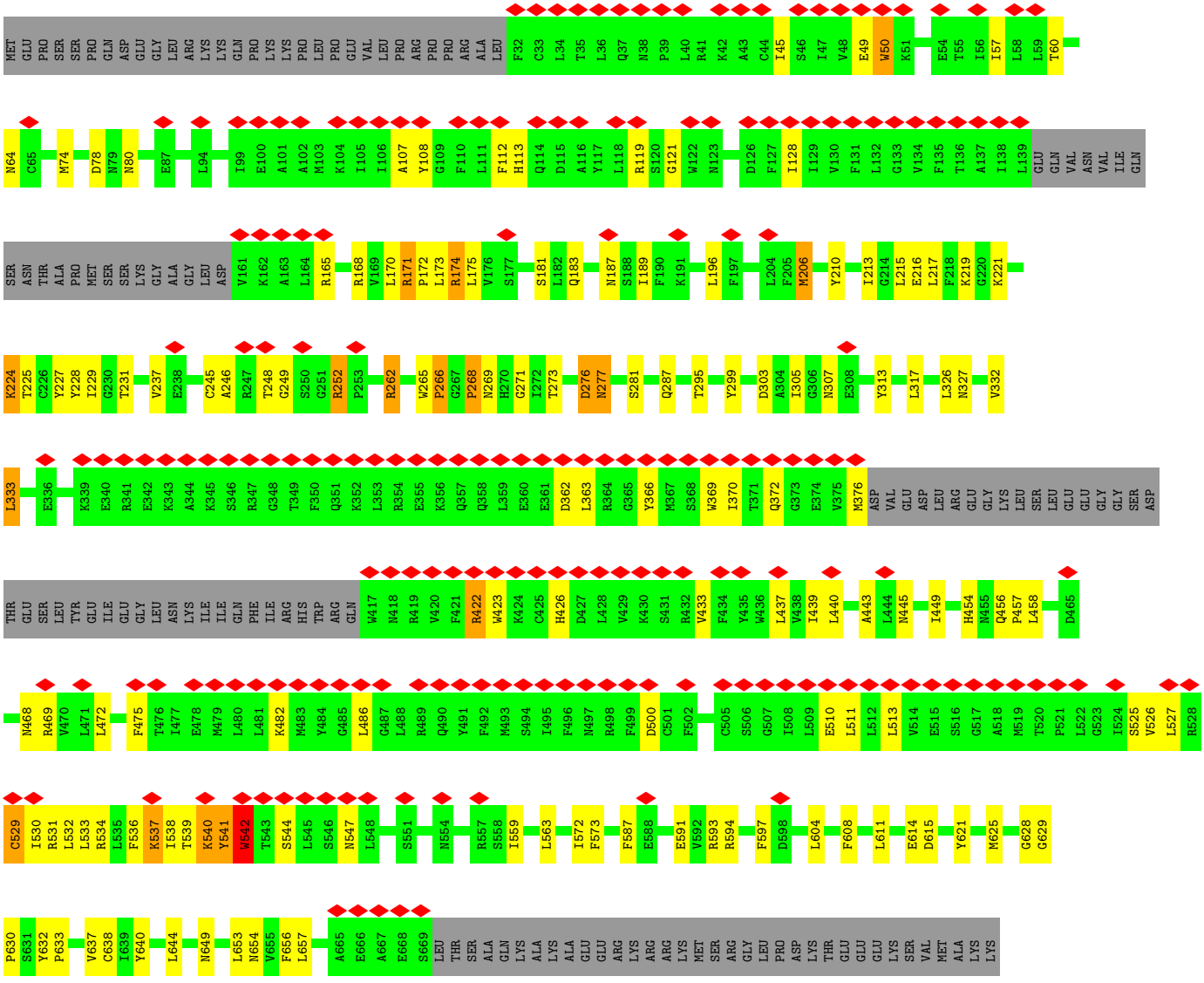
Mol	Chain	Residues	Atoms	AltConf
11	A	2	Total Ca 2 2	0
11	F	1	Total Ca 1 1	0

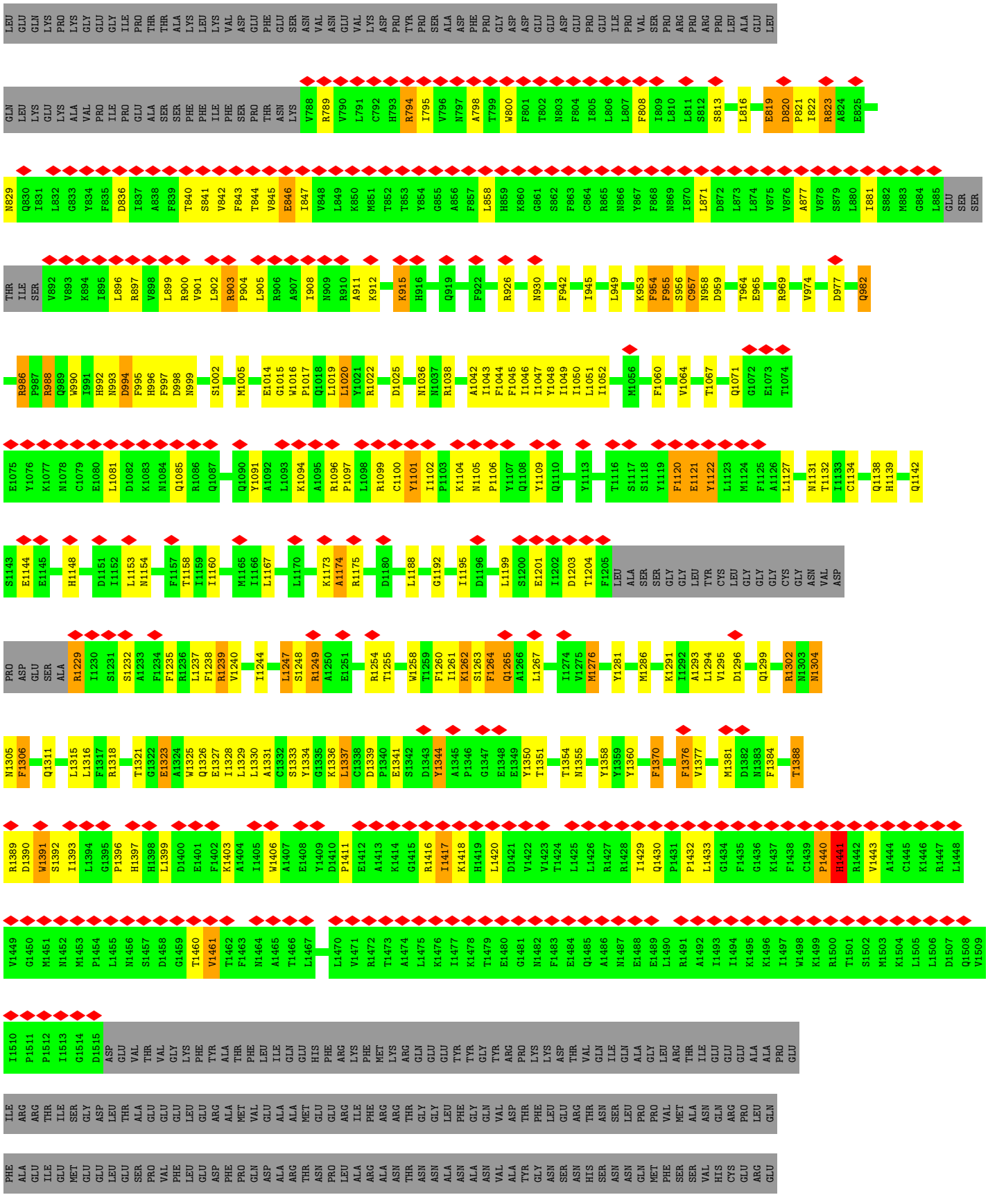
3 Residue-property plots (i)

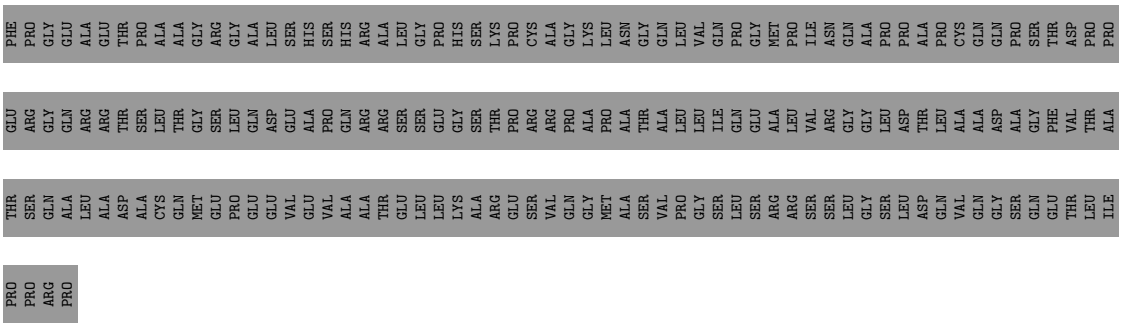
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Voltage-dependent L-type calcium channel subunit alpha-1S

Chain A:

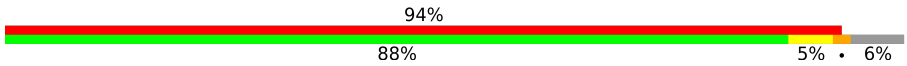


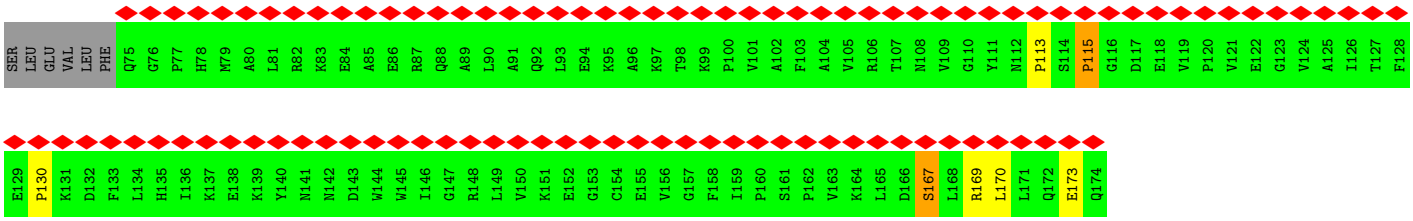

LEU GLU GLN LYS PRO LYS GLY GLU GLY ILE PRO THR THR ALA LYS LEU LYS VAL ASP GLU PHE GLU SER ASN VAL ASN GLU VAL LYS ASP PRO TYR PRO SER ALA ASP PHE PRO GLY ASP ASP GLU GLU ASP GLU PRO GLU ILE PRO VAL SER PRO ARG PRO ARG PRO LEU ALA GLU LEU
GLN LEU LYS GLU LYS ALA VAL PRO ILE PRO GLU ALA SER SER PHE PHE ILE PHE SER PRO THR ASN LYS V788 R789 V790 L791 C792 H793 R794 I795 V796 N797 A798 T799 W800 F801 T802 N803 F804 I805 L806 L807 F808 I809 L810 L811 S812 S813 L816 E819 D820 P821 I822 R823 A824 E825
N829 Q830 I831 L832 G833 Y834 F835 D836 I837 A838 F839 T840 S841 V842 F843 T844 V845 E846 I847 V848 L849 K850 M851 T852 T853 Y854 G855 A856 F857 L858 H859 K860 G861 S862 F863 C864 R865 N866 Y867 F868 N869 I870 L871 D872 L873 L874 V875 V876 A877 V878 S879 L880 I881 S882 M883 G884 L885 GLU SER SER
THR ILE SER V892 V893 K894 I895 L896 R897 V898 L899 R900 V901 L902 R903 P904 L905 R906 A907 I908 N909 R910 A911 K912 K915 H916 Q919 F922 R926 N930 F942 I945 L949 K953 F954 F955 S956 C957 N958 D959 T964 E965 R969 V974 D977 Q982
R986 P987 R988 Q989 W990 I991 H992 N993 D994 F995 H996 F997 D998 N999 S1002 M1005 E1014 G1015 W1016 P1017 Q1018 L1019 L1020 Y1021 R1022 D1025 N1036 N1037 R1038 A1042 I1043 F1044 F1045 I1046 I1047 Y1048 I1049 I1050 L1051 I1052 M1056 F1060 V1064 T1067 Q1071 G1072 E1073 T1074
E1075 Y1076 K1077 N1078 C1079 E1080 L1081 D1082 K1083 N1084 Q1085 R1086 Q1087 Q1090 Y1091 A1092 L1093 K1094 A1095 R1096 P1097 L1098 R1099 C1100 Y1101 I1102 P1103 K1104 N1105 P1106 Y1107 Q1108 Y1109 Q1110 Y1113 T1116 S1117 S1118 Y1119 F1120 E1121 Y1122 L1123 M1124 F1125 A1126 L1127 N1131 T1132 I1133 C1134 Q1138 H1139 Q1142
S1143 E1144 E1145 H1148 D1151 I1152 L1153 N1154 F1157 T1158 I1159 I1160 M1165 I1166 L1167 L1170 K1173 A1174 R1175 D1180 L1188 G1192 I1195 D1196 L1199 S1200 E1201 I1202 D1203 T1204 F1205 LEU ALA SER SER GLY GLY LEU TYR CYS LEU GLY GLY GLY CYS GLY ASN VAL ASP
PRO ASP GLU SER ALA R1229 T1230 S1231 S1232 A1233 F1234 F1235 R1236 L1237 F1238 R1239 V1240 I1244 L1247 S1248 R1249 A1250 E1251 R1254 T1255 W1258 T1259 F1260 I1261 K1262 S1263 F1264 Q1265 A1266 L1267 I1274 V1275 M1276 Y1281 M1286 K1291 I1292 A1293 L1294 V1295 D1296 Q1299 R1302 N1303 N1304
N1305 F1306 Q1311 L1315 L1316 F1317 R1318 T1321 G1322 E1323 A1324 W1325 Q1326 E1327 I1328 L1329 L1330 A1331 C1332 S1333 Y1334 G1335 K1336 L1337 C1338 D1339 P1340 E1341 S1342 D1343 Y1344 A1345 P1346 G1347 E1348 E1349 Y1350 T1351 T1354 N1355 Y1358 Y1359 Y1360 F1370 F1376 V1377 M1381 D1382 N1383 F1384 T1388
R1389 D1390 W1391 S1392 I1393 L1394 G1395 P1396 H1397 H1398 L1399 D1400 E1401 F1402 K1403 A1404 I1405 W1406 A1407 E1408 Y1409 D1410 P1411 E1412 A1413 K1414 G1415 R1416 I1417 K1418 H1419 L1420 D1421 V1422 V1423 T1424 L1425 L1426 R1427 R1428 I1429 Q1430 P1431 P1432 L1433 G1434 F1435 G1436 K1437 F1438 C1439 P1440 H1441 R1442 V1443 A1444 C1445 K1446 R1447 L1448
V1449 G1450 M1451 N1452 M1453 P1454 L1455 N1456 S1457 D1458 G1459 T1460 V1461 T1462 F1463 N1464 A1465 T1466 L1467 L1470 V1471 R1472 T1473 A1474 L1475 K1476 I1477 K1478 T1479 E1480 G1481 N1482 F1483 E1484 Q1485 A1486 N1487 E1488 E1489 L1490 R1491 A1492 I1493 I1494 K1495 K1496 I1497 W1498 K1499 R1500 T1501 S1502 M1503 K1504 L1505 L1506 D1507 Q1508 V1509
I1510 P1511 P1512 I1513 G1514 D1515 ASP GLU VAL VAL THR VAL GLY LYS PHE TYR ALA THR PHE LEU ILE GLN GLU HIS PHE ARG LYS PHE MET LYS ARG GLN GLU GLU TYR TYR GLY TYR ARG PRO LYS LYS ASP THR VAL GLN ILE GLN ALA GLY LEU ARG THR ILE GLU GLU GLU ALA ALA PRO
ILE ARG ARG THR ILE SER GLY ASP LEU THR ALA GLU GLU GLU LEU GLU ARG ALA MET VAL GLU ALA ALA MET GLU GLU ARG ILE PHE ARG ARG THR GLY GLY LEU PHE GLY GLN VAL ASP THR PHE LEU GLU SER ASN LEU PRO VAL MET PHE SER VAL HIS CYS GLU ARG GLU
PHE ALA GLU ILE GLU MET GLU GLU LEU GLU SER PRO VAL PHE LEU GLU ASP PHE PRO GLN ASP ALA ALA ARG THR ASN PRO LEU ALA ARG ALA ASN THR ASN ASN ALA ALA ASN ALA ALA VAL ALA TYR GLY ASN SER ASN HIS SER ASN ASN GLN MET PHE SER VAL HIS CYS GLU ARG GLU



• Molecule 2: Voltage-dependent L-type calcium channel subunit beta-1

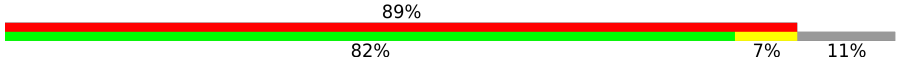
Chain B:

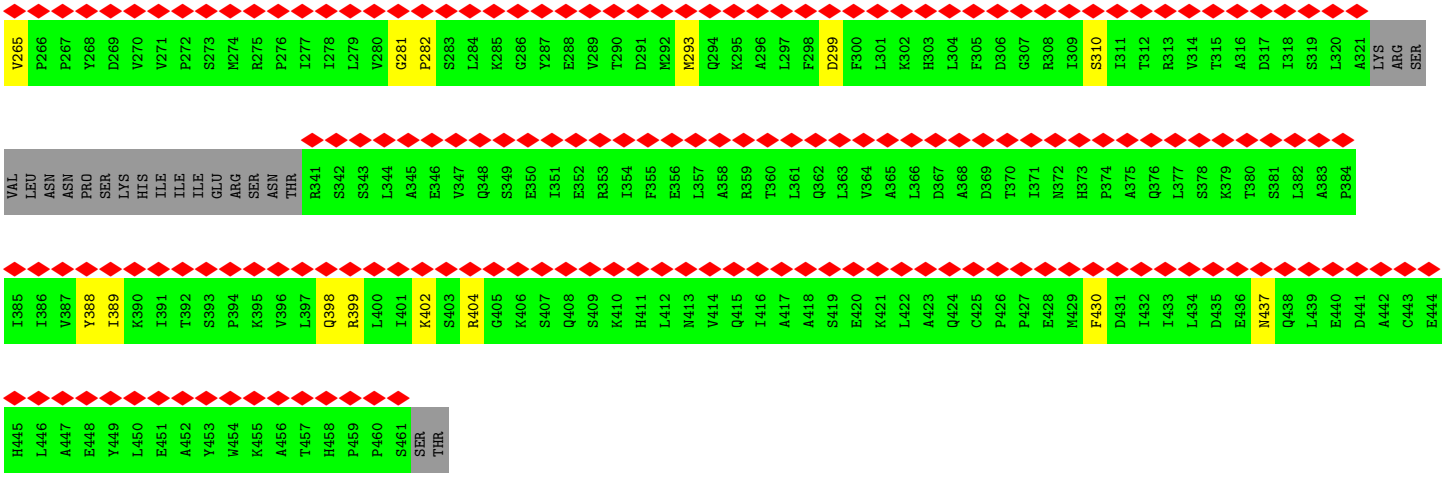




• Molecule 3: Voltage-dependent L-type calcium channel subunit beta-1

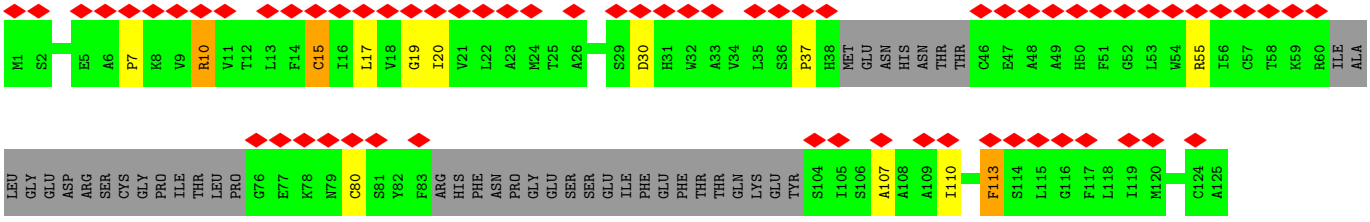
Chain C:

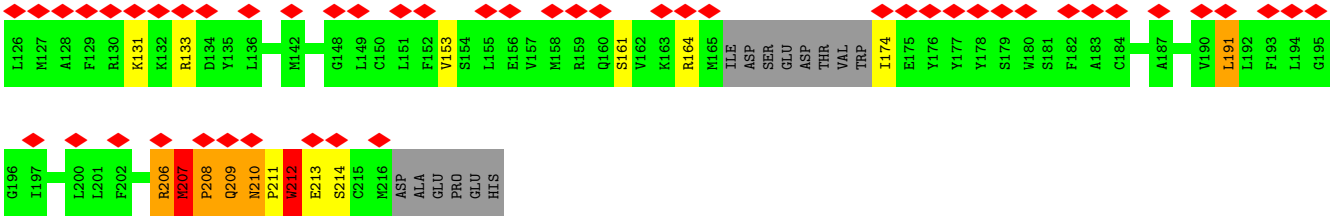




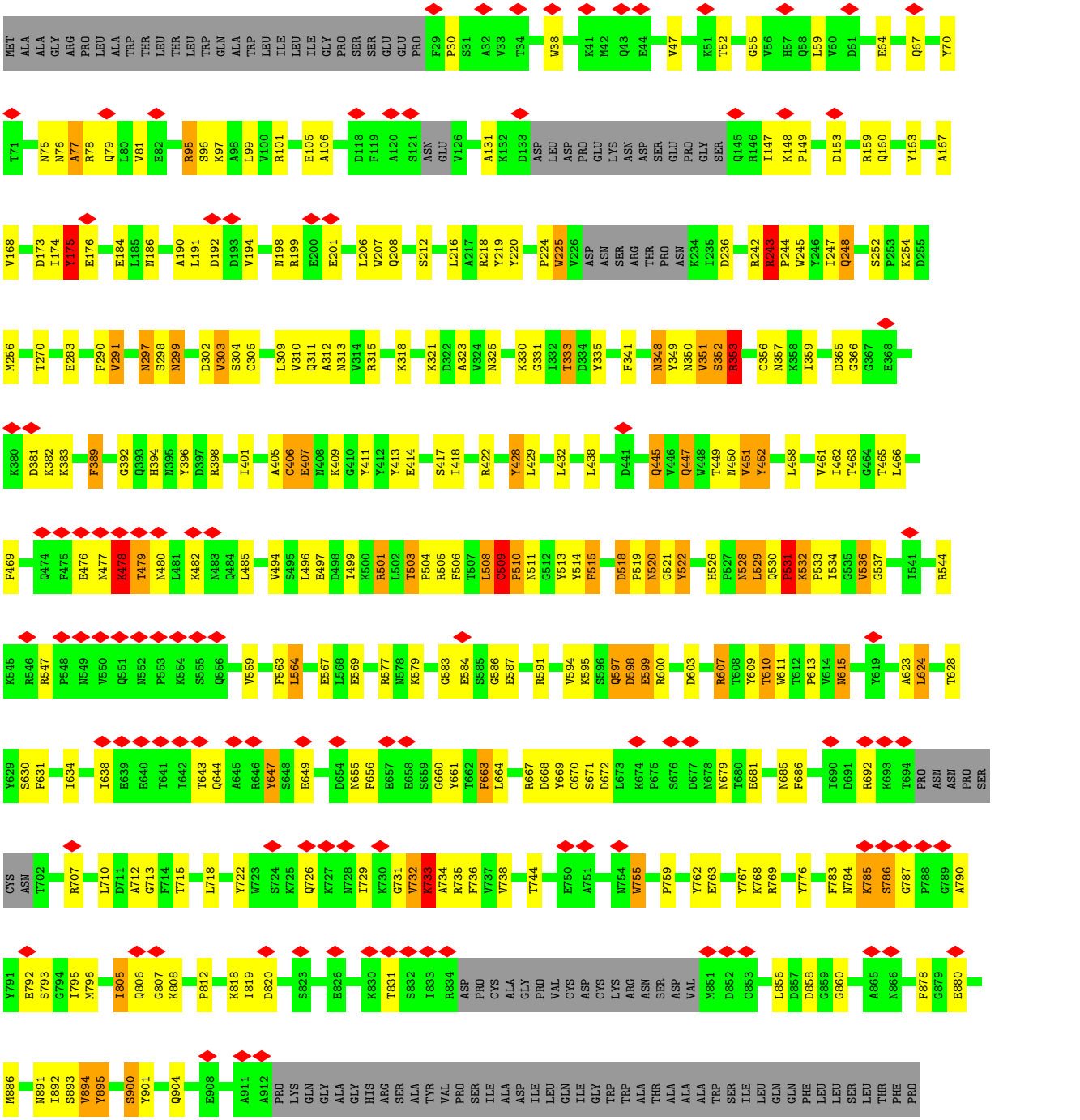
• Molecule 4: Voltage-dependent calcium channel gamma-1 subunit

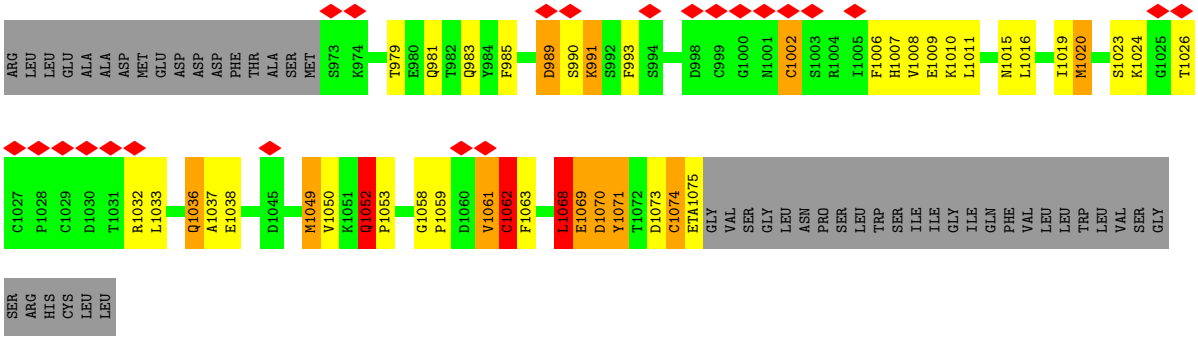
Chain E:





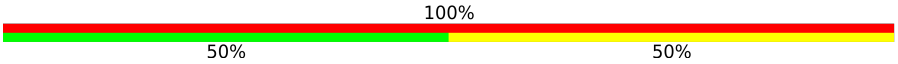
• Molecule 5: Voltage-dependent calcium channel subunit alpha-2/delta-1





• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:

• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	527833	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1.3	Depositor
Maximum defocus (nm)	2.9	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.294	Depositor
Minimum map value	-0.187	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.044	Depositor
Map size (Å)	337.92, 337.92, 337.92	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.32, 1.32, 1.32	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: ETA, PC1, CA, NAG, BMA

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	0.56	2/10431 (0.0%)	0.73	24/14157 (0.2%)
2	B	0.43	1/723 (0.1%)	0.65	3/979 (0.3%)
3	C	0.34	0/1394	0.50	0/1892
4	E	0.42	1/1336 (0.1%)	0.58	2/1802 (0.1%)
5	F	0.68	13/7721 (0.2%)	0.85	32/10463 (0.3%)
All	All	0.58	17/21605 (0.1%)	0.76	61/29293 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	11
3	C	0	2
5	F	0	14
All	All	0	27

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	171	ARG	C-O	13.19	1.48	1.23
5	F	647	TYR	C-N	10.24	1.57	1.34
5	F	312	ALA	C-O	7.40	1.37	1.23
2	B	167	SER	CB-OG	6.12	1.50	1.42
5	F	526	HIS	C-N	-6.02	1.22	1.34
5	F	1062	CYS	C-O	-5.84	1.12	1.23
5	F	504	PRO	N-CD	5.50	1.55	1.47
5	F	1053	PRO	N-CD	5.37	1.55	1.47
5	F	225	TRP	CB-CG	-5.31	1.40	1.50
5	F	533	PRO	N-CD	5.29	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	244	PRO	N-CD	5.27	1.55	1.47
5	F	510	PRO	N-CD	5.26	1.55	1.47
5	F	1059	PRO	N-CD	5.20	1.55	1.47
4	E	208	PRO	N-CD	5.19	1.55	1.47
5	F	531	PRO	N-CD	5.05	1.54	1.47
5	F	291	VAL	CB-CG1	-5.03	1.42	1.52
1	A	638	CYS	CB-SG	-5.03	1.73	1.81

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	518	ASP	CB-CA-C	-10.92	88.55	110.40
5	F	469	PHE	CB-CA-C	-9.64	91.12	110.40
5	F	445	GLN	CB-CA-C	9.59	129.57	110.40
1	A	1174	ALA	CB-CA-C	-8.28	97.69	110.10
5	F	175	TYR	N-CA-C	8.25	133.27	111.00
5	F	406	CYS	O-C-N	-8.24	109.52	122.70
5	F	609	TYR	CB-CA-C	7.89	126.17	110.40
5	F	663	PHE	CB-CA-C	-7.64	95.12	110.40
1	A	957	CYS	CB-CA-C	-7.37	95.67	110.40
1	A	181	SER	CB-CA-C	7.31	123.99	110.10
1	A	333	LEU	CA-CB-CG	7.24	131.95	115.30
5	F	607	ARG	N-CA-C	-7.20	91.56	111.00
5	F	216	LEU	CB-CA-C	-7.15	96.61	110.20
1	A	949	LEU	CA-CB-CG	7.10	131.62	115.30
1	A	1417	ILE	CB-CA-C	6.97	125.53	111.60
5	F	407	GLU	CB-CA-C	-6.90	96.59	110.40
5	F	522	TYR	CB-CA-C	-6.80	96.79	110.40
2	B	115	PRO	N-CA-CB	6.75	111.41	103.30
2	B	130	PRO	N-CA-CB	6.56	111.17	103.30
5	F	1002	CYS	CB-CA-C	6.53	123.45	110.40
1	A	281	SER	CB-CA-C	6.35	122.16	110.10
5	F	735	ARG	CB-CA-C	-6.34	97.73	110.40
1	A	954	PHE	CB-CG-CD1	6.32	125.22	120.80
1	A	1461	VAL	CB-CA-C	6.28	123.32	111.40
2	B	113	PRO	N-CA-CB	6.17	110.70	103.30
4	E	210	ASN	C-N-CD	6.10	141.22	128.40
5	F	1006	PHE	CB-CA-C	-6.04	98.31	110.40
1	A	326	LEU	CA-CB-CG	6.04	129.18	115.30
1	A	440	LEU	CB-CA-C	5.99	121.58	110.20
1	A	458	LEU	CA-CB-CG	5.96	129.01	115.30
5	F	664	LEU	CB-CA-C	-5.95	98.90	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	305	CYS	CA-CB-SG	5.92	124.65	114.00
5	F	603	ASP	CB-CA-C	-5.84	98.72	110.40
5	F	405	ALA	O-C-N	-5.83	113.37	122.70
5	F	254	LYS	CB-CA-C	-5.78	98.84	110.40
5	F	624	LEU	CB-CA-C	-5.76	99.25	110.20
1	A	644	LEU	CB-CG-CD2	-5.73	101.25	111.00
1	A	954	PHE	CB-CG-CD2	-5.72	116.80	120.80
5	F	1052	GLN	C-N-CD	5.70	140.37	128.40
4	E	207	MET	C-N-CD	5.68	140.34	128.40
5	F	900	SER	CB-CA-C	-5.64	99.39	110.10
5	F	243	ARG	C-N-CD	5.62	140.20	128.40
1	A	443	ALA	CB-CA-C	5.62	118.53	110.10
5	F	509	CYS	C-N-CD	5.60	140.17	128.40
5	F	1002	CYS	N-CA-C	-5.60	95.87	111.00
5	F	1058	GLY	C-N-CD	5.60	140.17	128.40
5	F	520	ASN	CB-CA-C	-5.57	99.27	110.40
1	A	997	PHE	CB-CG-CD1	5.56	124.69	120.80
1	A	1316	LEU	CB-CG-CD2	-5.53	101.60	111.00
1	A	196	LEU	CA-CB-CG	5.51	127.97	115.30
5	F	783	PHE	C-N-CA	5.47	135.38	121.70
5	F	607	ARG	C-N-CA	5.41	135.22	121.70
5	F	503	THR	C-N-CD	5.33	139.58	128.40
1	A	597	PHE	CB-CG-CD1	5.30	124.51	120.80
1	A	1188	LEU	CA-CB-CG	5.30	127.48	115.30
5	F	609	TYR	CA-CB-CG	5.30	123.46	113.40
1	A	858	LEU	CA-CB-CG	5.24	127.35	115.30
1	A	1337	LEU	CA-CB-CG	5.17	127.20	115.30
1	A	333	LEU	CB-CG-CD2	-5.16	102.22	111.00
5	F	610	THR	CB-CA-C	-5.15	97.68	111.60
1	A	653	LEU	CA-CB-CG	5.03	126.87	115.30

There are no chirality outliers.

All (27) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1344	TYR	Peptide
1	A	1440	PRO	Peptide
1	A	1441	HIS	Peptide
1	A	228	TYR	Peptide
1	A	229	ILE	Peptide
1	A	237	VAL	Peptide
1	A	266	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	A	268	PRO	Peptide
1	A	456	GLN	Peptide
1	A	628	GLY	Peptide
1	A	629	GLY	Peptide
3	C	281	GLY	Peptide,Mainchain
5	F	1023	SER	Peptide
5	F	1024	LYS	Peptide
5	F	1074	CYS	Peptide,Mainchain
5	F	175	TYR	Peptide
5	F	220	TYR	Peptide
5	F	406	CYS	Mainchain
5	F	476	GLU	Peptide
5	F	522	TYR	Peptide
5	F	600	ARG	Peptide
5	F	70	TYR	Peptide
5	F	785	LYS	Peptide
5	F	786	SER	Peptide
5	F	805	ILE	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10183	0	10143	394	0
2	B	710	0	633	1	0
3	C	1367	0	1343	9	0
4	E	1304	0	1330	66	0
5	F	7567	0	7399	316	0
6	D	28	0	25	0	0
6	G	28	0	25	5	0
6	J	28	0	25	1	0
6	K	28	0	25	0	0
7	H	39	0	34	0	0
7	I	39	0	34	0	0
8	L	42	0	37	0	0
9	A	14	0	13	0	0
9	F	98	0	91	0	0
10	A	426	0	675	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	A	2	0	0	0	0
11	F	1	0	0	0	0
All	All	21904	0	21832	768	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 18.

All (768) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1389:ARG:HD2	1:A:1391:TRP:CE3	1.43	1.51
5:F:669:TYR:HD1	5:F:670:CYS:N	1.28	1.29
4:E:208:PRO:CG	4:E:214:SER:HA	1.64	1.26
1:A:1203:ASP:OD2	1:A:1229:ARG:HD2	1.15	1.24
1:A:1389:ARG:HB2	1:A:1391:TRP:CZ3	1.71	1.24
5:F:411:TYR:CD1	5:F:1074:CYS:HA	1.71	1.22
4:E:15:CYS:SG	4:E:191:LEU:CD2	2.28	1.21
1:A:956:SER:HB3	1:A:1022:ARG:NH1	1.53	1.21
1:A:475:PHE:CE2	1:A:537:LYS:HE3	1.77	1.20
1:A:224:LYS:O	1:A:266:PRO:HG3	1.44	1.16
1:A:1389:ARG:HD2	1:A:1391:TRP:CD2	1.82	1.15
5:F:529:LEU:O	5:F:530:GLN:HG2	1.48	1.14
4:E:15:CYS:SG	4:E:191:LEU:HD21	1.87	1.13
5:F:315[B]:ARG:HH21	5:F:1049:MET:HE2	1.07	1.12
1:A:1060:PHE:HZ	1:A:1376:PHE:CE1	1.68	1.10
1:A:1015:GLY:HA3	1:A:1326:GLN:HE22	1.03	1.09
1:A:1389:ARG:CD	1:A:1391:TRP:CE3	2.34	1.09
1:A:956:SER:HB3	1:A:1022:ARG:HH11	0.92	1.08
4:E:208:PRO:HG3	4:E:214:SER:HA	1.28	1.08
1:A:1262:LYS:HE3	4:E:209:GLN:O	1.52	1.08
5:F:564:LEU:HD11	5:F:569:GLU:HG3	1.31	1.07
1:A:1046:ILE:HD12	10:A:1914:PC1:H392	1.36	1.06
5:F:174:ILE:HG22	5:F:175:TYR:H	1.21	1.06
5:F:669:TYR:CD1	5:F:670:CYS:N	2.09	1.05
1:A:128:ILE:HG13	1:A:171:ARG:HH11	1.16	1.05
1:A:1391:TRP:HE1	1:A:1397:HIS:CD2	1.73	1.04
5:F:564:LEU:CD1	5:F:569:GLU:HG3	1.87	1.04
4:E:19:GLY:HA3	4:E:191:LEU:CD1	1.88	1.04
1:A:587:PHE:HE2	1:A:625:MET:HE2	1.23	1.03
5:F:894:VAL:HG21	5:F:993:PHE:CE2	1.93	1.03
5:F:297:ASN:ND2	5:F:330:LYS:O	1.91	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:208:PRO:HG2	4:E:214:SER:HA	1.39	1.02
4:E:19:GLY:CA	4:E:191:LEU:CD1	2.38	1.02
5:F:661:TYR:CE2	5:F:663:PHE:CZ	2.48	1.02
1:A:362:ASP:OD1	3:C:437:ASN:ND2	1.93	1.01
5:F:643:THR:HG22	5:F:647:TYR:CE2	1.95	1.01
5:F:647:TYR:CE1	5:F:713:GLY:HA3	1.96	1.00
5:F:644:GLN:HA	5:F:647:TYR:HD2	1.25	1.00
5:F:534:ILE:HG22	5:F:904:GLN:HG2	1.40	0.99
1:A:1015:GLY:CA	1:A:1326:GLN:HE22	1.75	0.99
1:A:942:PHE:HD2	1:A:1048:TYR:CD1	1.81	0.99
1:A:1337:LEU:CD1	1:A:1350:TYR:HE1	1.76	0.98
5:F:248:GLN:OE1	5:F:447:GLN:HB3	1.63	0.98
1:A:1203:ASP:OD2	1:A:1229:ARG:CD	2.11	0.98
1:A:529:CYS:SG	1:A:945:ILE:HG13	2.03	0.97
1:A:1015:GLY:HA3	1:A:1326:GLN:NE2	1.80	0.97
4:E:19:GLY:CA	4:E:191:LEU:HD12	1.94	0.97
5:F:732:VAL:O	5:F:820:ASP:HB2	1.63	0.96
1:A:942:PHE:HD2	1:A:1048:TYR:HD1	1.00	0.96
5:F:174:ILE:HG22	5:F:175:TYR:N	1.75	0.96
5:F:315[B]:ARG:HH21	5:F:1049:MET:CE	1.78	0.96
1:A:955:PHE:CE1	1:A:992:HIS:ND1	2.34	0.95
4:E:19:GLY:HA3	4:E:191:LEU:HD13	1.48	0.95
1:A:1262:LYS:CE	4:E:209:GLN:O	2.15	0.95
5:F:528:ASN:O	5:F:528:ASN:ND2	1.98	0.95
1:A:955:PHE:CE1	1:A:992:HIS:CE1	2.54	0.95
1:A:614:GLU:OE2	1:A:615:ASP:HB2	1.68	0.94
6:G:1:NAG:C6	6:G:2:NAG:H82	1.98	0.94
4:E:19:GLY:N	4:E:191:LEU:CD1	2.32	0.93
1:A:1390:ASP:O	1:A:1392:SER:N	2.02	0.93
5:F:382:LYS:NZ	5:F:407:GLU:O	2.02	0.93
1:A:1042:ALA:O	1:A:1046:ILE:HG13	1.69	0.92
1:A:1389:ARG:HB2	1:A:1391:TRP:HZ3	1.25	0.92
5:F:174:ILE:CG2	5:F:175:TYR:H	1.81	0.92
5:F:1036:GLN:HE21	5:F:1037:ALA:H	1.17	0.92
5:F:661:TYR:CD2	5:F:663:PHE:CZ	2.58	0.92
1:A:1299:GLN:NE2	1:A:1327:GLU:OE1	2.03	0.92
1:A:836:ASP:OD2	1:A:900:ARG:NH1	2.02	0.92
5:F:290:PHE:HD2	5:F:310:VAL:O	1.52	0.91
5:F:647:TYR:CD1	5:F:713:GLY:HA3	2.05	0.91
1:A:942:PHE:CD2	1:A:1048:TYR:HD1	1.88	0.91
1:A:1043:ILE:HG12	1:A:1047:ILE:HD11	1.52	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1337:LEU:HG	1:A:1350:TYR:CE1	2.05	0.90
1:A:956:SER:CB	1:A:1022:ARG:HH11	1.84	0.90
1:A:1389:ARG:HB2	1:A:1391:TRP:CE3	2.06	0.89
1:A:1060:PHE:CZ	1:A:1376:PHE:CE1	2.60	0.89
5:F:30:PRO:CG	5:F:1020:MET:HE1	2.03	0.89
5:F:315[B]:ARG:NH2	5:F:1049:MET:HE2	1.88	0.88
1:A:587:PHE:HE2	1:A:625:MET:CE	1.85	0.88
1:A:820:ASP:HB2	1:A:821:PRO:HA	1.56	0.86
1:A:1096:ARG:NH2	4:E:213:GLU:OE2	2.08	0.86
5:F:1062:CYS:O	5:F:1063:PHE:CD1	2.28	0.86
5:F:510:PRO:HG2	5:F:767:TYR:CE2	2.11	0.86
5:F:536:VAL:HG12	5:F:537:GLY:H	1.37	0.86
5:F:478:LYS:O	5:F:480:ASN:N	2.09	0.85
5:F:477:ASN:O	5:F:478:LYS:HB2	1.75	0.85
1:A:510:GLU:OE2	1:A:531:ARG:HD3	1.76	0.85
5:F:297:ASN:HD21	5:F:331:GLY:HA3	1.40	0.85
1:A:1391:TRP:NE1	1:A:1397:HIS:CD2	2.45	0.85
4:E:15:CYS:SG	4:E:191:LEU:HD23	2.14	0.84
5:F:661:TYR:HD2	5:F:663:PHE:CE2	1.96	0.84
5:F:30:PRO:HG2	5:F:1020:MET:HE1	1.60	0.84
1:A:841:SER:O	1:A:845:VAL:HG23	1.76	0.84
5:F:1036:GLN:NE2	5:F:1037:ALA:H	1.75	0.84
5:F:643:THR:HG22	5:F:647:TYR:HE2	1.42	0.83
5:F:894:VAL:HG11	5:F:993:PHE:CE2	2.13	0.83
1:A:965:GLU:OE1	1:A:990:TRP:NE1	2.11	0.83
1:A:1134:CYS:SG	1:A:1153:LEU:CD1	2.67	0.83
1:A:1391:TRP:NE1	1:A:1397:HIS:HD2	1.76	0.83
5:F:534:ILE:HG22	5:F:904:GLN:CG	2.09	0.82
5:F:894:VAL:HG21	5:F:993:PHE:HE2	1.41	0.82
1:A:1262:LYS:HE3	4:E:209:GLN:C	1.98	0.82
1:A:538:ILE:O	1:A:541:TYR:HD1	1.62	0.82
5:F:290:PHE:CD2	5:F:310:VAL:O	2.32	0.82
5:F:661:TYR:HE2	5:F:663:PHE:CZ	1.94	0.81
5:F:894:VAL:HG21	5:F:993:PHE:CZ	2.14	0.81
4:E:208:PRO:HG2	4:E:214:SER:CA	2.10	0.81
5:F:515:PHE:HE2	5:F:563:PHE:CE1	1.97	0.81
5:F:247:ILE:HG23	5:F:429:LEU:HD11	1.61	0.81
1:A:262:ARG:HG2	1:A:262:ARG:HH11	1.46	0.81
1:A:1046:ILE:CD1	10:A:1914:PC1:H392	2.11	0.80
1:A:128:ILE:HG13	1:A:171:ARG:NH1	1.94	0.80
5:F:174:ILE:CG2	5:F:175:TYR:N	2.43	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1134:CYS:SG	1:A:1153:LEU:HD12	2.22	0.80
5:F:671:SER:O	5:F:672:ASP:OD1	1.99	0.80
1:A:840:THR:O	1:A:844:THR:HG23	1.82	0.79
5:F:733:LYS:NZ	5:F:792:GLU:O	2.14	0.79
1:A:1337:LEU:CD1	1:A:1350:TYR:CE1	2.66	0.79
1:A:955:PHE:HE1	1:A:992:HIS:CE1	2.00	0.79
1:A:1046:ILE:O	1:A:1049:ILE:HG22	1.84	0.78
1:A:591:GLU:OE2	1:A:593:ARG:NH1	2.15	0.78
5:F:353:ARG:HB2	5:F:353:ARG:HH11	1.48	0.78
1:A:955:PHE:CD1	1:A:992:HIS:ND1	2.51	0.78
1:A:587:PHE:CE2	1:A:625:MET:CE	2.68	0.77
1:A:1384:PHE:O	1:A:1388:THR:HG23	1.85	0.77
1:A:215:LEU:O	1:A:219:LYS:HG3	1.83	0.77
1:A:587:PHE:CE2	1:A:625:MET:HE2	2.15	0.77
5:F:644:GLN:HA	5:F:647:TYR:CD2	2.16	0.77
5:F:1061:VAL:HG23	5:F:1062:CYS:H	1.48	0.77
5:F:564:LEU:CD1	5:F:569:GLU:CG	2.63	0.77
1:A:821:PRO:HG3	1:A:1286:MET:HG2	1.67	0.77
5:F:411:TYR:CE1	5:F:1074:CYS:HA	2.19	0.77
5:F:894:VAL:HG11	5:F:993:PHE:HE2	1.49	0.77
1:A:1020:LEU:HD12	1:A:1020:LEU:O	1.85	0.76
1:A:903:ARG:HB2	1:A:904:PRO:HD3	1.66	0.76
1:A:1337:LEU:HD12	1:A:1350:TYR:HE1	1.50	0.76
1:A:820:ASP:H	1:A:821:PRO:HA	1.50	0.76
1:A:955:PHE:CD1	1:A:992:HIS:CE1	2.73	0.76
1:A:1390:ASP:HB3	1:A:1393:ILE:CD1	2.16	0.75
5:F:661:TYR:CD2	5:F:663:PHE:CE2	2.74	0.75
5:F:76:ASN:O	5:F:78:ARG:N	2.20	0.75
5:F:411:TYR:CD1	5:F:1074:CYS:CA	2.63	0.75
5:F:894:VAL:CG2	5:F:993:PHE:CE2	2.69	0.75
1:A:1060:PHE:HZ	1:A:1376:PHE:CD1	2.04	0.75
1:A:468:ASN:ND2	1:A:531:ARG:NH2	2.35	0.75
1:A:475:PHE:CZ	1:A:537:LYS:HE3	2.21	0.75
1:A:902:LEU:HD11	1:A:905:LEU:HD12	1.69	0.75
1:A:1325:TRP:HA	1:A:1328:ILE:HD12	1.68	0.74
4:E:19:GLY:CA	4:E:191:LEU:HD13	2.11	0.74
5:F:503:THR:HB	5:F:514:TYR:HD2	1.53	0.74
5:F:510:PRO:HG2	5:F:767:TYR:HE2	1.52	0.74
1:A:1389:ARG:CB	1:A:1391:TRP:CZ3	2.63	0.74
4:E:19:GLY:HA3	4:E:191:LEU:HD12	1.60	0.74
5:F:450:ASN:O	5:F:451:VAL:HG22	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:452:TYR:OH	5:F:463:THR:CG2	2.36	0.73
1:A:820:ASP:HB2	1:A:821:PRO:CA	2.18	0.73
5:F:661:TYR:CE2	5:F:663:PHE:HZ	2.02	0.73
1:A:171:ARG:O	1:A:174:ARG:HB2	1.88	0.73
1:A:819:GLU:CD	1:A:897:ARG:HH21	1.91	0.73
1:A:224:LYS:O	1:A:266:PRO:CG	2.32	0.73
5:F:315[B]:ARG:NH2	5:F:1049:MET:CE	2.46	0.73
5:F:598:ASP:C	5:F:599:GLU:HG3	2.08	0.73
5:F:732:VAL:HG23	5:F:733:LYS:N	2.02	0.73
1:A:1235:PHE:HE2	4:E:153:VAL:CG2	2.02	0.73
1:A:1389:ARG:HE	1:A:1391:TRP:HB2	1.54	0.72
1:A:902:LEU:CD1	1:A:905:LEU:HD12	2.19	0.72
5:F:478:LYS:O	5:F:479:THR:C	2.27	0.72
5:F:586:GLY:HA3	5:F:611:TRP:CZ2	2.24	0.72
1:A:262:ARG:HG2	1:A:262:ARG:NH1	1.99	0.72
1:A:820:ASP:CB	1:A:821:PRO:CA	2.68	0.72
4:E:19:GLY:H	4:E:191:LEU:CD1	2.01	0.72
5:F:530:GLN:OE1	5:F:532:LYS:NZ	2.22	0.72
1:A:1195:ILE:HD11	4:E:113:PHE:CD2	2.25	0.72
1:A:1299:GLN:HG2	1:A:1327:GLU:HB3	1.71	0.72
5:F:1074:CYS:SG	5:F:1075:ETA:N	2.63	0.72
5:F:30:PRO:HG3	5:F:1020:MET:CE	2.19	0.72
5:F:30:PRO:HG3	5:F:1020:MET:HE1	1.69	0.72
1:A:544:SER:OG	1:A:547:ASN:HB3	1.90	0.71
1:A:843:PHE:CE2	1:A:871:LEU:HA	2.25	0.71
1:A:1134:CYS:SG	1:A:1153:LEU:HD13	2.30	0.71
5:F:669:TYR:CE1	5:F:670:CYS:HB2	2.25	0.71
5:F:353:ARG:HB2	5:F:353:ARG:NH1	2.05	0.71
1:A:439:ILE:HG12	1:A:541:TYR:OH	1.91	0.71
5:F:366:GLY:HA2	5:F:401:ILE:HD11	1.72	0.71
1:A:1014:GLU:OE2	1:A:1326:GLN:NE2	2.23	0.71
1:A:1329:LEU:HD11	1:A:1358:TYR:CD1	2.26	0.70
1:A:908:ILE:HD11	1:A:1276:MET:HG2	1.74	0.70
5:F:409:LYS:HE2	5:F:1071:TYR:CE1	2.26	0.70
1:A:1391:TRP:CD1	1:A:1397:HIS:HD2	2.09	0.70
5:F:892:ILE:O	5:F:892:ILE:HD12	1.91	0.70
1:A:632:TYR:HB3	1:A:633:PRO:HD3	1.71	0.70
1:A:911:ALA:O	1:A:915:LYS:HE3	1.92	0.70
5:F:529:LEU:O	5:F:530:GLN:CG	2.35	0.70
1:A:1249[A]:ARG:O	1:A:1249[A]:ARG:HD3	1.92	0.69
1:A:538:ILE:O	1:A:541:TYR:CD1	2.46	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:595:LYS:HE3	5:F:983:GLN:HE22	1.56	0.69
1:A:245:CYS:SG	1:A:246:ALA:N	2.66	0.69
1:A:268:PRO:HB2	1:A:273:THR:HB	1.73	0.69
5:F:511:ASN:HB3	5:F:607:ARG:HH12	1.56	0.69
1:A:1235:PHE:HE2	4:E:153:VAL:HG21	1.58	0.69
1:A:994:ASP:HB3	1:A:1330:LEU:HD21	1.75	0.68
4:E:208:PRO:O	4:E:210:ASN:N	2.27	0.68
6:G:1:NAG:H62	6:G:2:NAG:H82	1.76	0.68
5:F:318:LYS:HG2	5:F:536:VAL:HG13	1.75	0.68
1:A:1235:PHE:CE2	4:E:153:VAL:HG21	2.28	0.68
1:A:1337:LEU:CG	1:A:1350:TYR:CE1	2.76	0.68
5:F:564:LEU:HD12	5:F:569:GLU:CG	2.24	0.68
1:A:820:ASP:CB	1:A:821:PRO:HA	2.19	0.68
1:A:1071:GLN:NE2	1:A:1381:MET:SD	2.67	0.68
5:F:351:VAL:HG12	5:F:352:SER:N	2.09	0.67
1:A:843:PHE:HE2	1:A:871:LEU:CA	2.07	0.67
1:A:1417:ILE:O	1:A:1460:THR:HA	1.95	0.67
1:A:1305:ASN:HD22	1:A:1311:GLN:HG3	1.59	0.66
1:A:1047:ILE:O	1:A:1051:LEU:HG	1.94	0.66
1:A:1391:TRP:CZ2	1:A:1396:PRO:HD2	2.30	0.66
5:F:77:ALA:O	5:F:81:VAL:HG23	1.95	0.66
6:G:1:NAG:H61	6:G:2:NAG:H82	1.75	0.66
5:F:503:THR:HB	5:F:514:TYR:CD2	2.29	0.66
1:A:843:PHE:O	1:A:846:GLU:HG3	1.95	0.66
5:F:649:GLU:OE1	5:F:655:ASN:ND2	2.29	0.66
5:F:302:ASP:O	5:F:304:SER:N	2.29	0.66
1:A:996:HIS:ND1	1:A:998:ASP:HB2	2.11	0.65
5:F:586:GLY:O	5:F:611:TRP:CD2	2.49	0.65
5:F:506:PHE:HA	5:F:762:TYR:HE2	1.60	0.65
5:F:991:LYS:HB3	5:F:1010:LYS:HB2	1.78	0.65
5:F:667:ARG:NH1	5:F:668:ASP:O	2.30	0.65
1:A:915:LYS:HD3	1:A:915:LYS:N	2.11	0.65
1:A:231:THR:O	1:A:262:ARG:NH2	2.29	0.65
1:A:1264:PHE:CE1	1:A:1267:LEU:HD23	2.32	0.65
1:A:1060:PHE:CZ	1:A:1376:PHE:CD1	2.82	0.65
1:A:1192:GLY:HA3	1:A:1238:PHE:CD2	2.31	0.65
1:A:45:ILE:HG12	1:A:107:ALA:HA	1.78	0.65
1:A:439:ILE:CG1	1:A:541:TYR:OH	2.45	0.65
1:A:843:PHE:CE2	1:A:871:LEU:CA	2.80	0.65
5:F:297:ASN:ND2	5:F:331:GLY:HA3	2.10	0.65
1:A:1430:GLN:HG3	1:A:1432:PRO:HD2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:536:VAL:HG12	5:F:537:GLY:N	2.10	0.64
1:A:1060:PHE:HZ	1:A:1376:PHE:CZ	2.14	0.64
1:A:1248:SER:HB3	1:A:1249[B]:ARG:HD3	1.78	0.64
5:F:647:TYR:CD1	5:F:713:GLY:CA	2.78	0.64
1:A:1334:TYR:CE1	1:A:1351:THR:HG23	2.33	0.64
5:F:449:THR:O	5:F:462:ILE:HG13	1.97	0.64
5:F:661:TYR:HE2	5:F:663:PHE:HZ	1.38	0.64
5:F:671:SER:C	5:F:672:ASP:OD1	2.35	0.64
5:F:736:PHE:CZ	5:F:796:MET:SD	2.90	0.64
1:A:1139:HIS:CD2	1:A:1142:GLN:HB3	2.33	0.64
5:F:76:ASN:ND2	5:F:79:GLN:HB2	2.13	0.64
5:F:283:GLU:OE2	5:F:321:LYS:NZ	2.31	0.64
5:F:597:GLN:NE2	5:F:763:GLU:O	2.31	0.63
5:F:153:ASP:OD1	5:F:160:GLN:HG2	1.98	0.63
1:A:303:ASP:OD2	1:A:1302:ARG:NH1	2.31	0.63
1:A:372:GLN:NE2	1:A:486:LEU:O	2.31	0.63
5:F:667:ARG:HH21	5:F:686:PHE:HE1	1.45	0.63
5:F:894:VAL:CB	5:F:993:PHE:CE2	2.82	0.63
1:A:1195:ILE:HD11	4:E:113:PHE:HD2	1.62	0.63
1:A:1389:ARG:HD2	1:A:1391:TRP:CZ3	2.25	0.63
5:F:407:GLU:O	5:F:407:GLU:HG2	1.98	0.63
5:F:452:TYR:OH	5:F:463:THR:HG21	1.99	0.62
1:A:468:ASN:HD21	1:A:531:ARG:HD3	1.65	0.62
4:E:206:ARG:O	4:E:207:MET:C	2.36	0.62
1:A:1019:LEU:HD21	1:A:1045:PHE:CZ	2.35	0.62
1:A:822:ILE:HD12	1:A:822:ILE:O	2.00	0.61
1:A:608:PHE:CZ	1:A:1050:ILE:HD11	2.35	0.61
1:A:820:ASP:N	1:A:821:PRO:HA	2.11	0.61
1:A:843:PHE:O	1:A:846:GLU:CG	2.48	0.61
1:A:1258:TRP:HE1	4:E:208:PRO:HD2	1.64	0.61
5:F:351:VAL:O	5:F:352:SER:HB3	1.98	0.61
5:F:482:LYS:O	5:F:482:LYS:HG2	1.99	0.61
5:F:647:TYR:HE1	5:F:713:GLY:HA3	1.60	0.61
1:A:1260:PHE:HA	1:A:1263:SER:OG	1.99	0.61
1:A:823:ARG:HG2	1:A:823:ARG:HH21	1.65	0.61
5:F:858:ASP:HB2	5:F:1015:ASN:OD1	1.99	0.61
5:F:669:TYR:HE1	5:F:670:CYS:HB2	1.64	0.61
5:F:163:TYR:OH	5:F:199:ARG:NH2	2.34	0.61
5:F:894:VAL:CG1	5:F:993:PHE:CE2	2.84	0.61
4:E:30:ASP:OD2	4:E:55:ARG:NH2	2.34	0.61
5:F:531:PRO:O	5:F:532:LYS:HG3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:731:GLY:O	5:F:732:VAL:HG22	2.01	0.60
5:F:310:VAL:HG12	5:F:1050:VAL:HG21	1.83	0.60
5:F:101:ARG:HH12	5:F:201:GLU:HG2	1.64	0.60
1:A:265:TRP:HZ2	1:A:271:GLY:HA2	1.66	0.60
1:A:823:ARG:HH21	1:A:823:ARG:CG	2.14	0.60
1:A:942:PHE:HA	1:A:945:ILE:HG22	1.83	0.60
1:A:1389:ARG:CB	1:A:1391:TRP:CE3	2.81	0.60
5:F:579:LYS:O	5:F:583:GLY:HA3	2.01	0.60
1:A:1016:TRP:CD1	1:A:1017:PRO:HD3	2.37	0.60
5:F:243:ARG:HH11	5:F:243:ARG:CG	2.15	0.60
5:F:411:TYR:HD1	5:F:1074:CYS:HA	1.56	0.59
1:A:637:VAL:HG22	10:A:1903:PC1:H291	1.84	0.59
1:A:541:TYR:O	1:A:542:TRP:HB2	2.02	0.59
5:F:309:LEU:HD12	5:F:353:ARG:HD2	1.84	0.59
5:F:981:GLN:NE2	5:F:1038:GLU:OE2	2.35	0.59
1:A:587:PHE:CE2	1:A:625:MET:HE3	2.38	0.59
5:F:529:LEU:C	5:F:530:GLN:HG2	2.20	0.59
5:F:586:GLY:O	5:F:611:TRP:CE2	2.56	0.59
1:A:1195:ILE:CD1	4:E:113:PHE:CD2	2.86	0.59
5:F:256:MET:HB3	5:F:291:VAL:HG12	1.83	0.59
5:F:303:VAL:O	5:F:303:VAL:HG22	2.02	0.59
5:F:309:LEU:HD12	5:F:353:ARG:CD	2.33	0.59
1:A:206:MET:HE2	1:A:317:LEU:HD12	1.85	0.58
5:F:302:ASP:OD1	5:F:341:PHE:HE2	1.86	0.58
5:F:894:VAL:CG1	5:F:993:PHE:HE2	2.15	0.58
5:F:643:THR:O	5:F:647:TYR:CD2	2.57	0.58
1:A:822:ILE:HG21	1:A:1291:LYS:H	1.68	0.58
1:A:982:GLN:HG2	5:F:547:ARG:HE	1.67	0.58
5:F:225:TRP:NE1	5:F:236:ASP:OD2	2.36	0.58
1:A:469:ARG:HG2	1:A:511:LEU:HD11	1.85	0.58
1:A:1016:TRP:O	1:A:1020:LEU:N	2.28	0.58
4:E:208:PRO:CG	4:E:214:SER:CA	2.58	0.58
5:F:206:LEU:HD13	5:F:458:LEU:HD21	1.85	0.58
1:A:262:ARG:HH11	1:A:262:ARG:CG	2.15	0.58
5:F:894:VAL:CG2	5:F:993:PHE:HE2	2.10	0.58
1:A:108:TYR:HB2	1:A:112:PHE:HB2	1.86	0.57
1:A:482:LYS:HE2	1:A:486:LEU:HD22	1.86	0.57
1:A:183:GLN:O	1:A:187:ASN:ND2	2.38	0.57
1:A:591:GLU:OE2	1:A:593:ARG:NH2	2.36	0.57
5:F:365:ASP:O	5:F:394:HIS:NE2	2.37	0.57
5:F:679:ASN:HD21	5:F:759:PRO:HG3	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:THR:HG23	1:A:266:PRO:HB3	1.86	0.57
1:A:1094:LYS:HD3	4:E:212:TRP:CZ2	2.40	0.57
1:A:900:ARG:HD2	1:A:903:ARG:HH11	1.70	0.57
1:A:1262:LYS:HE2	4:E:209:GLN:OE1	2.04	0.57
1:A:1416:ARG:HA	1:A:1461:VAL:O	2.04	0.57
1:A:369:TRP:HD1	1:A:369:TRP:O	1.87	0.57
1:A:468:ASN:HD22	1:A:531:ARG:NH2	2.02	0.57
1:A:1249[A]:ARG:HH21	1:A:1249[A]:ARG:CG	2.17	0.57
5:F:505:ARG:O	5:F:505:ARG:HG2	2.03	0.57
5:F:586:GLY:CA	5:F:611:TRP:CZ2	2.88	0.57
1:A:965:GLU:CD	1:A:990:TRP:HE1	2.08	0.57
1:A:529:CYS:SG	1:A:945:ILE:CG1	2.89	0.56
1:A:1244:ILE:CG2	1:A:1247:LEU:HD21	2.35	0.56
1:A:206:MET:CE	1:A:317:LEU:HD12	2.34	0.56
1:A:475:PHE:CE2	1:A:537:LYS:CE	2.70	0.56
4:E:206:ARG:HB3	4:E:206:ARG:CZ	2.33	0.56
5:F:638:ILE:HG21	5:F:644:GLN:HB3	1.87	0.56
1:A:542:TRP:HE3	1:A:542:TRP:N	2.04	0.56
4:E:19:GLY:N	4:E:191:LEU:HD13	2.14	0.56
1:A:1144:GLU:O	1:A:1148:HIS:ND1	2.30	0.56
1:A:1390:ASP:HB3	1:A:1393:ILE:HD12	1.86	0.56
1:A:1339:ASP:O	1:A:1341:GLU:N	2.34	0.56
5:F:981:GLN:HG2	5:F:1038:GLU:HG2	1.87	0.56
5:F:515:PHE:HD1	5:F:623:ALA:O	1.89	0.56
1:A:252:ARG:HD2	1:A:1302:ARG:HH11	1.70	0.56
5:F:270:THR:HG22	5:F:392:GLY:HA3	1.87	0.56
5:F:356:CYS:SG	5:F:357:ASN:N	2.76	0.56
1:A:843:PHE:CD2	1:A:871:LEU:HA	2.41	0.56
1:A:959:ASP:OD2	1:A:988:ARG:NH1	2.38	0.56
1:A:1099:ARG:O	1:A:1100:CYS:SG	2.63	0.56
1:A:1389:ARG:CD	1:A:1391:TRP:CD2	2.73	0.56
1:A:454:HIS:HB2	1:A:998:ASP:OD1	2.05	0.56
5:F:64:GLU:O	5:F:67:GLN:NE2	2.38	0.55
1:A:1264:PHE:CE1	1:A:1267:LEU:CD2	2.90	0.55
5:F:452:TYR:N	5:F:452:TYR:CD1	2.73	0.55
1:A:445:ASN:HD21	1:A:534:ARG:HD3	1.71	0.55
10:A:1911:PC1:H322	10:A:1911:PC1:H262	1.89	0.55
5:F:389:PHE:N	5:F:389:PHE:CD1	2.73	0.55
5:F:497:GLU:O	5:F:501:ARG:HD3	2.05	0.55
5:F:1036:GLN:HE21	5:F:1037:ALA:N	1.97	0.55
1:A:1389:ARG:CG	1:A:1391:TRP:CE3	2.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:732:VAL:O	5:F:820:ASP:CB	2.48	0.55
1:A:1139:HIS:HD2	1:A:1142:GLN:HB3	1.69	0.55
1:A:1020:LEU:HD12	1:A:1020:LEU:C	2.27	0.55
5:F:530:GLN:HG2	5:F:904:GLN:HE22	1.70	0.55
1:A:74:MET:HB3	1:A:78:ASP:HB3	1.88	0.55
1:A:1043:ILE:O	1:A:1047:ILE:HG13	2.07	0.55
5:F:518:ASP:O	5:F:520:ASN:N	2.40	0.55
1:A:1391:TRP:CE2	1:A:1396:PRO:HD2	2.42	0.55
1:A:1019:LEU:CD2	1:A:1045:PHE:CZ	2.90	0.54
1:A:1046:ILE:O	1:A:1050:ILE:HG12	2.07	0.54
4:E:15:CYS:O	4:E:191:LEU:HD11	2.07	0.54
5:F:510:PRO:HG3	5:F:762:TYR:CD1	2.42	0.54
5:F:647:TYR:HD1	5:F:713:GLY:CA	2.20	0.54
4:E:37:PRO:HA	4:E:174:ILE:HA	1.90	0.54
5:F:880:GLU:HA	5:F:1033:LEU:HD22	1.89	0.54
1:A:1046:ILE:HD13	10:A:1914:PC1:H381	1.90	0.54
5:F:247:ILE:HG22	5:F:247:ILE:O	2.08	0.54
1:A:513:LEU:HD23	1:A:527:LEU:HD11	1.90	0.54
1:A:216:GLU:OE2	1:A:1239:ARG:NH2	2.37	0.54
1:A:1262:LYS:CD	4:E:209:GLN:O	2.56	0.54
4:E:19:GLY:N	4:E:191:LEU:HD11	2.18	0.54
4:E:206:ARG:HB3	4:E:206:ARG:NH1	2.23	0.54
1:A:820:ASP:OD2	1:A:829:ASN:ND2	2.40	0.54
1:A:1173:LYS:O	1:A:1175:ARG:N	2.40	0.54
1:A:957:CYS:SG	1:A:958:ASN:N	2.81	0.54
1:A:1043:ILE:CG2	10:A:1904:PC1:H291	2.37	0.54
1:A:1016:TRP:CG	1:A:1017:PRO:HD3	2.43	0.54
1:A:369:TRP:NE1	3:C:293:MET:HA	2.23	0.53
5:F:510:PRO:HG2	5:F:767:TYR:CD2	2.42	0.53
5:F:634:ILE:HB	5:F:707:ARG:HH12	1.73	0.53
1:A:1244:ILE:O	1:A:1247:LEU:HD23	2.09	0.53
1:A:573:PHE:O	1:A:640:TYR:OH	2.25	0.53
1:A:942:PHE:CD2	1:A:1048:TYR:CD1	2.73	0.53
1:A:969:ARG:HB3	5:F:176:GLU:HG3	1.90	0.53
1:A:541:TYR:CD1	1:A:541:TYR:N	2.76	0.53
5:F:252:SER:OG	5:F:357:ASN:OD1	2.26	0.53
1:A:1264:PHE:CZ	1:A:1267:LEU:HD23	2.44	0.53
1:A:1334:TYR:CE1	1:A:1351:THR:CG2	2.92	0.53
5:F:452:TYR:N	5:F:452:TYR:HD1	2.05	0.53
5:F:669:TYR:CD1	5:F:670:CYS:CB	2.92	0.53
5:F:1061:VAL:HG23	5:F:1062:CYS:N	2.20	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:LEU:HD11	1:A:1064:VAL:HG11	1.91	0.53
1:A:820:ASP:HB2	1:A:821:PRO:C	2.30	0.53
1:A:1101:TYR:H	1:A:1101:TYR:HD1	1.56	0.53
1:A:1337:LEU:HD12	1:A:1350:TYR:CE1	2.39	0.53
1:A:1101:TYR:CD1	1:A:1101:TYR:N	2.74	0.53
5:F:55:GLY:HA3	5:F:718:LEU:HD11	1.91	0.52
1:A:542:TRP:N	1:A:542:TRP:CE3	2.76	0.52
1:A:816:LEU:HD21	1:A:901:VAL:HG12	1.91	0.52
5:F:411:TYR:CE1	5:F:1074:CYS:CA	2.88	0.52
1:A:1014:GLU:OE2	1:A:1015:GLY:N	2.43	0.52
1:A:1015:GLY:CA	1:A:1326:GLN:NE2	2.55	0.52
5:F:669:TYR:HD1	5:F:670:CYS:CA	2.15	0.52
5:F:77:ALA:HA	5:F:624:LEU:CD2	2.38	0.52
5:F:515:PHE:CD1	5:F:623:ALA:O	2.63	0.52
5:F:515:PHE:CE2	5:F:563:PHE:CE1	2.88	0.52
1:A:953:LYS:HE2	1:A:1038:ARG:HH12	1.75	0.52
5:F:359:ILE:HD11	5:F:432:LEU:HD21	1.91	0.52
1:A:217:LEU:HD11	1:A:1237:LEU:HD11	1.91	0.52
1:A:276:ASP:O	1:A:277:ASN:CB	2.57	0.52
1:A:366:TYR:O	1:A:369:TRP:HB3	2.10	0.52
1:A:632:TYR:HB3	1:A:633:PRO:CD	2.39	0.52
5:F:243:ARG:NH1	5:F:243:ARG:HG3	2.24	0.52
5:F:303:VAL:O	5:F:323:ALA:HB1	2.10	0.52
5:F:321:LYS:O	5:F:325:ASN:ND2	2.43	0.52
5:F:733:LYS:NZ	5:F:793:SER:HA	2.25	0.52
5:F:805:ILE:O	5:F:807:GLY:N	2.38	0.52
1:A:1306:PHE:CD2	1:A:1315:LEU:HD13	2.45	0.52
4:E:7:PRO:HA	4:E:10:ARG:HB2	1.92	0.52
5:F:1011:LEU:HD22	5:F:1016:LEU:HD12	1.92	0.51
1:A:1016:TRP:N	1:A:1017:PRO:CD	2.73	0.51
5:F:1007:HIS:NE2	5:F:1009:GLU:OE2	2.43	0.51
1:A:843:PHE:HE2	1:A:871:LEU:HA	1.68	0.51
5:F:309:LEU:HD12	5:F:353:ARG:CG	2.40	0.51
1:A:819:GLU:CG	1:A:897:ARG:HH21	2.24	0.51
1:A:843:PHE:HE2	1:A:871:LEU:N	2.09	0.51
1:A:1416:ARG:HB3	1:A:1460:THR:HB	1.91	0.51
5:F:1008:VAL:HG22	5:F:1019:ILE:HG12	1.92	0.51
1:A:225:THR:HA	1:A:266:PRO:HB3	1.92	0.51
4:E:131:LYS:HB3	4:E:133:ARG:HE	1.76	0.51
5:F:398:ARG:NH1	5:F:414:GLU:OE2	2.43	0.51
5:F:510:PRO:HG3	5:F:762:TYR:CE1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:ASN:HD21	1:A:531:ARG:HH21	1.59	0.51
5:F:669:TYR:CD1	5:F:670:CYS:HB2	2.46	0.51
1:A:1249[A]:ARG:NH2	1:A:1249[A]:ARG:HG2	2.24	0.51
4:E:19:GLY:H	4:E:191:LEU:HD13	1.70	0.51
5:F:198:ASN:HB2	5:F:208:GLN:HE22	1.76	0.51
5:F:894:VAL:HG11	5:F:993:PHE:CD2	2.44	0.51
1:A:287:GLN:NE2	1:A:621:TYR:OH	2.35	0.51
3:C:265:VAL:HG12	3:C:265:VAL:O	2.10	0.51
5:F:131:ALA:HB2	5:F:167:ALA:HB1	1.92	0.51
1:A:468:ASN:ND2	1:A:531:ARG:HH21	2.08	0.50
5:F:243:ARG:CG	5:F:243:ARG:NH1	2.73	0.50
1:A:974:VAL:HG21	1:A:986:ARG:HD2	1.93	0.50
1:A:1235:PHE:CE2	4:E:153:VAL:CG2	2.87	0.50
1:A:1244:ILE:HG23	1:A:1247:LEU:HD21	1.93	0.50
5:F:1052:GLN:O	5:F:1052:GLN:HG2	2.12	0.50
6:G:1:NAG:H61	6:G:2:NAG:C8	2.41	0.50
1:A:526:VAL:O	1:A:530:ILE:HG13	2.10	0.50
1:A:1337:LEU:HD11	1:A:1350:TYR:HE1	1.70	0.50
5:F:886:MET:CE	5:F:895:TYR:HH	2.25	0.50
5:F:77:ALA:HA	5:F:624:LEU:HD21	1.93	0.50
5:F:993:PHE:HB2	5:F:1008:VAL:HB	1.94	0.50
1:A:1005:MET:HB2	10:A:1911:PC1:H352	1.92	0.50
5:F:245:TRP:O	5:F:465:THR:HG21	2.12	0.50
1:A:1418:LYS:HG3	1:A:1420:LEU:H	1.77	0.50
5:F:75:ASN:O	5:F:76:ASN:HB3	2.11	0.50
5:F:173:ASP:CB	5:F:422:ARG:HH22	2.25	0.50
1:A:57:ILE:HA	1:A:60:THR:HG22	1.93	0.50
1:A:529:CYS:HA	1:A:532:LEU:HD12	1.94	0.50
1:A:591:GLU:OE2	1:A:593:ARG:CZ	2.59	0.50
4:E:107:ALA:HA	4:E:110:ILE:HD12	1.93	0.50
5:F:428:TYR:CD1	5:F:428:TYR:C	2.85	0.49
5:F:638:ILE:HD11	5:F:710:LEU:HB2	1.94	0.49
1:A:1106:PRO:HA	1:A:1109:TYR:HB3	1.95	0.49
1:A:915:LYS:HD3	1:A:915:LYS:H	1.75	0.49
1:A:170:LEU:HD12	1:A:173:LEU:HD13	1.95	0.49
10:A:1902:PC1:H221	10:A:1902:PC1:H321	1.94	0.49
5:F:438:LEU:HD12	5:F:1068:LEU:HD12	1.95	0.49
1:A:844:THR:O	1:A:847:ILE:HG13	2.12	0.49
1:A:993:ASN:O	1:A:995:PHE:N	2.39	0.49
1:A:1046:ILE:CD1	10:A:1914:PC1:C39	2.89	0.49
5:F:394:HIS:HD2	5:F:396:TYR:HB2	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:985:PHE:HZ	6:J:1:NAG:H61	1.77	0.49
5:F:389:PHE:N	5:F:389:PHE:HD1	2.10	0.49
5:F:482:LYS:HE3	5:F:485:LEU:HD12	1.93	0.49
5:F:584:GLU:O	5:F:613:PRO:HD3	2.12	0.49
5:F:153:ASP:OD1	5:F:160:GLN:CG	2.59	0.49
5:F:564:LEU:HD12	5:F:569:GLU:CB	2.43	0.49
5:F:744:THR:HG1	5:F:755:TRP:HZ3	1.60	0.49
1:A:49:GLU:O	1:A:50:TRP:O	2.31	0.49
1:A:1060:PHE:CZ	1:A:1376:PHE:CZ	2.96	0.49
1:A:363:LEU:HD22	3:C:399:ARG:HD3	1.95	0.49
1:A:1334:TYR:CZ	1:A:1351:THR:HG23	2.47	0.49
5:F:417:SER:OG	5:F:418:ILE:N	2.46	0.49
5:F:513:TYR:OH	5:F:567:GLU:OE2	2.28	0.49
5:F:95:ARG:HD3	5:F:494:VAL:HG22	1.95	0.49
1:A:808:PHE:HE2	1:A:903:ARG:HH22	1.61	0.48
5:F:333:THR:HG21	5:F:335:TYR:CE2	2.47	0.48
5:F:564:LEU:CD1	5:F:569:GLU:CB	2.90	0.48
5:F:733:LYS:HD2	5:F:793:SER:O	2.13	0.48
5:F:733:LYS:HZ3	5:F:793:SER:HA	1.78	0.48
1:A:842:VAL:O	1:A:845:VAL:HB	2.14	0.48
5:F:333:THR:HG21	5:F:335:TYR:HE2	1.78	0.48
5:F:733:LYS:CD	5:F:793:SER:O	2.61	0.48
1:A:974:VAL:HG23	1:A:986:ARG:HG3	1.95	0.48
1:A:1293:ALA:HB2	1:A:1339:ASP:H	1.77	0.48
1:A:1318:ARG:HH21	1:A:1328:ILE:HD11	1.79	0.48
4:E:208:PRO:HG2	4:E:214:SER:CB	2.43	0.48
5:F:184:GLU:OE2	5:F:212:SER:OG	2.27	0.48
5:F:744:THR:HB	5:F:755:TRP:CH2	2.48	0.48
1:A:269:ASN:ND2	1:A:273:THR:OG1	2.42	0.48
5:F:1062:CYS:O	5:F:1063:PHE:HD1	1.88	0.48
1:A:510:GLU:OE2	1:A:531:ARG:CD	2.55	0.48
1:A:542:TRP:HE3	1:A:542:TRP:H	1.61	0.48
1:A:820:ASP:CG	1:A:829:ASN:HD21	2.17	0.48
1:A:1081:LEU:HD22	1:A:1085:GLN:HE21	1.79	0.48
4:E:161:SER:HA	4:E:164:ARG:HD3	1.95	0.48
5:F:105:GLU:HG3	5:F:194:VAL:HG21	1.95	0.48
1:A:172:PRO:HB2	1:A:572:ILE:HD11	1.95	0.48
1:A:974:VAL:CG2	1:A:986:ARG:HG3	2.44	0.48
5:F:173:ASP:OD2	5:F:422:ARG:NH2	2.47	0.48
5:F:531:PRO:C	5:F:532:LYS:HG3	2.34	0.48
5:F:726:GLN:HB3	5:F:729:ILE:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:586:GLY:C	5:F:611:TRP:CZ2	2.87	0.48
1:A:500:ASP:OD1	1:A:537:LYS:NZ	2.47	0.47
1:A:1258:TRP:NE1	4:E:208:PRO:HD2	2.29	0.47
5:F:478:LYS:O	5:F:480:ASN:CG	2.52	0.47
5:F:478:LYS:C	5:F:480:ASN:N	2.66	0.47
4:E:207:MET:O	4:E:209:GLN:N	2.47	0.47
5:F:615:ASN:OD1	6:G:1:NAG:O5	2.32	0.47
1:A:587:PHE:CD2	1:A:625:MET:HE3	2.50	0.47
1:A:1262:LYS:CG	4:E:209:GLN:O	2.62	0.47
4:E:19:GLY:HA2	4:E:191:LEU:HD12	1.87	0.47
5:F:732:VAL:HG23	5:F:733:LYS:H	1.74	0.47
5:F:644:GLN:CA	5:F:647:TYR:HD2	2.12	0.47
1:A:534:ARG:O	1:A:537:LYS:HB2	2.14	0.47
1:A:594:ARG:NH2	1:A:1025:ASP:OD1	2.31	0.47
1:A:965:GLU:HA	1:A:990:TRP:CZ2	2.49	0.47
1:A:1390:ASP:HB3	1:A:1393:ILE:HD13	1.94	0.47
5:F:348:ASN:O	5:F:350:ASN:N	2.47	0.47
1:A:433:VAL:O	1:A:437:LEU:N	2.44	0.47
1:A:813:SER:HA	1:A:816:LEU:HB3	1.96	0.47
1:A:1199:LEU:HD12	1:A:1232:SER:HB3	1.96	0.47
1:A:1296:ASP:OD2	1:A:1302:ARG:NH2	2.47	0.47
4:E:15:CYS:O	4:E:191:LEU:HD21	2.15	0.47
5:F:38:TRP:HE1	5:F:831:THR:HB	1.79	0.47
1:A:820:ASP:CB	1:A:821:PRO:C	2.83	0.47
1:A:843:PHE:CE2	1:A:871:LEU:CB	2.98	0.47
1:A:1067:THR:HG21	1:A:1377:VAL:HG13	1.97	0.47
1:A:1429:ILE:HG21	1:A:1433:LEU:HD12	1.96	0.46
5:F:302:ASP:OD1	5:F:341:PHE:CE2	2.67	0.46
5:F:598:ASP:O	5:F:599:GLU:HG3	2.14	0.46
5:F:669:TYR:HD1	5:F:670:CYS:CB	2.26	0.46
5:F:1068:LEU:N	5:F:1068:LEU:HD23	2.30	0.46
4:E:211:PRO:O	4:E:212:TRP:CD1	2.68	0.46
5:F:536:VAL:CG1	5:F:537:GLY:H	2.18	0.46
5:F:563:PHE:HB3	5:F:577:ARG:HD3	1.97	0.46
1:A:165:ARG:HG3	1:A:165:ARG:HH11	1.80	0.46
1:A:533:LEU:HG	1:A:533:LEU:O	2.14	0.46
1:A:1154:ASN:O	1:A:1158:THR:HG23	2.15	0.46
5:F:297:ASN:HD21	5:F:331:GLY:CA	2.21	0.46
5:F:656:PHE:O	5:F:660:GLY:HA2	2.14	0.46
1:A:213:ILE:HG13	1:A:1240:VAL:HG11	1.97	0.46
5:F:159:ARG:NH2	5:F:224:PRO:O	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:219:TYR:O	5:F:219:TYR:CD2	2.68	0.46
5:F:597:GLN:HB2	5:F:768:LYS:HZ1	1.80	0.46
1:A:332:VAL:HB	1:A:657:LEU:HD11	1.97	0.46
5:F:106:ALA:HB2	5:F:191:LEU:HD21	1.97	0.46
5:F:563:PHE:HD2	5:F:577:ARG:HD3	1.80	0.46
1:A:121:GLY:HA3	1:A:174:ARG:NH2	2.31	0.46
1:A:912[B]:LYS:HA	1:A:915:LYS:HE3	1.97	0.46
5:F:518:ASP:O	5:F:521:GLY:N	2.39	0.46
5:F:795:ILE:O	5:F:819:ILE:N	2.49	0.46
1:A:911:ALA:O	1:A:915:LYS:CE	2.63	0.46
1:A:1016:TRP:CZ3	1:A:1020:LEU:HD23	2.51	0.46
1:A:823:ARG:CG	1:A:823:ARG:NH2	2.73	0.46
5:F:30:PRO:CG	5:F:1020:MET:CE	2.79	0.46
5:F:979:THR:HB	5:F:1038:GLU:HB3	1.98	0.46
10:A:1915:PC1:H321	10:A:1915:PC1:H31	1.71	0.45
5:F:458:LEU:HD23	5:F:461:VAL:HG11	1.97	0.45
5:F:445:GLN:O	5:F:466:LEU:CD1	2.64	0.45
1:A:1305:ASN:HD22	1:A:1311:GLN:CG	2.28	0.45
5:F:242:ARG:HA	5:F:247:ILE:HD11	1.99	0.45
5:F:1073:ASP:O	5:F:1074:CYS:C	2.54	0.45
1:A:614:GLU:HG3	1:A:1017:PRO:HG2	1.99	0.45
1:A:877:ALA:O	1:A:881:ILE:N	2.46	0.45
1:A:903:ARG:CB	1:A:904:PRO:HD3	2.42	0.45
1:A:1016:TRP:CZ3	1:A:1020:LEU:CD2	3.00	0.45
5:F:586:GLY:O	5:F:611:TRP:CE3	2.69	0.45
5:F:207:TRP:HE1	5:F:458:LEU:HD22	1.82	0.45
1:A:1261:ILE:HG22	4:E:207:MET:SD	2.57	0.45
1:A:276:ASP:O	1:A:277:ASN:HB3	2.16	0.45
1:A:1281:TYR:O	1:A:1360:TYR:OH	2.33	0.45
5:F:47:VAL:HG13	5:F:776:TYR:HE2	1.81	0.45
5:F:531:PRO:C	5:F:532:LYS:CG	2.85	0.45
5:F:587:GLU:HB3	5:F:610:THR:HG22	1.99	0.45
5:F:733:LYS:HB3	5:F:818:LYS:O	2.17	0.45
5:F:1068:LEU:HB2	5:F:1069:GLU:H	1.66	0.45
1:A:295:THR:HG22	1:A:1323:GLU:OE2	2.17	0.44
1:A:1334:TYR:CG	1:A:1334:TYR:O	2.70	0.44
1:A:376:MET:SD	1:A:422:ARG:NH1	2.90	0.44
5:F:1020:MET:HE2	5:F:1020:MET:HB3	1.77	0.44
1:A:1254:ARG:HG3	1:A:1255:THR:N	2.32	0.44
5:F:900:SER:OG	5:F:901:TYR:N	2.50	0.44
1:A:210:TYR:O	1:A:313:TYR:OH	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:820:ASP:N	1:A:821:PRO:CA	2.79	0.44
1:A:964:THR:OG1	1:A:965:GLU:N	2.50	0.44
1:A:305:ILE:HG23	10:A:1902:PC1:H121	1.99	0.44
1:A:896:LEU:HD23	1:A:899:LEU:HD12	2.00	0.44
4:E:19:GLY:H	4:E:191:LEU:HD11	1.77	0.44
5:F:96:SER:O	5:F:99:LEU:HB2	2.18	0.44
1:A:587:PHE:HB3	1:A:593:ARG:HH21	1.82	0.44
1:A:1094:LYS:HD3	4:E:212:TRP:CH2	2.53	0.44
1:A:1244:ILE:O	1:A:1247:LEU:CD2	2.65	0.44
5:F:894:VAL:HA	5:F:895:TYR:HA	1.68	0.44
1:A:536:PHE:O	1:A:539:THR:OG1	2.30	0.44
1:A:1262:LYS:CE	4:E:209:GLN:OE1	2.65	0.44
5:F:147:ILE:HG22	5:F:149:PRO:HD3	1.99	0.44
1:A:468:ASN:ND2	1:A:531:ARG:CZ	2.81	0.44
1:A:475:PHE:CZ	1:A:537:LYS:CE	2.99	0.44
1:A:1120:PHE:HZ	1:A:1167:LEU:HD12	1.83	0.44
1:A:1121:GLU:CG	1:A:1249[A]:ARG:HH22	2.30	0.44
4:E:209:GLN:HG3	4:E:210:ASN:N	2.33	0.44
5:F:564:LEU:HD12	5:F:569:GLU:HB2	1.99	0.44
5:F:738:VAL:HG13	5:F:744:THR:HG22	2.00	0.44
5:F:892:ILE:O	5:F:893:SER:HB3	2.18	0.44
1:A:539:THR:C	1:A:541:TYR:N	2.68	0.43
1:A:902:LEU:HD12	1:A:905:LEU:HD12	1.95	0.43
1:A:1046:ILE:HA	1:A:1049:ILE:HG22	2.00	0.43
1:A:1334:TYR:O	1:A:1334:TYR:CD1	2.70	0.43
3:C:398:GLN:HG2	3:C:402:LYS:HD2	2.00	0.43
5:F:428:TYR:CD1	5:F:428:TYR:O	2.70	0.43
5:F:508:LEU:N	5:F:508:LEU:HD23	2.33	0.43
1:A:423:TRP:HA	1:A:426:HIS:HD2	1.83	0.43
5:F:168:VAL:HG22	5:F:218:ARG:HG2	2.00	0.43
5:F:594:VAL:HG21	5:F:607:ARG:HH21	1.84	0.43
5:F:1068:LEU:O	5:F:1070:ASP:N	2.52	0.43
1:A:468:ASN:HD21	1:A:531:ARG:CD	2.30	0.43
5:F:190:ALA:C	5:F:192:ASP:H	2.21	0.43
5:F:509:CYS:O	5:F:511:ASN:N	2.52	0.43
5:F:860:GLY:O	5:F:878:PHE:N	2.44	0.43
1:A:225:THR:HG21	1:A:227:TYR:CZ	2.53	0.43
1:A:1016:TRP:HZ3	1:A:1020:LEU:CD2	2.31	0.43
1:A:307:ASN:OD1	1:A:307:ASN:N	2.46	0.43
1:A:540:LYS:HE3	1:A:540:LYS:HB2	1.74	0.43
1:A:846:GLU:HG3	1:A:847:ILE:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:656:PHE:CD1	5:F:660:GLY:O	2.71	0.43
1:A:794[B]:ARG:HE	1:A:794[B]:ARG:HB3	1.54	0.43
1:A:1044:PHE:HB2	10:A:1904:PC1:H2A1	2.00	0.43
5:F:298:SER:OG	5:F:299:ASN:N	2.51	0.43
5:F:598:ASP:N	5:F:598:ASP:OD1	2.50	0.43
1:A:1263:SER:O	1:A:1265:GLN:N	2.41	0.43
1:A:1403:LYS:HA	1:A:1406:TRP:HD1	1.83	0.43
2:B:169:ARG:NH1	2:B:173:GLU:OE1	2.51	0.43
4:E:17:LEU:HD23	4:E:20:ILE:HD12	2.00	0.43
1:A:1384:PHE:CE1	1:A:1388:THR:HG21	2.53	0.43
5:F:411:TYR:HA	5:F:1074:CYS:HB2	1.99	0.43
1:A:1046:ILE:C	1:A:1049:ILE:HG22	2.37	0.43
1:A:1321:THR:HG22	10:A:1909:PC1:H3D2	2.00	0.43
1:A:1331:ALA:O	1:A:1336:LYS:HG3	2.19	0.43
1:A:1370:PHE:CD1	1:A:1370:PHE:C	2.91	0.43
5:F:712:ALA:HA	5:F:715:THR:HG22	2.01	0.43
1:A:165:ARG:O	1:A:168:ARG:HG2	2.19	0.42
1:A:172:PRO:O	1:A:175:LEU:HB3	2.19	0.42
1:A:252:ARG:HD2	1:A:1302:ARG:NH1	2.33	0.42
1:A:449:ILE:HD12	1:A:449:ILE:HA	1.90	0.42
1:A:1244:ILE:HG22	1:A:1247:LEU:HD21	2.00	0.42
5:F:661:TYR:HD2	5:F:663:PHE:CZ	2.13	0.42
5:F:790:ALA:N	5:F:793:SER:OG	2.52	0.42
1:A:1091:TYR:CZ	1:A:1399:LEU:HB3	2.54	0.42
1:A:1104:LYS:HG3	1:A:1105:ASN:H	1.84	0.42
1:A:1389:ARG:HE	1:A:1391:TRP:CB	2.29	0.42
10:A:1912:PC1:H142	10:A:1912:PC1:H112	1.86	0.42
5:F:989:ASP:HB3	5:F:990:SER:H	1.69	0.42
1:A:370:ILE:HG21	3:C:404:ARG:NH1	2.34	0.42
5:F:309:LEU:HD12	5:F:353:ARG:HG2	2.00	0.42
5:F:509:CYS:C	5:F:511:ASN:N	2.73	0.42
1:A:1127:LEU:HD13	1:A:1160:ILE:HG21	2.00	0.42
5:F:381:ASP:HB3	5:F:383:LYS:HE3	2.00	0.42
1:A:165:ARG:HG3	1:A:165:ARG:NH1	2.33	0.42
1:A:559:ILE:HG22	1:A:563:LEU:HB2	2.01	0.42
1:A:614:GLU:HG3	1:A:1017:PRO:CG	2.49	0.42
1:A:1195:ILE:CD1	4:E:113:PHE:CE2	3.03	0.42
5:F:52:THR:O	5:F:722:TYR:OH	2.30	0.42
5:F:784:ASN:O	5:F:787:GLY:N	2.50	0.42
1:A:1293:ALA:O	1:A:1295:VAL:N	2.52	0.42
4:E:55:ARG:HD2	4:E:80:CYS:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1249[A]:ARG:CG	1:A:1249[A]:ARG:NH2	2.75	0.42
5:F:248:GLN:HE21	5:F:248:GLN:HB3	1.66	0.42
5:F:515:PHE:HE2	5:F:563:PHE:HE1	1.59	0.42
1:A:902:LEU:O	1:A:905:LEU:HB2	2.20	0.42
1:A:1132:THR:HG21	10:A:1912:PC1:H3A1	2.01	0.42
5:F:805:ILE:HB	5:F:808:LYS:HE2	2.02	0.42
5:F:886:MET:SD	5:F:895:TYR:CE1	3.13	0.42
5:F:496:LEU:HD23	5:F:499:ILE:HD12	2.02	0.42
1:A:1020:LEU:HD13	1:A:1045:PHE:HD2	1.85	0.42
1:A:632:TYR:CB	1:A:633:PRO:CD	2.98	0.41
1:A:945:ILE:HD11	10:A:1904:PC1:H361	2.02	0.41
1:A:1262:LYS:HG2	4:E:209:GLN:HA	2.01	0.41
1:A:1304:ASN:HD22	1:A:1304:ASN:HA	1.60	0.41
5:F:586:GLY:CA	5:F:611:TRP:CE2	3.02	0.41
5:F:594:VAL:HG21	5:F:607:ARG:HE	1.85	0.41
5:F:856:LEU:HD12	5:F:856:LEU:HA	1.91	0.41
5:F:1061:VAL:CG2	5:F:1062:CYS:H	2.19	0.41
1:A:1265:GLN:HE21	1:A:1265:GLN:HB3	1.65	0.41
1:A:1389:ARG:HH21	1:A:1389:ARG:HG2	1.84	0.41
5:F:348:ASN:C	5:F:350:ASN:N	2.71	0.41
5:F:598:ASP:C	5:F:599:GLU:CG	2.85	0.41
5:F:1073:ASP:O	5:F:1074:CYS:O	2.38	0.41
1:A:632:TYR:CD1	1:A:632:TYR:C	2.92	0.41
1:A:1049:ILE:HG23	1:A:1050:ILE:N	2.34	0.41
1:A:265:TRP:CZ2	1:A:271:GLY:HA2	2.52	0.41
1:A:1096:ARG:HB3	1:A:1097:PRO:HD2	2.02	0.41
1:A:1102:ILE:HG13	1:A:1411:PRO:HB2	2.02	0.41
3:C:282:PRO:HA	3:C:389:ILE:O	2.21	0.41
5:F:76:ASN:HD22	5:F:79:GLN:HB2	1.84	0.41
5:F:413:TYR:OH	5:F:428:TYR:HA	2.20	0.41
5:F:767:TYR:OH	5:F:812:PRO:O	2.35	0.41
5:F:769:ARG:HH22	5:F:858:ASP:HB3	1.86	0.41
5:F:878:PHE:HB3	5:F:886:MET:HE3	2.02	0.41
1:A:472:LEU:HD23	1:A:472:LEU:HA	1.92	0.41
1:A:526:VAL:HG22	10:A:1904:PC1:H331	2.02	0.41
5:F:509:CYS:HB2	5:F:630:SER:HB3	2.03	0.41
1:A:999:ASN:HB2	1:A:1002:SER:H	1.86	0.41
1:A:1052:ILE:HD13	1:A:1052:ILE:HA	1.90	0.41
10:A:1903:PC1:H2E2	10:A:1903:PC1:H3C2	2.03	0.41
5:F:55:GLY:O	5:F:59:LEU:N	2.46	0.41
5:F:382:LYS:NZ	5:F:407:GLU:HG2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:681:GLU:O	5:F:685:ASN:ND2	2.54	0.41
5:F:894:VAL:CB	5:F:993:PHE:HE2	2.29	0.41
1:A:113:HIS:O	1:A:119:ARG:NE	2.36	0.41
1:A:1389:ARG:NE	1:A:1391:TRP:HB2	2.29	0.41
10:A:1909:PC1:H3C2	10:A:1909:PC1:H391	1.74	0.41
5:F:243:ARG:HH11	5:F:243:ARG:HG3	1.84	0.41
5:F:303:VAL:O	5:F:303:VAL:HG13	2.21	0.41
1:A:189:ILE:HG13	1:A:654:ASN:HD22	1.85	0.41
1:A:248:THR:HG22	1:A:249:GLY:H	1.86	0.41
1:A:369:TRP:O	1:A:369:TRP:CD1	2.71	0.41
1:A:604:LEU:HA	1:A:604:LEU:HD12	1.89	0.41
1:A:794[B]:ARG:NH2	1:A:795:ILE:HD11	2.36	0.41
1:A:821:PRO:HG3	1:A:1286:MET:CG	2.42	0.41
1:A:965:GLU:HA	1:A:990:TRP:HZ2	1.85	0.41
1:A:1043:ILE:CG1	1:A:1047:ILE:HD11	2.37	0.41
10:A:1912:PC1:H231	10:A:1912:PC1:H261	1.53	0.41
5:F:736:PHE:CE1	5:F:796:MET:SD	3.14	0.41
4:E:113:PHE:HD1	4:E:113:PHE:HA	1.69	0.41
4:E:211:PRO:C	4:E:212:TRP:CD1	2.95	0.41
4:E:207:MET:C	4:E:209:GLN:N	2.75	0.40
1:A:794[A]:ARG:NH1	1:A:798:ALA:CB	2.84	0.40
1:A:1201:GLU:O	1:A:1204:THR:OG1	2.37	0.40
1:A:1391:TRP:CD1	1:A:1397:HIS:CD2	2.98	0.40
4:E:207:MET:C	4:E:209:GLN:H	2.24	0.40
5:F:628:THR:HA	5:F:631:PHE:HE2	1.86	0.40
1:A:656:PHE:CE1	1:A:1060:PHE:HD2	2.39	0.40
1:A:1122:TYR:HD1	1:A:1122:TYR:HA	1.77	0.40
1:A:1391:TRP:CZ2	1:A:1396:PRO:CD	3.02	0.40
3:C:388:TYR:HB2	3:C:430:PHE:CD1	2.56	0.40
5:F:530:GLN:CG	5:F:904:GLN:HE22	2.34	0.40
5:F:895:TYR:CD1	5:F:895:TYR:N	2.90	0.40
1:A:299:TYR:O	1:A:303:ASP:HB2	2.22	0.40
1:A:369:TRP:CD1	3:C:293:MET:HA	2.56	0.40
1:A:611:LEU:HD12	1:A:611:LEU:HA	1.86	0.40
4:E:15:CYS:O	4:E:191:LEU:CD1	2.70	0.40
5:F:451:VAL:HG23	5:F:559:VAL:O	2.20	0.40
5:F:584:GLU:O	5:F:613:PRO:CD	2.69	0.40
1:A:1249[B]:ARG:HA	1:A:1249[B]:ARG:HD2	1.97	0.40
1:A:1441:HIS:HB3	1:A:1443:VAL:N	2.36	0.40
5:F:1002:CYS:SG	5:F:1026:THR:OG1	2.76	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	1268/1873 (68%)	1103 (87%)	143 (11%)	22 (2%)	9 45
2	B	98/106 (92%)	90 (92%)	8 (8%)	0	100 100
3	C	174/199 (87%)	171 (98%)	3 (2%)	0	100 100
4	E	156/222 (70%)	142 (91%)	12 (8%)	2 (1%)	12 50
5	F	929/1106 (84%)	764 (82%)	137 (15%)	28 (3%)	4 33
All	All	2625/3506 (75%)	2270 (86%)	303 (12%)	52 (2%)	11 41

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	TRP
1	A	977	ASP
1	A	1174	ALA
1	A	1391	TRP
1	A	1441	HIS
5	F	77	ALA
5	F	303	VAL
5	F	351	VAL
5	F	352	SER
5	F	451	VAL
5	F	478	LYS
5	F	479	THR
5	F	536	VAL
5	F	598	ASP
5	F	785	LYS
5	F	806	GLN
5	F	1061	VAL
1	A	80	ASN
1	A	1440	PRO
4	E	209	GLN
5	F	732	VAL

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Mol	Chain	Res	Type
5	F	733	LYS
5	F	1068	LEU
1	A	819	GLU
1	A	1344	TYR
1	A	1354	THR
5	F	297	ASN
5	F	349	TYR
5	F	353	ARG
5	F	531	PRO
5	F	786	SER
1	A	994	ASP
1	A	1138	GLN
1	A	1333	SER
1	A	1355	ASN
5	F	175	TYR
5	F	313	ASN
5	F	734	ALA
5	F	1069	GLU
1	A	820	ASP
1	A	903	ARG
1	A	1323	GLU
4	E	212	TRP
1	A	542	TRP
1	A	1294	LEU
5	F	532	LYS
5	F	894	VAL
5	F	1062	CYS
5	F	519	PRO
1	A	457	PRO
1	A	252	ARG
1	A	630	PRO

5.3.2 Protein sidechains (i)

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1073/1628 (66%)	1020 (95%)	53 (5%)	25	59
2	B	59/91 (65%)	56 (95%)	3 (5%)	24	58
3	C	143/179 (80%)	141 (99%)	2 (1%)	67	85
4	E	141/192 (73%)	134 (95%)	7 (5%)	24	59
5	F	837/974 (86%)	793 (95%)	44 (5%)	22	58
All	All	2253/3064 (74%)	2144 (95%)	109 (5%)	29	60

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	174	ARG
1	A	206	MET
1	A	221	LYS
1	A	224	LYS
1	A	262	ARG
1	A	276	ASP
1	A	277	ASN
1	A	327	ASN
1	A	422	ARG
1	A	525	SER
1	A	529	CYS
1	A	537	LYS
1	A	540	LYS
1	A	541	TYR
1	A	542	TRP
1	A	649	ASN
1	A	789	ARG
1	A	794[A]	ARG
1	A	794[B]	ARG
1	A	800	TRP
1	A	823	ARG
1	A	846	GLU
1	A	915	LYS
1	A	926	ARG
1	A	930	ASN
1	A	954	PHE
1	A	955	PHE

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Mol	Chain	Res	Type
1	A	982	GLN
1	A	986	ARG
1	A	988	ARG
1	A	1020	LEU
1	A	1036	ASN
1	A	1101	TYR
1	A	1120	PHE
1	A	1121	GLU
1	A	1122	TYR
1	A	1131	ASN
1	A	1229	ARG
1	A	1239	ARG
1	A	1247	LEU
1	A	1249[A]	ARG
1	A	1249[B]	ARG
1	A	1262	LYS
1	A	1264	PHE
1	A	1265	GLN
1	A	1276	MET
1	A	1302	ARG
1	A	1304	ASN
1	A	1306	PHE
1	A	1370	PHE
1	A	1376	PHE
1	A	1388	THR
2	B	115	PRO
2	B	167	SER
2	B	170	LEU
3	C	299	ASP
3	C	310	SER
4	E	10	ARG
4	E	15	CYS
4	E	113	PHE
4	E	191	LEU
4	E	206	ARG
4	E	207	MET
4	E	212	TRP
5	F	95	ARG
5	F	97	LYS
5	F	148	LYS
5	F	186	ASN
5	F	243	ARG

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Mol	Chain	Res	Type
5	F	248	GLN
5	F	299	ASN
5	F	311	GLN
5	F	333	THR
5	F	348	ASN
5	F	353	ARG
5	F	389	PHE
5	F	428	TYR
5	F	447	GLN
5	F	452	TYR
5	F	478	LYS
5	F	501	ARG
5	F	508	LEU
5	F	509	CYS
5	F	515	PHE
5	F	528	ASN
5	F	529	LEU
5	F	544	ARG
5	F	564	LEU
5	F	591	ARG
5	F	597	GLN
5	F	599	GLU
5	F	615	ASN
5	F	692	ARG
5	F	733	LYS
5	F	755	TRP
5	F	891	ASN
5	F	895	TYR
5	F	989	ASP
5	F	991	LYS
5	F	1020	MET
5	F	1032	ARG
5	F	1036	GLN
5	F	1049	MET
5	F	1052	GLN
5	F	1062	CYS
5	F	1068	LEU
5	F	1070	ASP
5	F	1071	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	269	ASN
1	A	372	GLN
1	A	426	HIS
1	A	445	ASN
1	A	468	ASN
1	A	916	HIS
1	A	1036	ASN
1	A	1071	GLN
1	A	1085	GLN
1	A	1139	HIS
1	A	1154	ASN
1	A	1265	GLN
1	A	1304	ASN
1	A	1305	ASN
1	A	1311	GLN
1	A	1326	GLN
1	A	1397	HIS
5	F	76	ASN
5	F	311	GLN
5	F	313	ASN
5	F	316	ASN
5	F	348	ASN
5	F	480	ASN
5	F	511	ASN
5	F	556	GLN
5	F	655	ASN
5	F	679	ASN
5	F	685	ASN
5	F	1036	GLN
5	F	1052	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
5	ETA	F	1075	5	3,3,3	0.43	0	2,2,2	0.53	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ETA	F	1075	5	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	1075	ETA	O-C-CA-N

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	1075	ETA	1	0

5.5 Carbohydrates (i)

17 monosaccharides 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	$\#\|Z\|>2$
6	NAG	D	1	5,6	14,14,15	0.61	1 (7%)	17,19,21	0.92	1 (5%)
6	NAG	D	2	6	14,14,15	0.47	0	17,19,21	0.42	0
6	NAG	G	1	5,6	14,14,15	0.30	0	17,19,21	0.61	0
6	NAG	G	2	6	14,14,15	0.30	0	17,19,21	0.61	0
7	NAG	H	1	5,7	14,14,15	0.65	1 (7%)	17,19,21	0.58	0
7	NAG	H	2	7	14,14,15	0.26	0	17,19,21	0.80	1 (5%)
7	BMA	H	3	7	11,11,12	0.87	0	15,15,17	0.81	0
7	NAG	I	1	5,7	14,14,15	0.31	0	17,19,21	0.77	0
7	NAG	I	2	7	14,14,15	0.31	0	17,19,21	0.57	0
7	BMA	I	3	7	11,11,12	0.61	0	15,15,17	0.93	2 (13%)
6	NAG	J	1	5,6	14,14,15	0.26	0	17,19,21	0.50	0
6	NAG	J	2	6	14,14,15	0.28	0	17,19,21	0.50	0
6	NAG	K	1	5,6	14,14,15	0.58	0	17,19,21	0.95	1 (5%)
6	NAG	K	2	6	14,14,15	0.58	0	17,19,21	1.02	1 (5%)
8	NAG	L	1	8,5	14,14,15	0.35	0	17,19,21	0.63	0
8	NAG	L	2	8	14,14,15	0.32	0	17,19,21	0.86	1 (5%)
8	NAG	L	3	8	14,14,15	0.43	0	17,19,21	0.67	1 (5%)

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
6	NAG	D	1	5,6	-	3/6/23/26	0/1/1/1
6	NAG	D	2	6	-	2/6/23/26	0/1/1/1
6	NAG	G	1	5,6	-	2/6/23/26	0/1/1/1
6	NAG	G	2	6	-	4/6/23/26	0/1/1/1
7	NAG	H	1	5,7	-	2/6/23/26	0/1/1/1
7	NAG	H	2	7	-	2/6/23/26	0/1/1/1
7	BMA	H	3	7	-	0/2/19/22	0/1/1/1
7	NAG	I	1	5,7	-	2/6/23/26	0/1/1/1
7	NAG	I	2	7	-	2/6/23/26	0/1/1/1
7	BMA	I	3	7	-	2/2/19/22	0/1/1/1
6	NAG	J	1	5,6	-	1/6/23/26	0/1/1/1
6	NAG	J	2	6	-	2/6/23/26	0/1/1/1
6	NAG	K	1	5,6	-	2/6/23/26	0/1/1/1
6	NAG	K	2	6	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	L	1	8,5	-	1/6/23/26	0/1/1/1
8	NAG	L	2	8	-	2/6/23/26	0/1/1/1
8	NAG	L	3	8	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	1	NAG	C1-C2	2.14	1.55	1.52
7	H	1	NAG	O5-C1	-2.02	1.40	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	K	1	NAG	C1-O5-C5	3.39	116.79	112.19
6	K	2	NAG	C2-N2-C7	3.03	127.21	122.90
8	L	2	NAG	C1-O5-C5	2.89	116.11	112.19
6	D	1	NAG	C2-N2-C7	2.77	126.85	122.90
7	H	2	NAG	C1-O5-C5	2.66	115.80	112.19
8	L	3	NAG	C1-O5-C5	2.34	115.36	112.19
7	I	3	BMA	C1-O5-C5	2.23	115.21	112.19
7	I	3	BMA	O2-C2-C3	-2.02	106.10	110.14

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	L	2	NAG	O5-C5-C6-O6
8	L	3	NAG	O5-C5-C6-O6
7	I	3	BMA	O5-C5-C6-O6
7	I	3	BMA	C4-C5-C6-O6
6	K	1	NAG	O5-C5-C6-O6
7	I	2	NAG	O5-C5-C6-O6
6	J	2	NAG	O5-C5-C6-O6
7	H	2	NAG	O5-C5-C6-O6
6	D	1	NAG	C4-C5-C6-O6
6	D	2	NAG	O5-C5-C6-O6
7	I	1	NAG	C4-C5-C6-O6
6	D	1	NAG	O5-C5-C6-O6
6	J	2	NAG	C4-C5-C6-O6
7	H	2	NAG	C4-C5-C6-O6
6	K	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	L	2	NAG	C4-C5-C6-O6
6	D	2	NAG	C4-C5-C6-O6
7	H	1	NAG	O5-C5-C6-O6
7	I	1	NAG	O5-C5-C6-O6
8	L	3	NAG	C4-C5-C6-O6
6	G	2	NAG	O5-C5-C6-O6
7	I	2	NAG	C4-C5-C6-O6
6	G	1	NAG	O5-C5-C6-O6
6	J	1	NAG	O5-C5-C6-O6
7	H	1	NAG	C4-C5-C6-O6
6	G	2	NAG	C4-C5-C6-O6
6	K	2	NAG	C4-C5-C6-O6
6	K	2	NAG	O5-C5-C6-O6
6	K	2	NAG	C3-C2-N2-C7
8	L	1	NAG	C4-C5-C6-O6
6	G	1	NAG	C4-C5-C6-O6
6	G	2	NAG	C8-C7-N2-C2
6	D	1	NAG	C3-C2-N2-C7
6	G	2	NAG	O7-C7-N2-C2

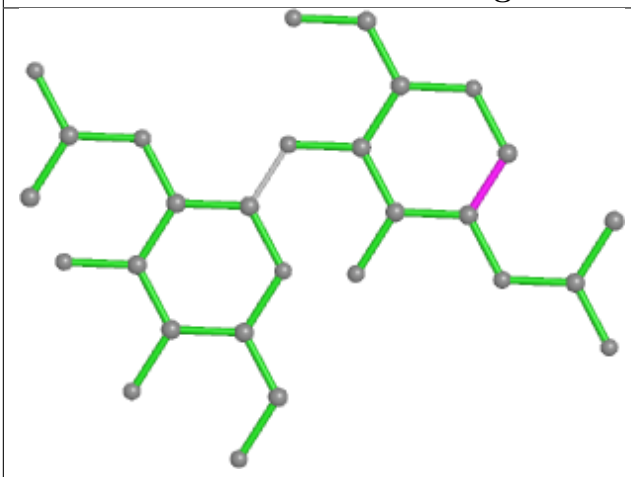
There are no ring outliers.

3 monomers are involved in 6 short contacts:

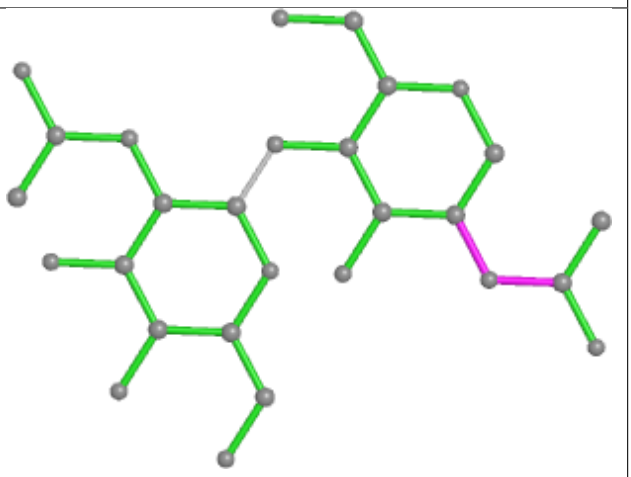
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	J	1	NAG	1	0
6	G	2	NAG	4	0
6	G	1	NAG	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

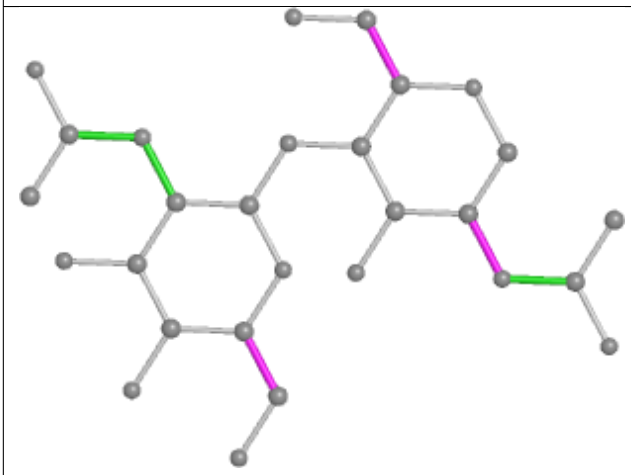
Oligosaccharide Chain D



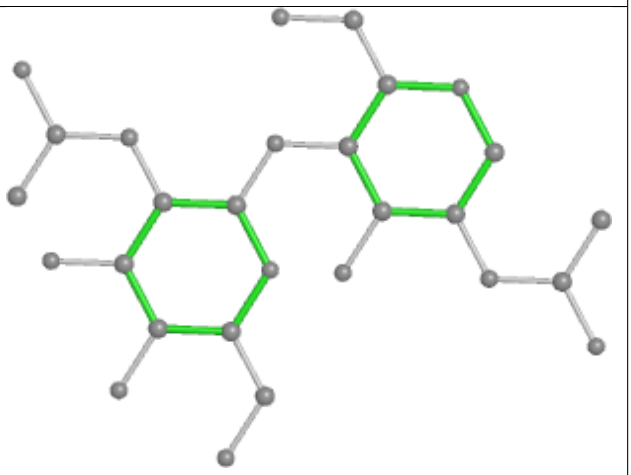
Bond lengths



Bond angles

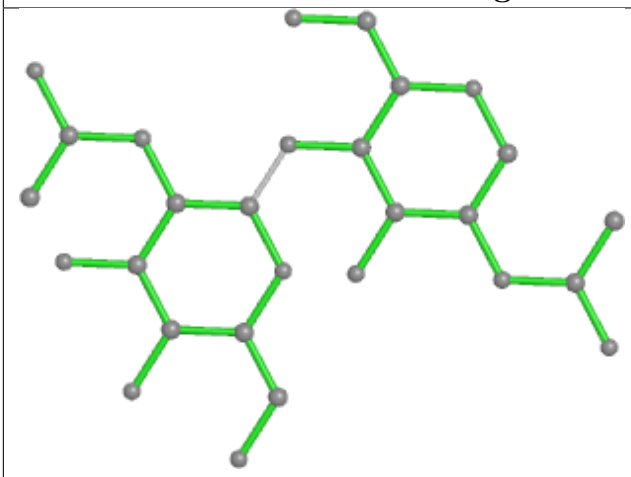


Torsions

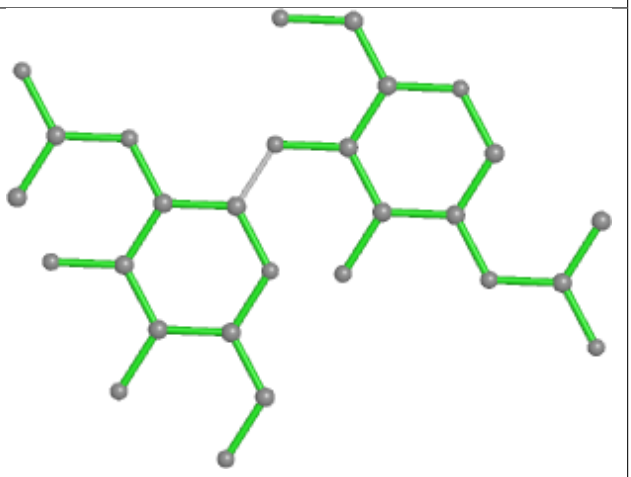


Rings

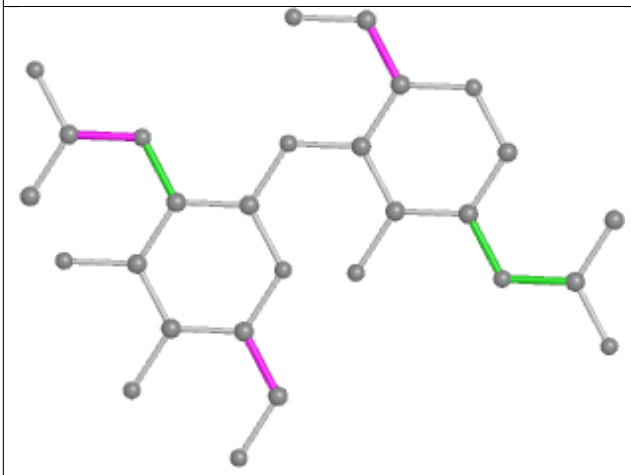
Oligosaccharide Chain G



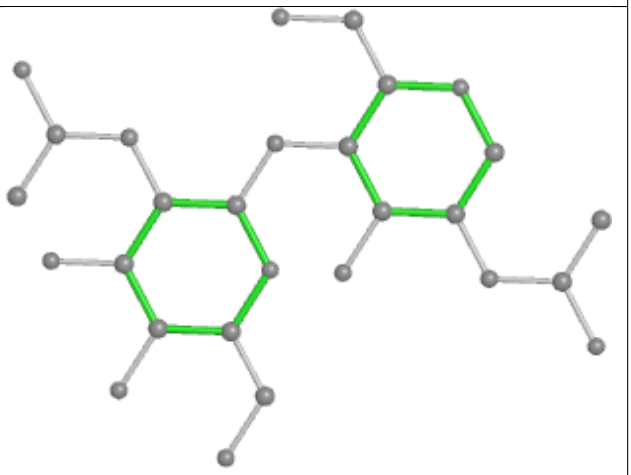
Bond lengths



Bond angles

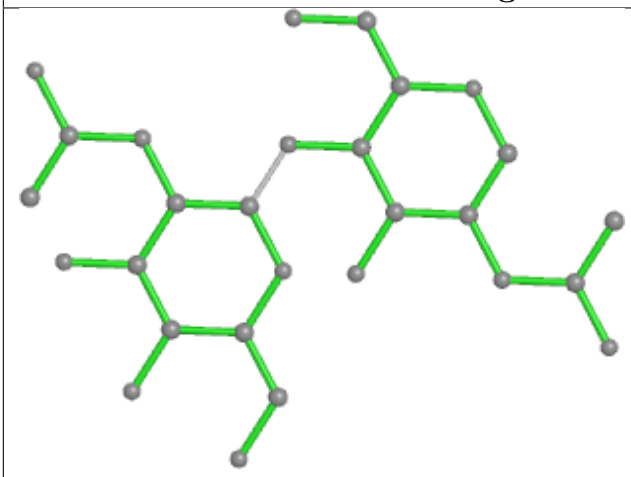


Torsions

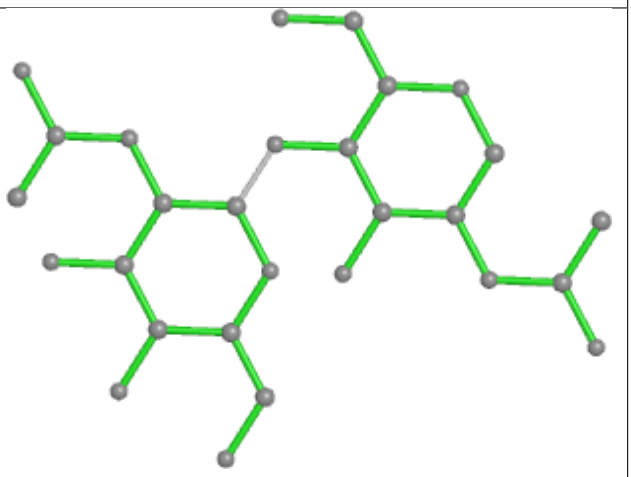


Rings

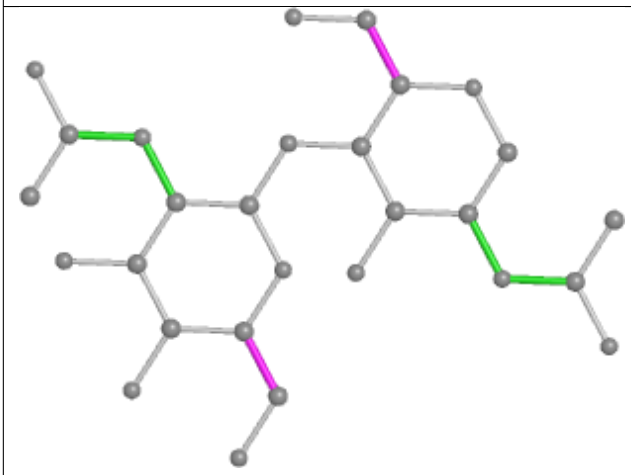
Oligosaccharide Chain J



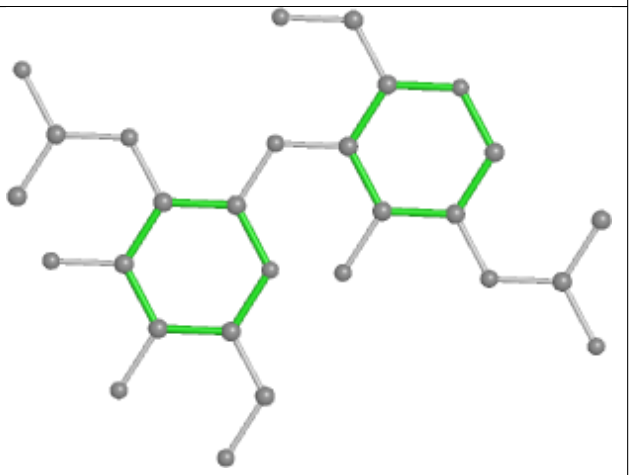
Bond lengths



Bond angles

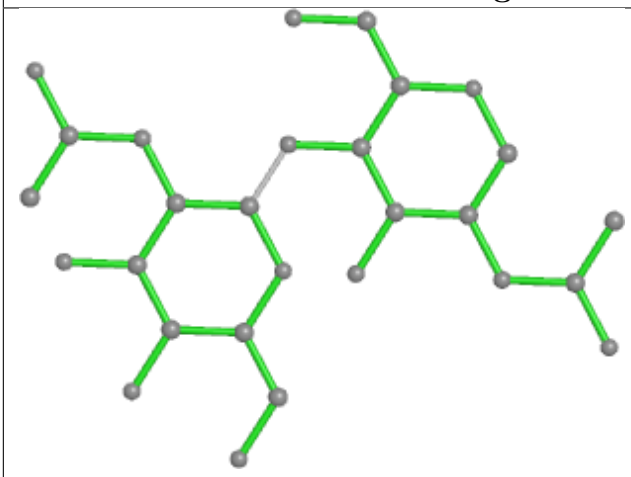


Torsions

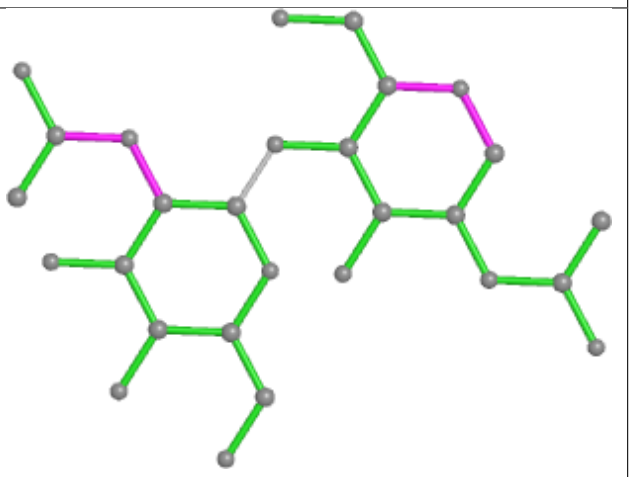


Rings

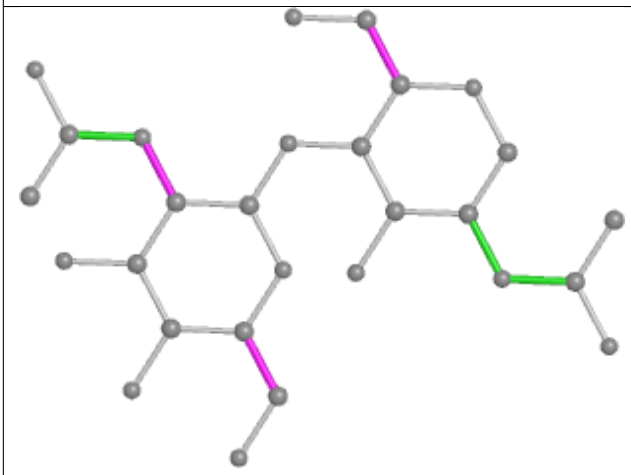
Oligosaccharide Chain K



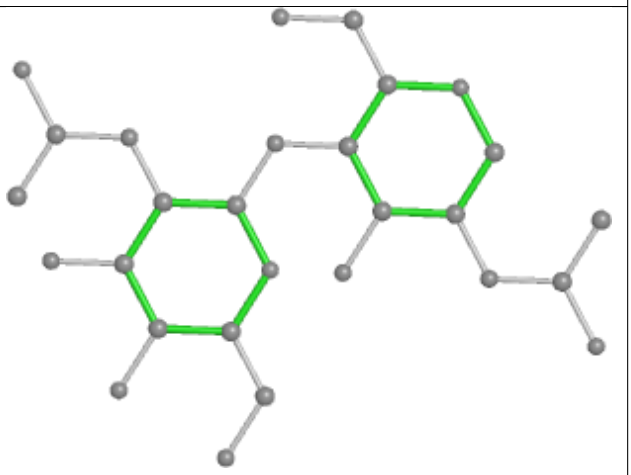
Bond lengths



Bond angles

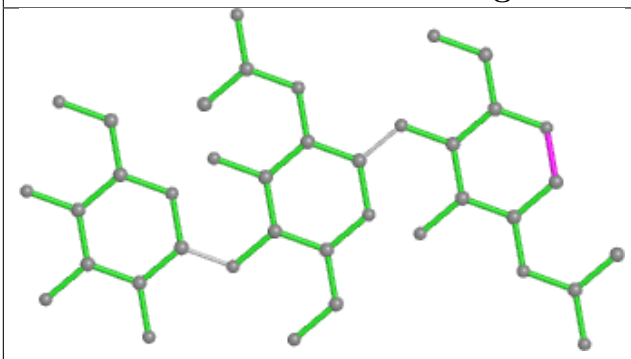


Torsions

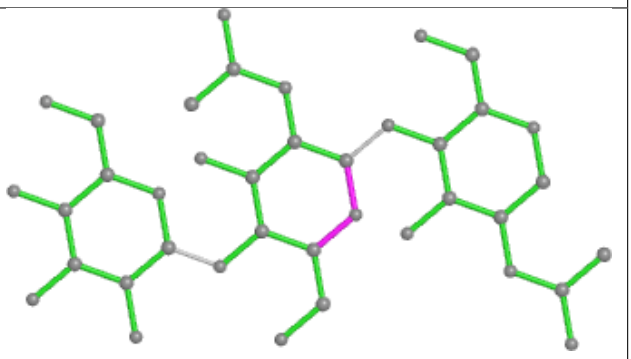


Rings

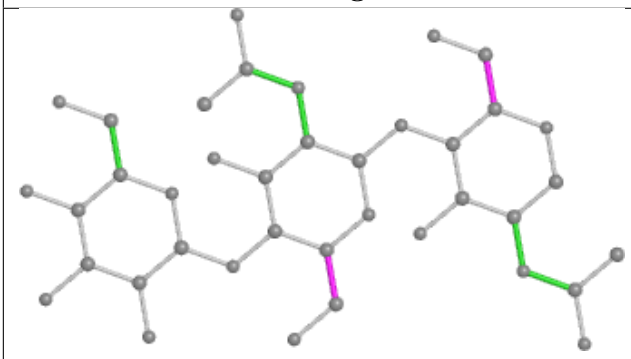
Oligosaccharide Chain H



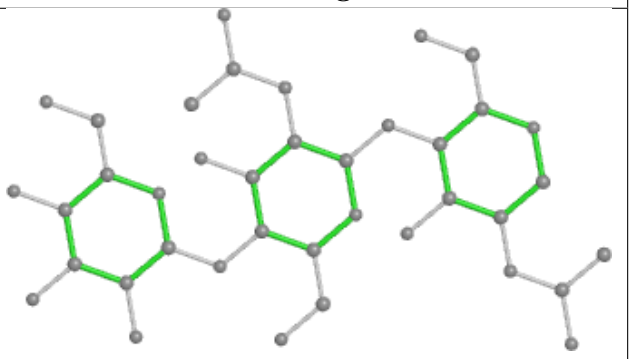
Bond lengths



Bond angles

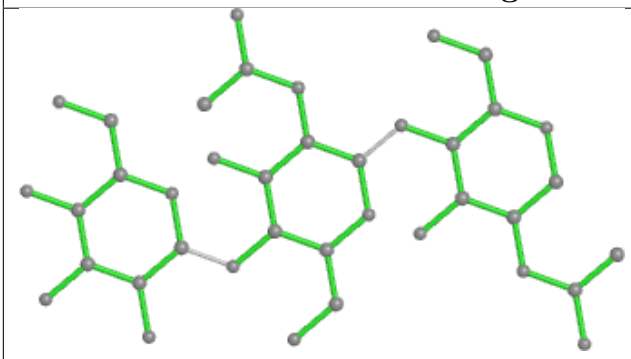


Torsions

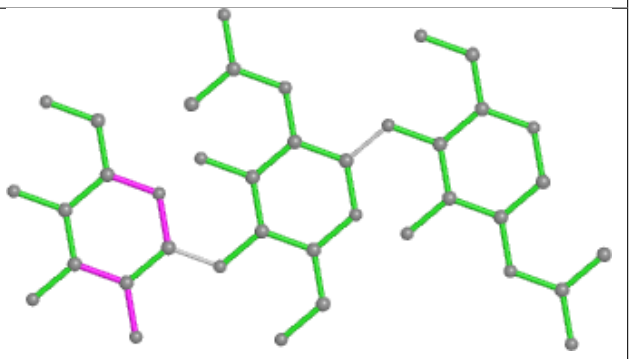


Rings

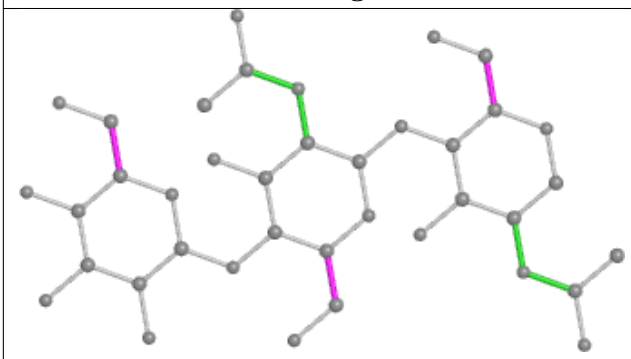
Oligosaccharide Chain I



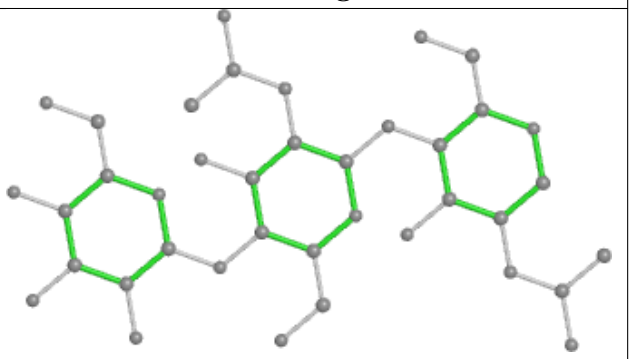
Bond lengths



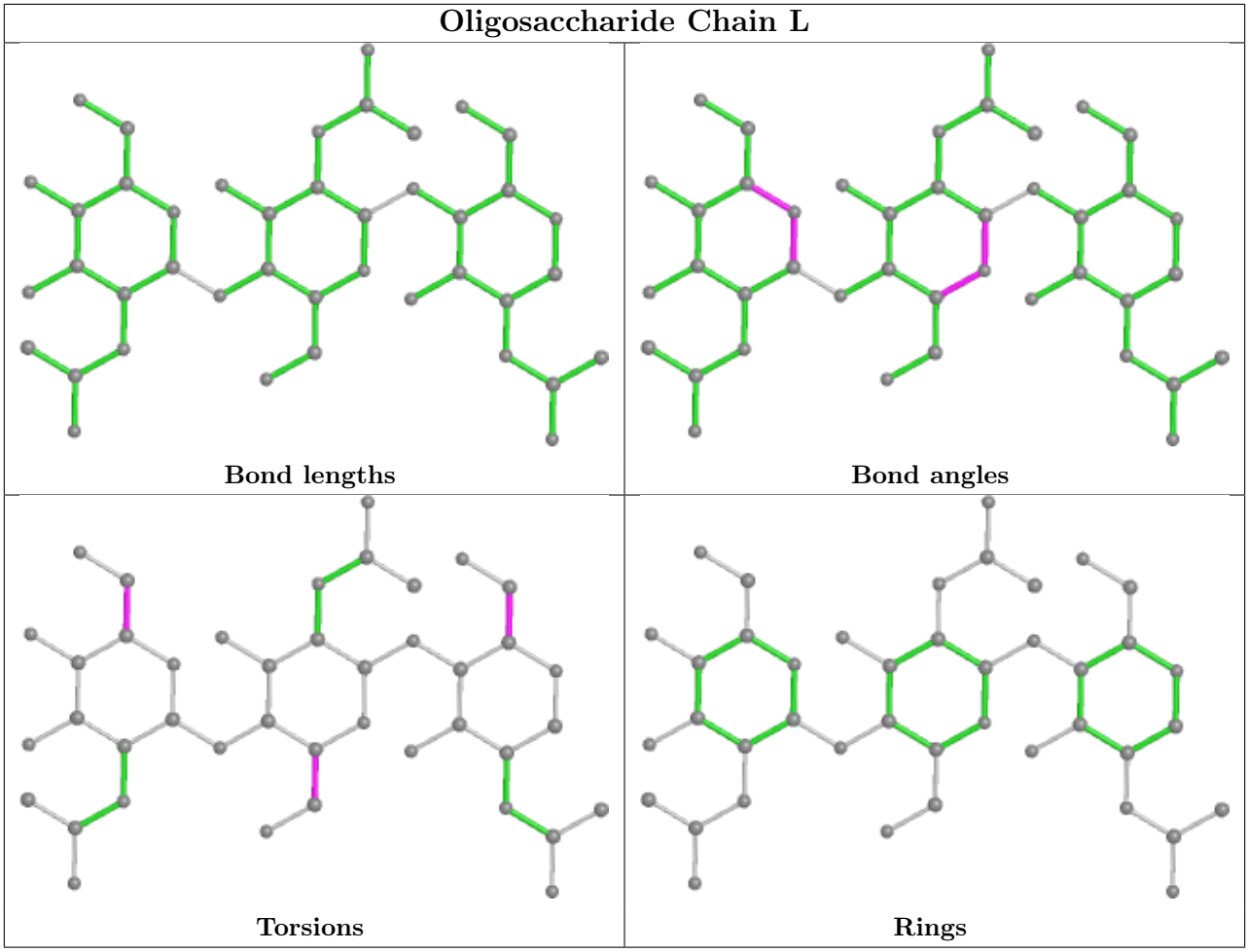
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 25 ligands modelled in this entry, 3 are monoatomic - leaving 22 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
10	PC1	A	1906	-	17,17,53	0.69	0	16,16,61	0.48	0
10	PC1	A	1915	-	47,47,53	1.17	3 (6%)	53,55,61	1.21	4 (7%)
9	NAG	F	1219	5	14,14,15	0.38	0	17,19,21	0.45	0
9	NAG	F	1214	5	14,14,15	0.64	0	17,19,21	0.57	0
10	PC1	A	1912	-	44,44,53	1.18	3 (6%)	50,52,61	1.10	3 (6%)
10	PC1	A	1908	-	11,11,53	0.61	0	10,10,61	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	PC1	A	1913	-	17,17,53	0.72	0	16,16,61	0.39	0
10	PC1	A	1914	-	13,13,53	0.57	0	12,12,61	0.49	0
10	PC1	A	1903	-	53,53,53	1.09	3 (5%)	59,61,61	1.02	3 (5%)
9	NAG	F	1206	5	14,14,15	0.50	0	17,19,21	0.38	0
10	PC1	A	1909	-	14,14,53	0.62	0	13,13,61	0.44	0
9	NAG	F	1213	5	14,14,15	0.45	0	17,19,21	0.69	1 (5%)
10	PC1	A	1910	-	17,17,53	0.77	0	16,16,61	0.38	0
10	PC1	A	1902	-	43,43,53	1.18	5 (11%)	49,51,61	1.19	3 (6%)
10	PC1	A	1904	-	41,41,53	1.22	3 (7%)	47,49,61	1.19	4 (8%)
10	PC1	A	1911	-	47,47,53	1.08	3 (6%)	53,55,61	1.10	4 (7%)
9	NAG	F	1220	5	14,14,15	0.81	1 (7%)	17,19,21	1.05	1 (5%)
9	NAG	F	1221	5	14,14,15	0.59	1 (7%)	17,19,21	0.60	0
10	PC1	A	1905	-	37,37,53	1.23	2 (5%)	43,45,61	1.14	3 (6%)
10	PC1	A	1907	-	11,11,53	0.70	0	10,10,61	0.37	0
9	NAG	F	1203	5	14,14,15	0.30	0	17,19,21	0.47	0
9	NAG	A	1901	1	14,14,15	0.39	0	17,19,21	0.55	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
10	PC1	A	1906	-	-	9/15/15/57	-
10	PC1	A	1915	-	-	29/51/51/57	-
9	NAG	F	1219	5	-	2/6/23/26	0/1/1/1
9	NAG	F	1214	5	-	0/6/23/26	0/1/1/1
10	PC1	A	1912	-	-	25/48/48/57	-
10	PC1	A	1908	-	-	5/9/9/57	-
10	PC1	A	1913	-	-	4/15/15/57	-
10	PC1	A	1914	-	-	6/11/11/57	-
10	PC1	A	1903	-	-	27/57/57/57	-
9	NAG	F	1206	5	-	0/6/23/26	0/1/1/1
10	PC1	A	1909	-	-	7/12/12/57	-
9	NAG	F	1213	5	-	2/6/23/26	0/1/1/1
10	PC1	A	1910	-	-	9/15/15/57	-
10	PC1	A	1902	-	-	23/47/47/57	-
10	PC1	A	1904	-	-	19/45/45/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	PC1	A	1911	-	-	30/51/51/57	-
9	NAG	F	1220	5	-	0/6/23/26	0/1/1/1
9	NAG	F	1221	5	-	1/6/23/26	0/1/1/1
10	PC1	A	1905	-	-	29/41/41/57	-
10	PC1	A	1907	-	-	4/9/9/57	-
9	NAG	F	1203	5	-	0/6/23/26	0/1/1/1
9	NAG	A	1901	1	-	2/6/23/26	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1904	PC1	O31-C31	3.29	1.43	1.33
10	A	1902	PC1	O21-C21	3.24	1.43	1.34
10	A	1912	PC1	O31-C31	3.22	1.42	1.33
10	A	1903	PC1	O31-C31	3.22	1.42	1.33
10	A	1915	PC1	O31-C31	3.19	1.42	1.33
10	A	1905	PC1	O21-C21	3.11	1.43	1.34
10	A	1915	PC1	O21-C21	3.09	1.43	1.34
10	A	1905	PC1	O31-C31	3.02	1.42	1.33
10	A	1902	PC1	O31-C31	2.97	1.42	1.33
10	A	1903	PC1	O21-C21	2.95	1.42	1.34
10	A	1904	PC1	O21-C21	2.88	1.42	1.34
10	A	1911	PC1	O21-C2	-2.77	1.39	1.46
10	A	1912	PC1	O21-C21	2.74	1.42	1.34
10	A	1912	PC1	O21-C2	-2.68	1.39	1.46
10	A	1911	PC1	O31-C31	2.67	1.41	1.33
10	A	1915	PC1	O21-C2	-2.65	1.40	1.46
10	A	1911	PC1	O21-C21	2.57	1.41	1.34
10	A	1903	PC1	O21-C2	-2.45	1.40	1.46
10	A	1904	PC1	O21-C2	-2.43	1.40	1.46
9	F	1220	NAG	C1-C2	2.31	1.55	1.52
10	A	1902	PC1	O21-C2	-2.17	1.41	1.46
10	A	1902	PC1	C22-C21	2.12	1.56	1.50
10	A	1902	PC1	P-O11	2.01	1.67	1.59
9	F	1221	NAG	O5-C1	2.01	1.46	1.43

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	1915	PC1	O21-C21-C22	5.40	123.15	111.50
10	A	1902	PC1	O21-C21-C22	5.05	122.38	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	1912	PC1	O21-C21-C22	4.37	120.91	111.50
10	A	1904	PC1	O21-C21-C22	4.07	120.28	111.50
10	A	1904	PC1	C15-N-C13	4.02	119.32	108.97
10	A	1905	PC1	C15-N-C13	3.82	118.80	108.97
9	F	1220	NAG	C1-O5-C5	3.73	117.24	112.19
10	A	1911	PC1	C15-N-C13	3.70	118.49	108.97
10	A	1902	PC1	C15-N-C13	3.70	118.49	108.97
10	A	1903	PC1	C15-N-C13	3.63	118.32	108.97
10	A	1903	PC1	O21-C21-C22	3.55	119.16	111.50
10	A	1905	PC1	O21-C21-C22	3.52	119.10	111.50
10	A	1912	PC1	C15-N-C13	3.52	118.02	108.97
10	A	1911	PC1	O21-C21-C22	3.43	118.89	111.50
10	A	1915	PC1	C15-N-C13	3.35	117.60	108.97
10	A	1904	PC1	O31-C31-C32	3.30	122.25	111.91
10	A	1915	PC1	O31-C31-C32	2.96	121.19	111.91
10	A	1903	PC1	O31-C31-C32	2.82	120.76	111.91
10	A	1902	PC1	O31-C31-C32	2.62	120.13	111.91
10	A	1912	PC1	O31-C31-C32	2.47	119.66	111.91
10	A	1911	PC1	O31-C31-C32	2.40	119.44	111.91
10	A	1915	PC1	O21-C21-O22	-2.35	118.03	123.70
9	F	1213	NAG	C1-O5-C5	2.25	115.24	112.19
10	A	1905	PC1	O31-C31-C32	2.19	118.79	111.91
10	A	1904	PC1	O31-C31-O32	-2.10	118.30	123.59
10	A	1911	PC1	C2-O21-C21	-2.03	112.79	117.79

There are no chirality outliers.

All (233) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	1902	PC1	C1-O11-P-O12
10	A	1902	PC1	O13-C11-C12-N
10	A	1903	PC1	C11-O13-P-O14
10	A	1903	PC1	C22-C21-O21-C2
10	A	1904	PC1	C11-O13-P-O12
10	A	1904	PC1	C11-O13-P-O14
10	A	1904	PC1	O13-C11-C12-N
10	A	1904	PC1	O11-C1-C2-O21
10	A	1904	PC1	O22-C21-O21-C2
10	A	1904	PC1	O32-C31-O31-C3
10	A	1904	PC1	C32-C31-O31-C3
10	A	1905	PC1	C11-O13-P-O14
10	A	1905	PC1	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
10	A	1905	PC1	C1-O11-P-O14
10	A	1905	PC1	C22-C21-O21-C2
10	A	1911	PC1	C11-O13-P-O12
10	A	1911	PC1	C11-O13-P-O14
10	A	1911	PC1	C1-O11-P-O12
10	A	1911	PC1	C1-O11-P-O14
10	A	1911	PC1	C1-O11-P-O13
10	A	1911	PC1	O13-C11-C12-N
10	A	1911	PC1	O22-C21-O21-C2
10	A	1912	PC1	C1-O11-P-O12
10	A	1912	PC1	C1-O11-P-O14
10	A	1912	PC1	O13-C11-C12-N
10	A	1912	PC1	C22-C21-O21-C2
10	A	1915	PC1	C11-O13-P-O12
10	A	1915	PC1	C1-O11-P-O12
10	A	1915	PC1	C1-O11-P-O14
10	A	1915	PC1	C1-O11-P-O13
10	A	1915	PC1	O22-C21-O21-C2
10	A	1915	PC1	C22-C21-O21-C2
10	A	1915	PC1	O32-C31-O31-C3
10	A	1915	PC1	C32-C31-O31-C3
9	A	1901	NAG	O5-C5-C6-O6
10	A	1903	PC1	O22-C21-O21-C2
10	A	1905	PC1	O22-C21-O21-C2
10	A	1912	PC1	O22-C21-O21-C2
9	F	1213	NAG	C4-C5-C6-O6
10	A	1904	PC1	C22-C21-O21-C2
10	A	1911	PC1	C22-C21-O21-C2
9	F	1213	NAG	O5-C5-C6-O6
10	A	1908	PC1	C39-C3A-C3B-C3C
10	A	1911	PC1	C32-C31-O31-C3
9	F	1219	NAG	O5-C5-C6-O6
9	A	1901	NAG	C4-C5-C6-O6
10	A	1910	PC1	C2E-C2F-C2G-C2H
10	A	1911	PC1	O32-C31-O31-C3
9	F	1219	NAG	C4-C5-C6-O6
10	A	1915	PC1	C36-C37-C38-C39
10	A	1912	PC1	C31-C32-C33-C34
10	A	1902	PC1	O21-C2-C3-O31
10	A	1912	PC1	C23-C24-C25-C26
10	A	1902	PC1	C22-C23-C24-C25
10	A	1909	PC1	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
10	A	1904	PC1	C21-C22-C23-C24
10	A	1902	PC1	C1-O11-P-O13
10	A	1903	PC1	C11-O13-P-O11
10	A	1904	PC1	C11-O13-P-O11
10	A	1904	PC1	C1-O11-P-O13
10	A	1911	PC1	C11-O13-P-O11
10	A	1912	PC1	C1-O11-P-O13
10	A	1915	PC1	C11-O13-P-O11
10	A	1906	PC1	C29-C2A-C2B-C2C
10	A	1909	PC1	C3B-C3C-C3D-C3E
10	A	1902	PC1	C34-C35-C36-C37
10	A	1911	PC1	C28-C29-C2A-C2B
10	A	1911	PC1	C2D-C2E-C2F-C2G
10	A	1915	PC1	C26-C27-C28-C29
10	A	1915	PC1	C2A-C2B-C2C-C2D
10	A	1905	PC1	C25-C26-C27-C28
10	A	1906	PC1	C24-C25-C26-C27
10	A	1915	PC1	C38-C39-C3A-C3B
10	A	1905	PC1	C1-C2-O21-C21
10	A	1911	PC1	C2B-C2C-C2D-C2E
10	A	1915	PC1	C2E-C2F-C2G-C2H
10	A	1912	PC1	C34-C35-C36-C37
10	A	1914	PC1	C3B-C3C-C3D-C3E
10	A	1903	PC1	C2E-C2F-C2G-C2H
10	A	1906	PC1	C25-C26-C27-C28
10	A	1910	PC1	C25-C26-C27-C28
10	A	1902	PC1	C33-C34-C35-C36
10	A	1915	PC1	C22-C23-C24-C25
10	A	1903	PC1	C22-C23-C24-C25
10	A	1903	PC1	C37-C38-C39-C3A
10	A	1906	PC1	C27-C28-C29-C2A
10	A	1915	PC1	C24-C25-C26-C27
10	A	1915	PC1	C34-C35-C36-C37
10	A	1902	PC1	C3A-C3B-C3C-C3D
10	A	1913	PC1	C27-C28-C29-C2A
10	A	1904	PC1	C27-C28-C29-C2A
10	A	1902	PC1	C24-C25-C26-C27
10	A	1914	PC1	C3E-C3F-C3G-C3H
10	A	1905	PC1	C21-C22-C23-C24
10	A	1903	PC1	C25-C26-C27-C28
10	A	1906	PC1	C2D-C2E-C2F-C2G
10	A	1912	PC1	C27-C28-C29-C2A

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Mol	Chain	Res	Type	Atoms
10	A	1905	PC1	C22-C23-C24-C25
10	A	1911	PC1	C37-C38-C39-C3A
10	A	1905	PC1	C34-C35-C36-C37
10	A	1903	PC1	C3D-C3E-C3F-C3G
10	A	1903	PC1	C3E-C3F-C3G-C3H
10	A	1912	PC1	C24-C25-C26-C27
10	A	1912	PC1	C36-C37-C38-C39
10	A	1903	PC1	C26-C27-C28-C29
10	A	1904	PC1	C24-C25-C26-C27
10	A	1903	PC1	C29-C2A-C2B-C2C
10	A	1911	PC1	C25-C26-C27-C28
10	A	1912	PC1	C33-C34-C35-C36
10	A	1902	PC1	C22-C21-O21-C2
10	A	1915	PC1	C33-C34-C35-C36
10	A	1915	PC1	C23-C24-C25-C26
10	A	1902	PC1	O22-C21-O21-C2
10	A	1902	PC1	C35-C36-C37-C38
10	A	1915	PC1	C21-C22-C23-C24
10	A	1915	PC1	C37-C38-C39-C3A
10	A	1903	PC1	C32-C31-O31-C3
10	A	1913	PC1	C26-C27-C28-C29
9	F	1221	NAG	O5-C5-C6-O6
10	A	1904	PC1	C22-C23-C24-C25
10	A	1903	PC1	C35-C36-C37-C38
10	A	1911	PC1	C24-C25-C26-C27
10	A	1907	PC1	C32-C33-C34-C35
10	A	1909	PC1	C39-C3A-C3B-C3C
10	A	1903	PC1	O32-C31-O31-C3
10	A	1905	PC1	C32-C31-O31-C3
10	A	1903	PC1	C24-C25-C26-C27
10	A	1911	PC1	O21-C2-C3-O31
10	A	1912	PC1	C38-C39-C3A-C3B
10	A	1905	PC1	C1-O11-P-O13
10	A	1910	PC1	C22-C23-C24-C25
10	A	1915	PC1	C29-C2A-C2B-C2C
10	A	1902	PC1	C1-C2-C3-O31
10	A	1910	PC1	C23-C24-C25-C26
10	A	1903	PC1	C38-C39-C3A-C3B
10	A	1907	PC1	C39-C3A-C3B-C3C
10	A	1912	PC1	C21-C22-C23-C24
10	A	1903	PC1	C2F-C2G-C2H-C2I
10	A	1904	PC1	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
10	A	1905	PC1	O32-C31-O31-C3
10	A	1915	PC1	C32-C33-C34-C35
10	A	1903	PC1	C34-C35-C36-C37
10	A	1905	PC1	C37-C38-C39-C3A
10	A	1902	PC1	O11-C1-C2-O21
10	A	1903	PC1	C32-C33-C34-C35
10	A	1905	PC1	C23-C24-C25-C26
10	A	1911	PC1	C36-C37-C38-C39
10	A	1912	PC1	C22-C23-C24-C25
10	A	1915	PC1	C39-C3A-C3B-C3C
10	A	1902	PC1	O11-C1-C2-C3
10	A	1904	PC1	O11-C1-C2-C3
10	A	1908	PC1	C3A-C3B-C3C-C3D
10	A	1905	PC1	C33-C34-C35-C36
10	A	1906	PC1	C2C-C2D-C2E-C2F
10	A	1908	PC1	C3E-C3F-C3G-C3H
10	A	1910	PC1	C27-C28-C29-C2A
10	A	1911	PC1	C1-C2-C3-O31
10	A	1910	PC1	C2B-C2C-C2D-C2E
10	A	1911	PC1	C22-C23-C24-C25
10	A	1912	PC1	C25-C26-C27-C28
10	A	1903	PC1	C31-C32-C33-C34
10	A	1914	PC1	C38-C39-C3A-C3B
10	A	1914	PC1	C3C-C3D-C3E-C3F
10	A	1905	PC1	C2-C1-O11-P
10	A	1911	PC1	C2-C1-O11-P
10	A	1911	PC1	C32-C33-C34-C35
10	A	1904	PC1	C35-C36-C37-C38
10	A	1911	PC1	O11-C1-C2-C3
10	A	1911	PC1	C23-C24-C25-C26
10	A	1907	PC1	C35-C36-C37-C38
10	A	1909	PC1	C37-C38-C39-C3A
10	A	1915	PC1	C2F-C2G-C2H-C2I
10	A	1912	PC1	C1-C2-C3-O31
10	A	1911	PC1	C29-C2A-C2B-C2C
10	A	1912	PC1	O21-C2-C3-O31
10	A	1915	PC1	O21-C2-C3-O31
10	A	1902	PC1	C3D-C3E-C3F-C3G
10	A	1914	PC1	C37-C38-C39-C3A
10	A	1905	PC1	C11-O13-P-O11
10	A	1902	PC1	C1-O11-P-O14
10	A	1903	PC1	C11-O13-P-O12

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Mol	Chain	Res	Type	Atoms
10	A	1904	PC1	C1-O11-P-O12
10	A	1905	PC1	C11-O13-P-O12
10	A	1906	PC1	C2E-C2F-C2G-C2H
10	A	1915	PC1	C12-C11-O13-P
10	A	1912	PC1	C32-C33-C34-C35
10	A	1911	PC1	O11-C1-C2-O21
10	A	1903	PC1	O13-C11-C12-N
10	A	1905	PC1	O13-C11-C12-N
10	A	1915	PC1	O13-C11-C12-N
10	A	1911	PC1	C33-C34-C35-C36
10	A	1912	PC1	C2A-C2B-C2C-C2D
10	A	1902	PC1	C23-C24-C25-C26
10	A	1908	PC1	C3F-C3G-C3H-C3I
10	A	1913	PC1	C24-C25-C26-C27
10	A	1905	PC1	C11-C12-N-C15
10	A	1905	PC1	C26-C27-C28-C29
10	A	1902	PC1	C11-O13-P-O11
10	A	1912	PC1	C11-O13-P-O11
10	A	1905	PC1	C38-C39-C3A-C3B
10	A	1905	PC1	C32-C33-C34-C35
10	A	1910	PC1	C29-C2A-C2B-C2C
10	A	1906	PC1	C23-C24-C25-C26
10	A	1909	PC1	C3F-C3G-C3H-C3I
10	A	1914	PC1	C36-C37-C38-C39
10	A	1908	PC1	C3D-C3E-C3F-C3G
10	A	1911	PC1	C34-C35-C36-C37
10	A	1903	PC1	C3C-C3D-C3E-C3F
10	A	1910	PC1	C24-C25-C26-C27
10	A	1910	PC1	C2C-C2D-C2E-C2F
10	A	1902	PC1	O32-C31-O31-C3
10	A	1902	PC1	C32-C31-O31-C3
10	A	1905	PC1	O21-C21-C22-C23
10	A	1906	PC1	C21-C22-C23-C24
10	A	1907	PC1	C34-C35-C36-C37
10	A	1905	PC1	C11-C12-N-C14
10	A	1913	PC1	C2D-C2E-C2F-C2G
10	A	1903	PC1	O31-C31-C32-C33
10	A	1909	PC1	C34-C35-C36-C37
10	A	1912	PC1	O31-C31-C32-C33
10	A	1905	PC1	O22-C21-C22-C23
10	A	1902	PC1	C3C-C3D-C3E-C3F
10	A	1902	PC1	C3B-C3C-C3D-C3E

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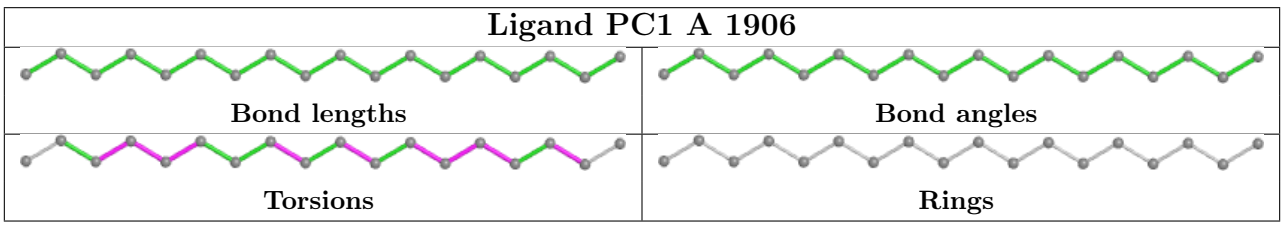
Mol	Chain	Res	Type	Atoms
10	A	1903	PC1	C27-C28-C29-C2A
10	A	1903	PC1	O32-C31-C32-C33
10	A	1912	PC1	O32-C31-C32-C33
10	A	1911	PC1	O21-C21-C22-C23
10	A	1905	PC1	C12-C11-O13-P
10	A	1912	PC1	C12-C11-O13-P
10	A	1909	PC1	C3A-C3B-C3C-C3D
10	A	1915	PC1	O31-C31-C32-C33
10	A	1904	PC1	C34-C35-C36-C37
10	A	1905	PC1	C31-C32-C33-C34

There are no ring outliers.

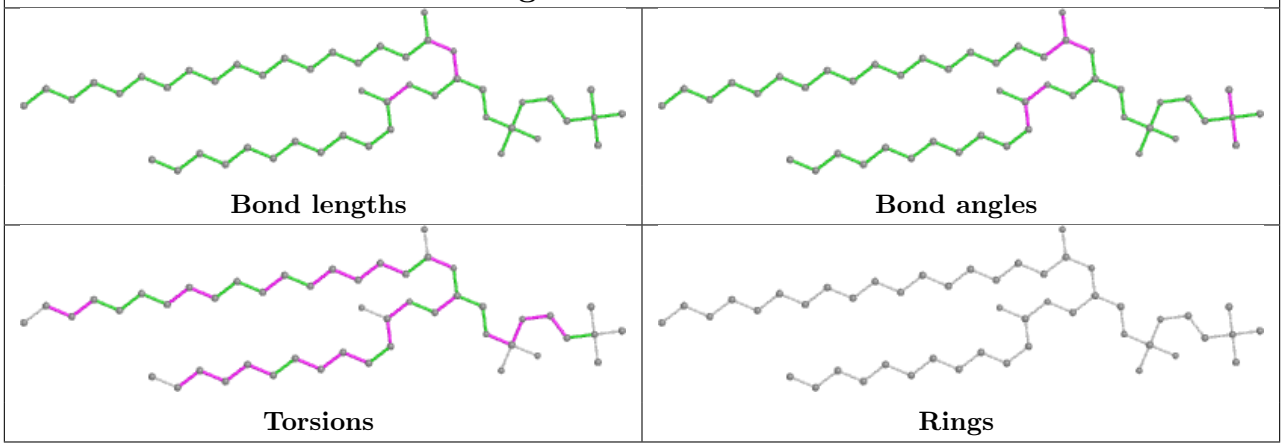
8 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	1915	PC1	1	0
10	A	1912	PC1	3	0
10	A	1914	PC1	4	0
10	A	1903	PC1	2	0
10	A	1909	PC1	2	0
10	A	1902	PC1	2	0
10	A	1904	PC1	4	0
10	A	1911	PC1	2	0

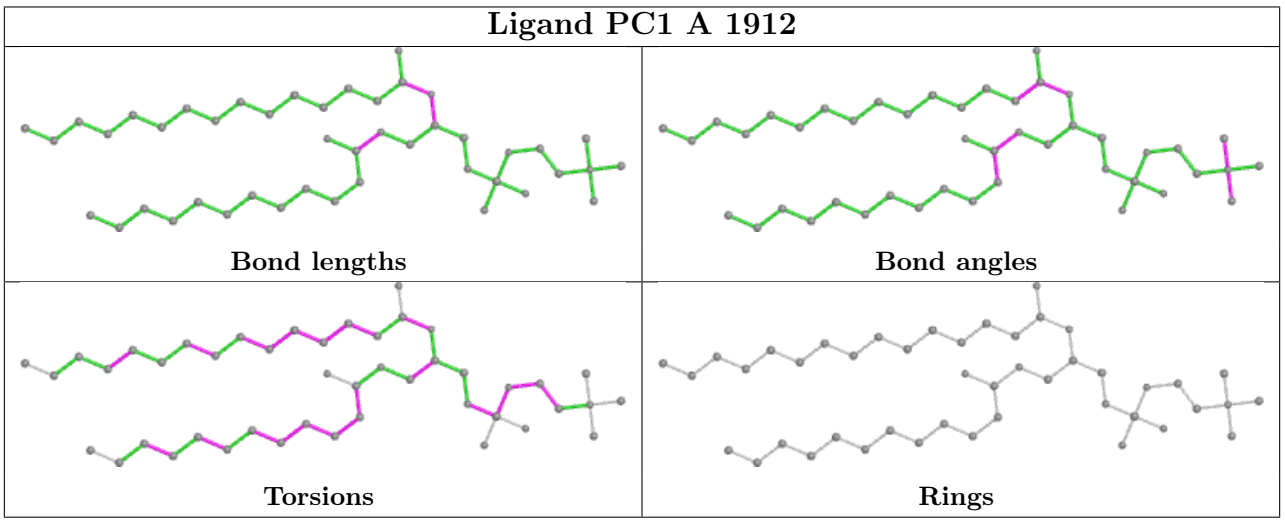
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



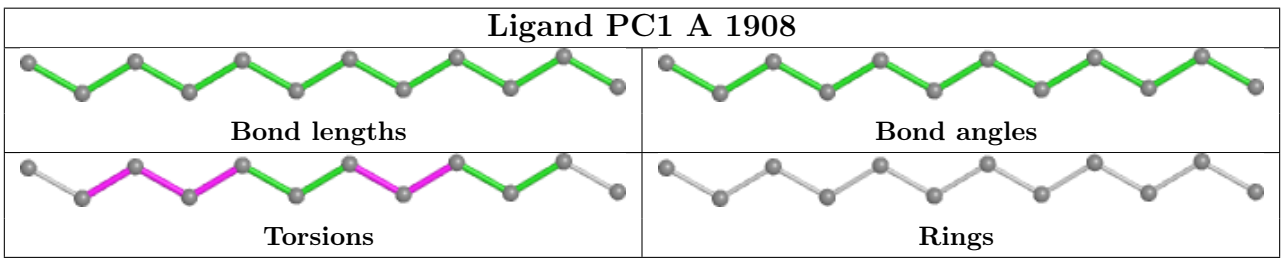
Ligand PC1 A 1915



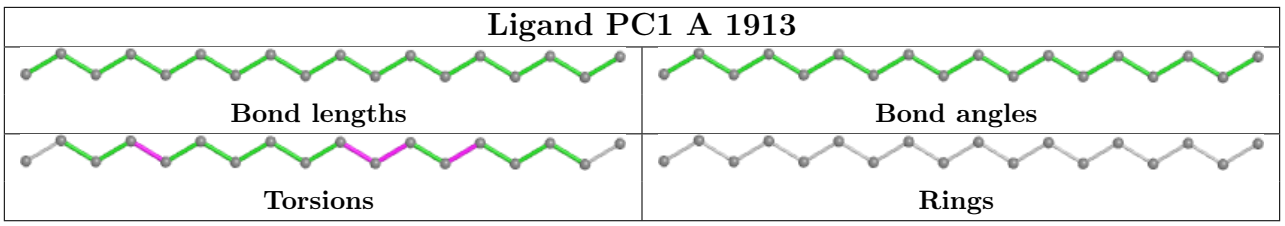
Ligand PC1 A 1912



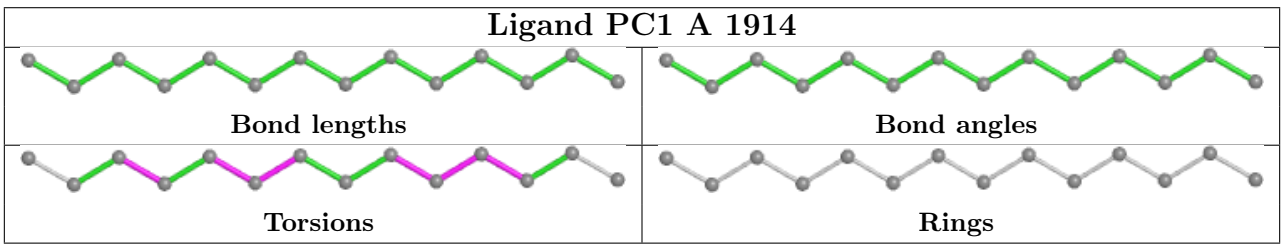
Ligand PC1 A 1908



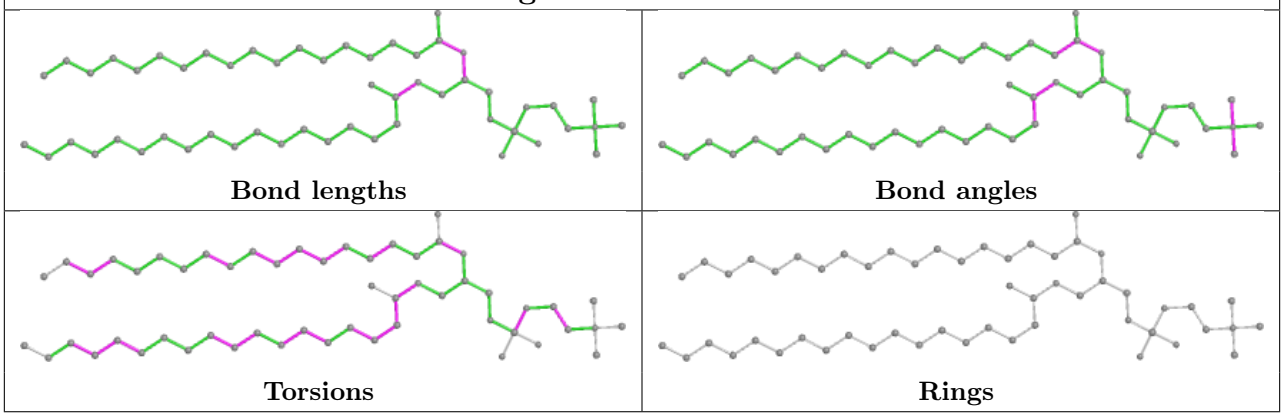
Ligand PC1 A 1913



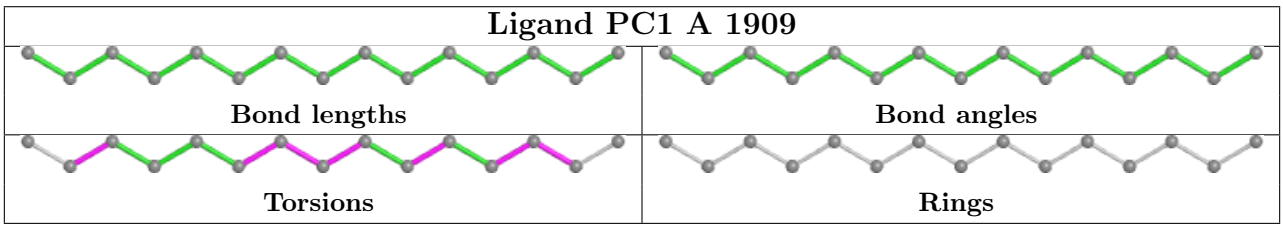
Ligand PC1 A 1914



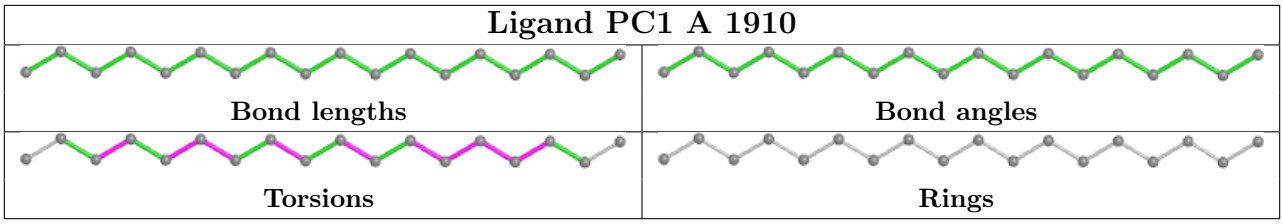
Ligand PC1 A 1903



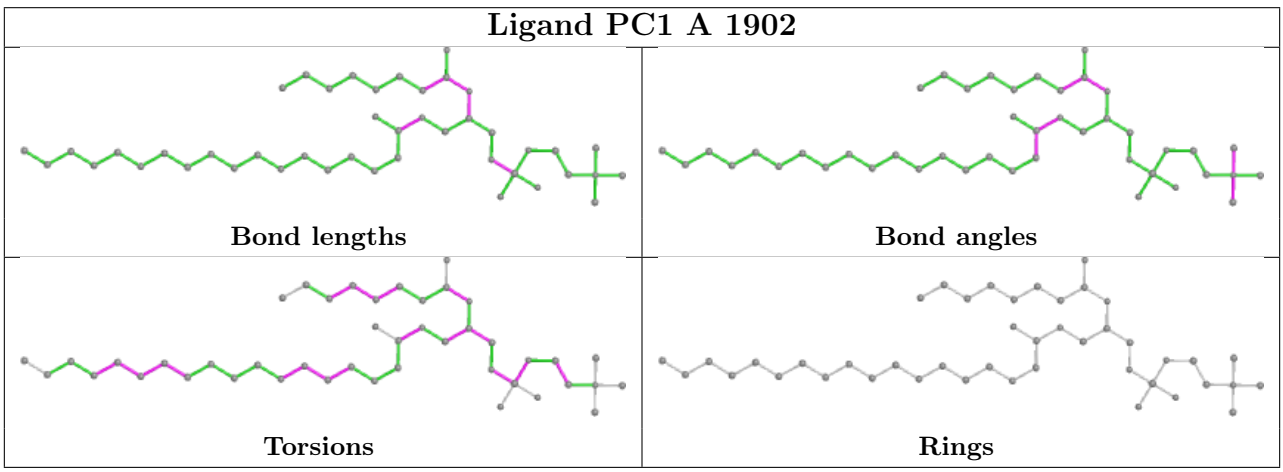
Ligand PC1 A 1909



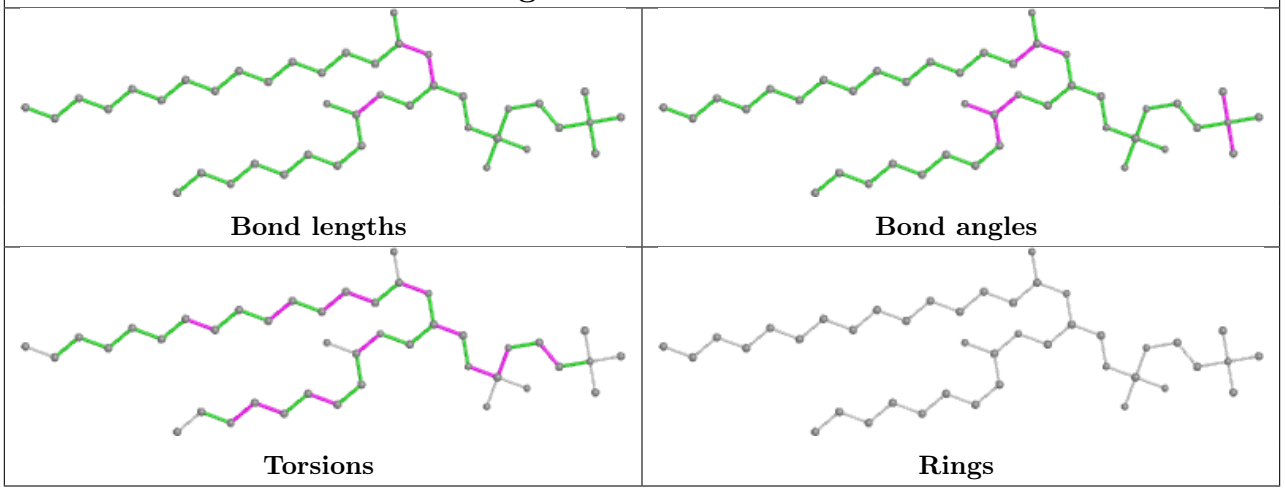
Ligand PC1 A 1910



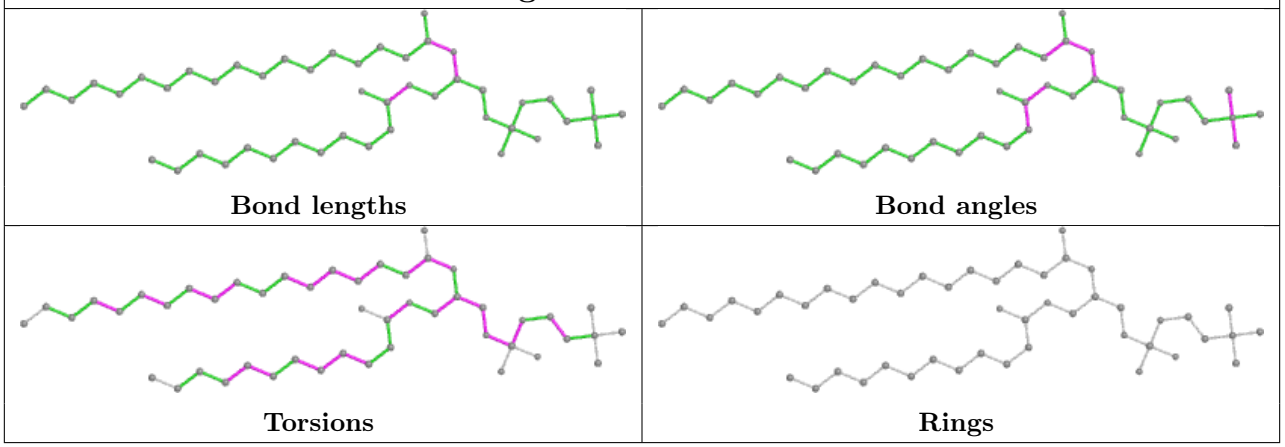
Ligand PC1 A 1902



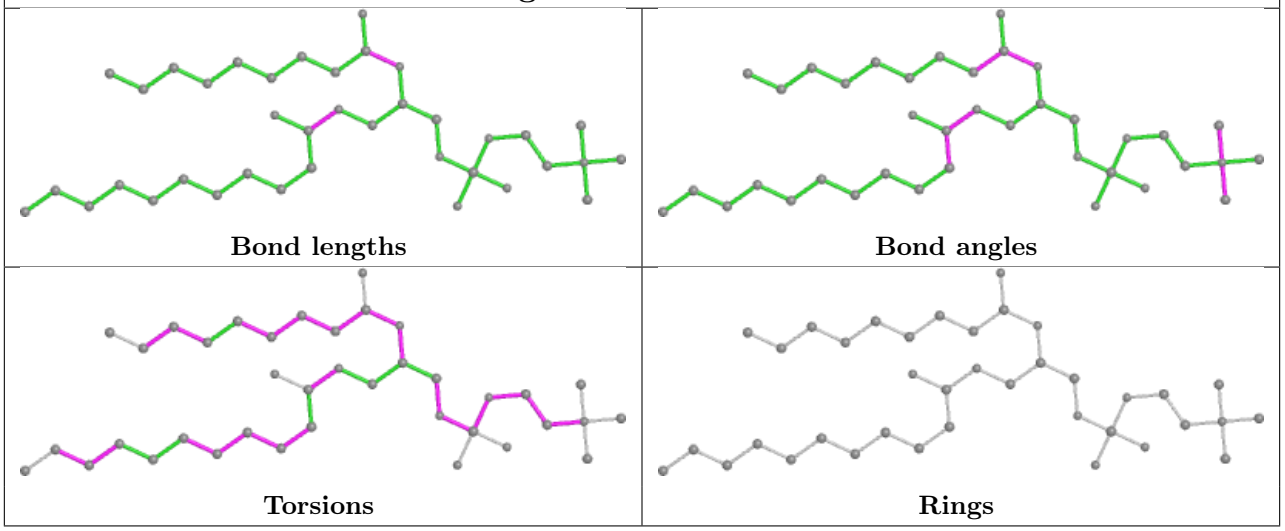
Ligand PC1 A 1904

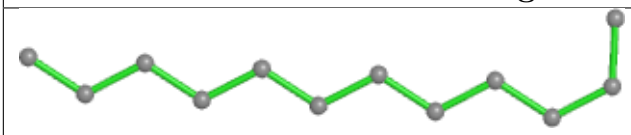
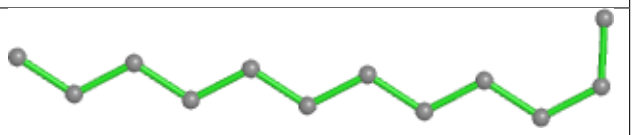
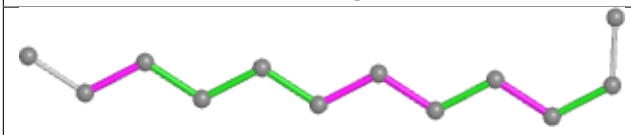
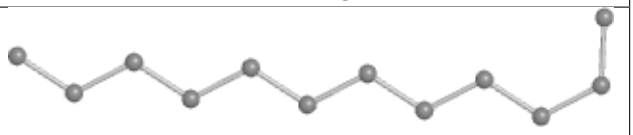


Ligand PC1 A 1911



Ligand PC1 A 1905



Ligand PC1 A 1907	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

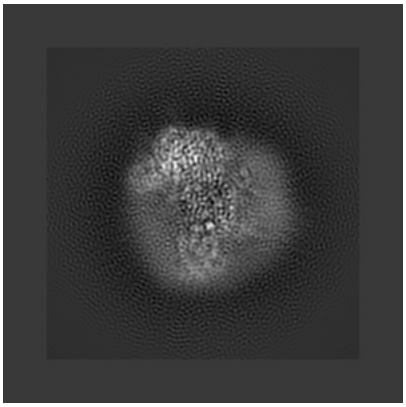
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9513. These allow visual inspection of the internal detail of the map and identification of artifacts.

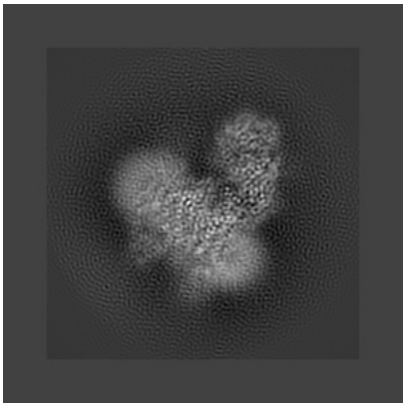
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

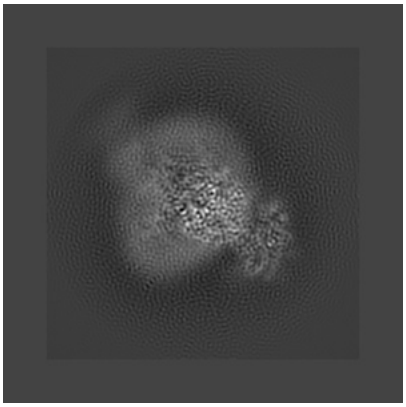
6.1.1 Primary map



X



Y

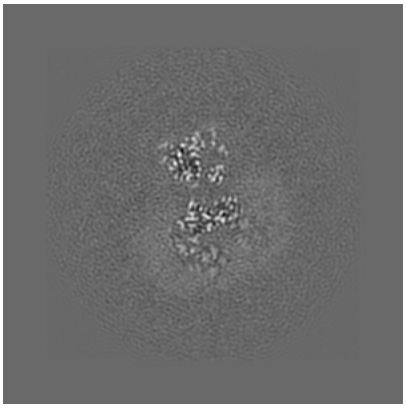


Z

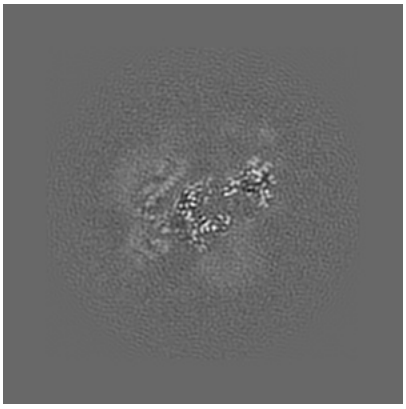
The images above show the map projected in three orthogonal directions.

6.2 Central slices

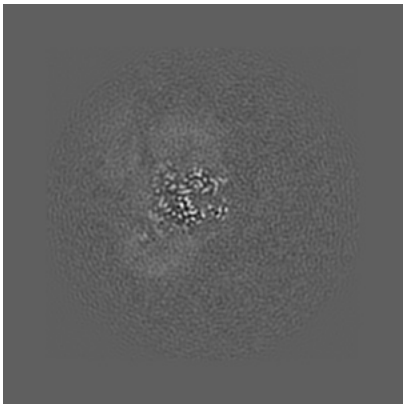
6.2.1 Primary map



X Index: 128



Y Index: 128

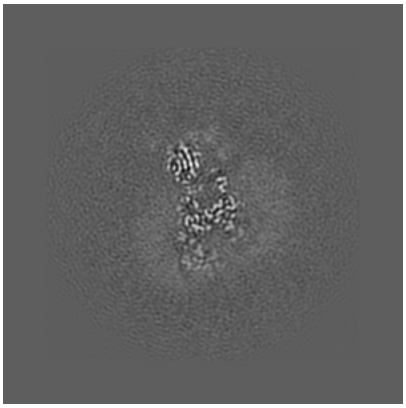


Z Index: 128

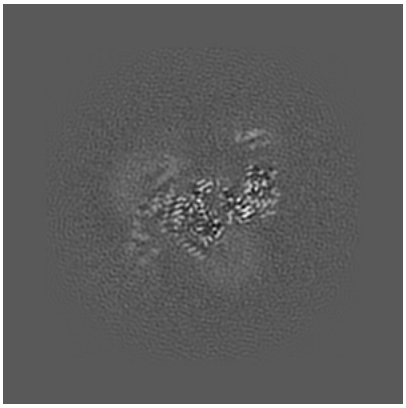
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

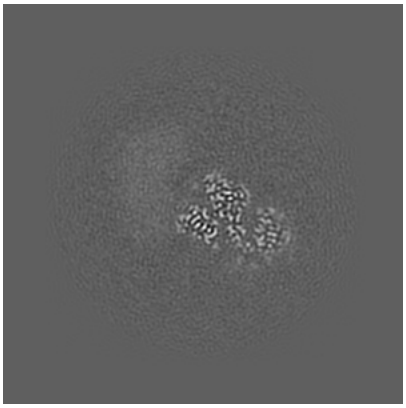
6.3.1 Primary map



X Index: 123



Y Index: 123

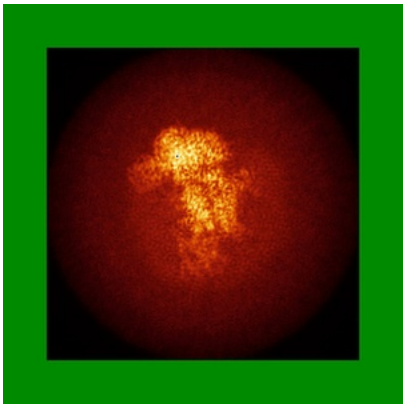


Z Index: 159

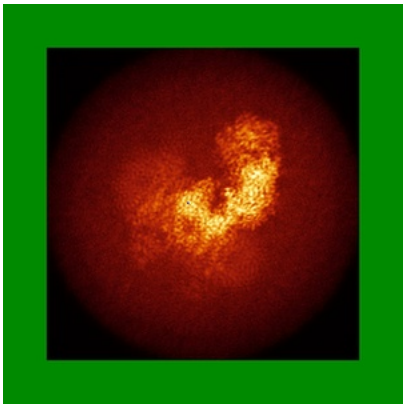
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

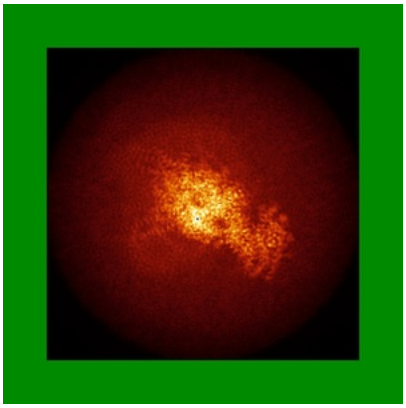
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.044. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

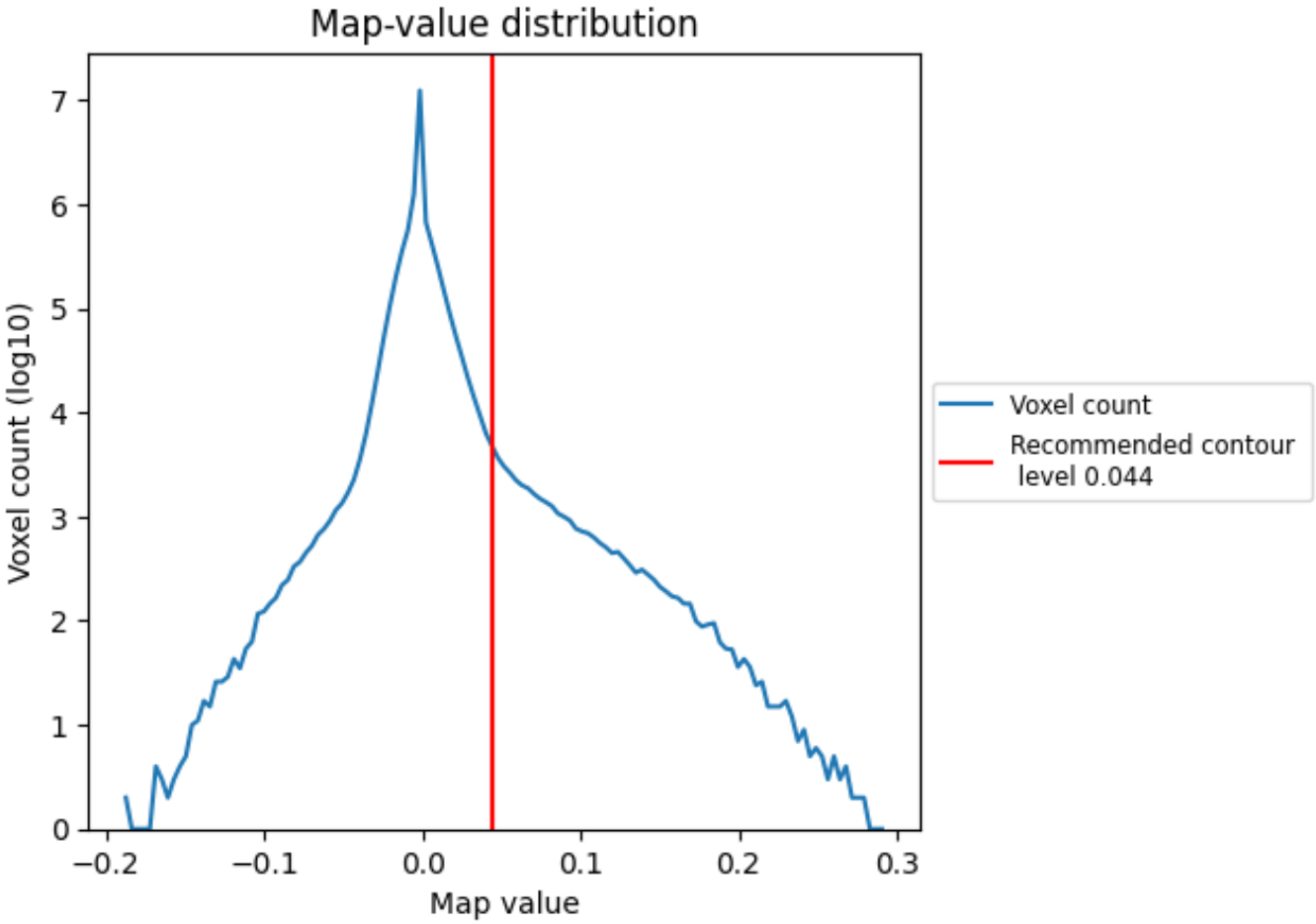
6.6 Mask visualisation (i)

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

7 Map analysis

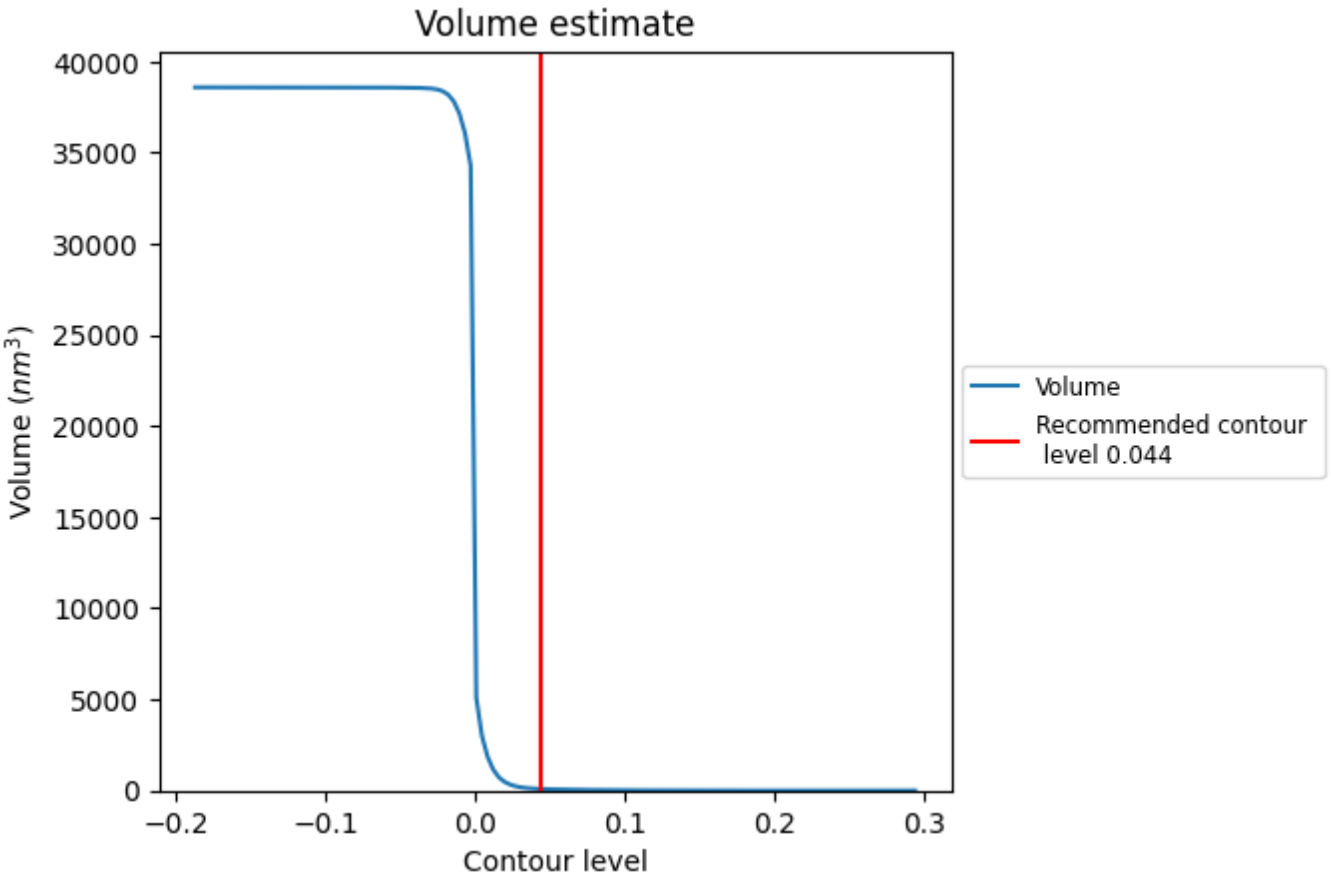
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

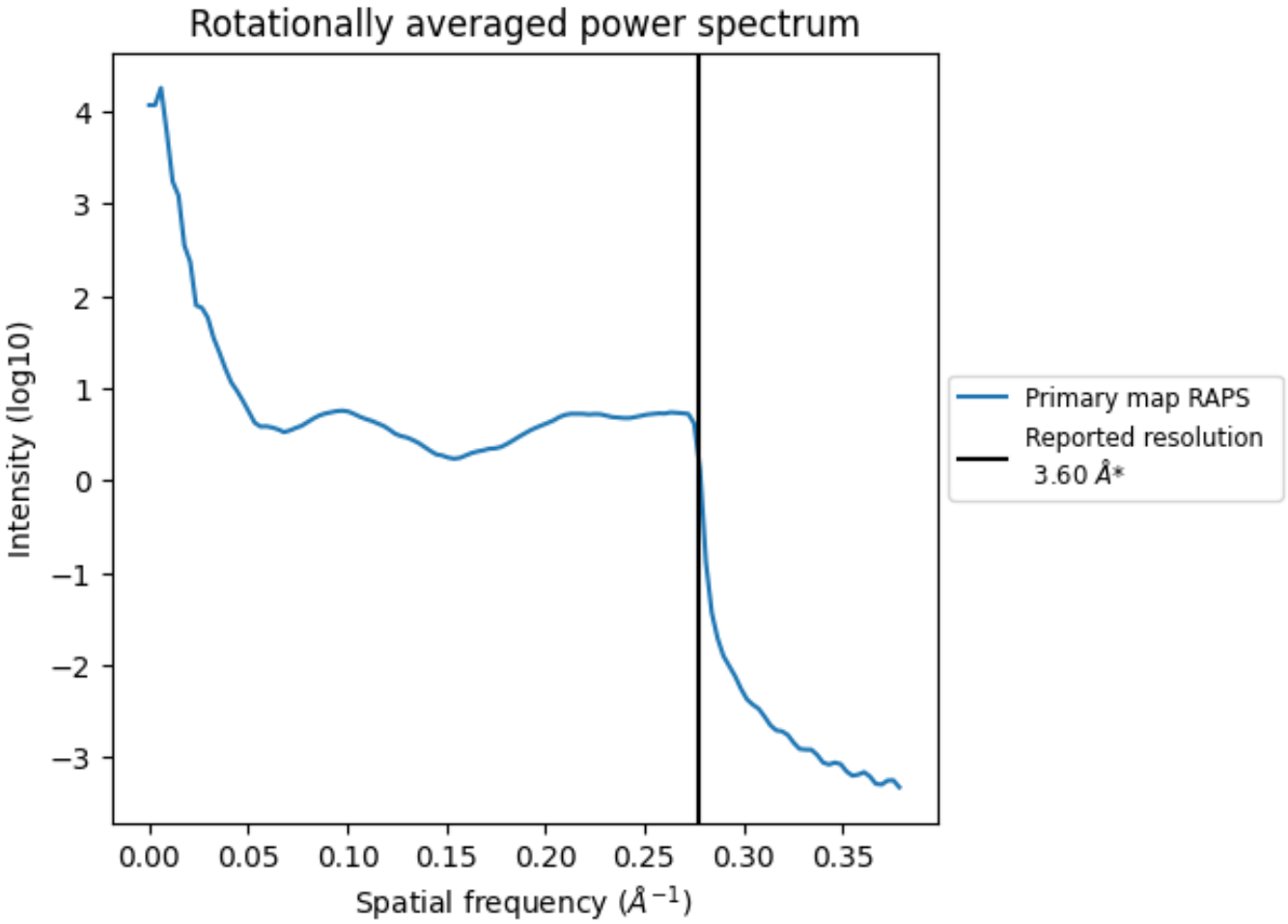
7.2 Volume estimate



The volume at the recommended contour level is 87 nm^3; this corresponds to an approximate mass of 79 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

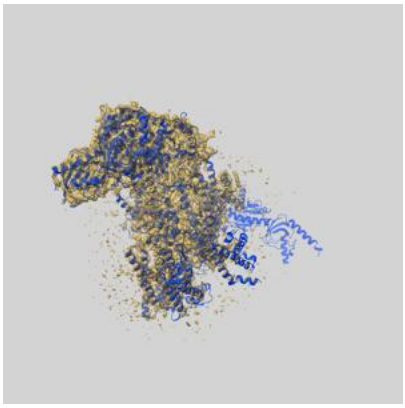
8 Fourier-Shell correlation (i)

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

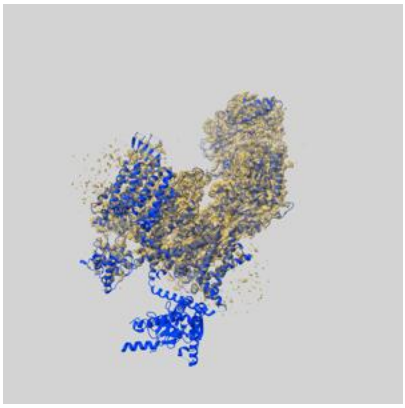
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9513 and PDB model 5GJV. Per-residue inclusion information can be found in section 3 on page 9.

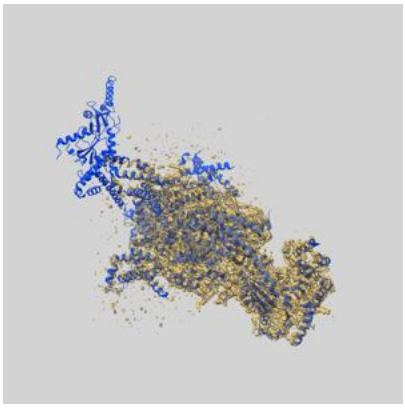
9.1 Map-model overlay



X



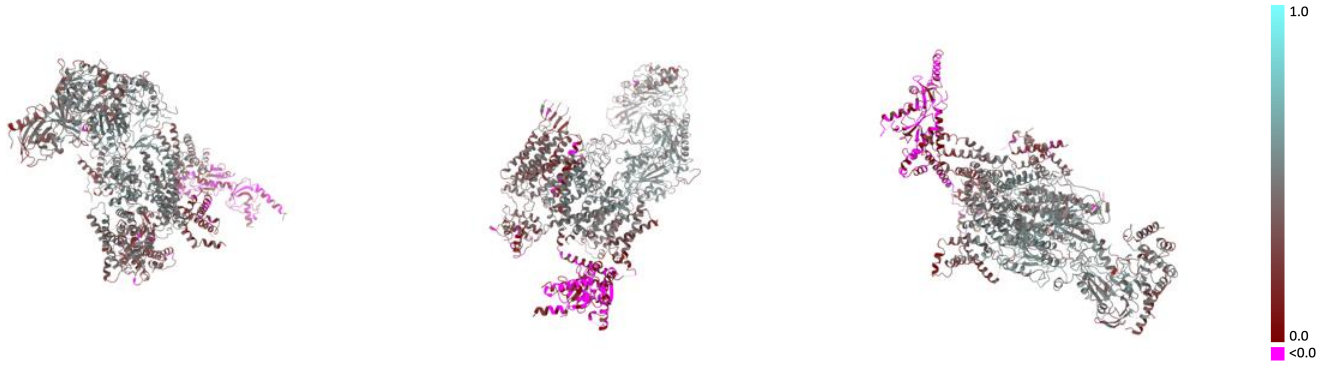
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.044 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.

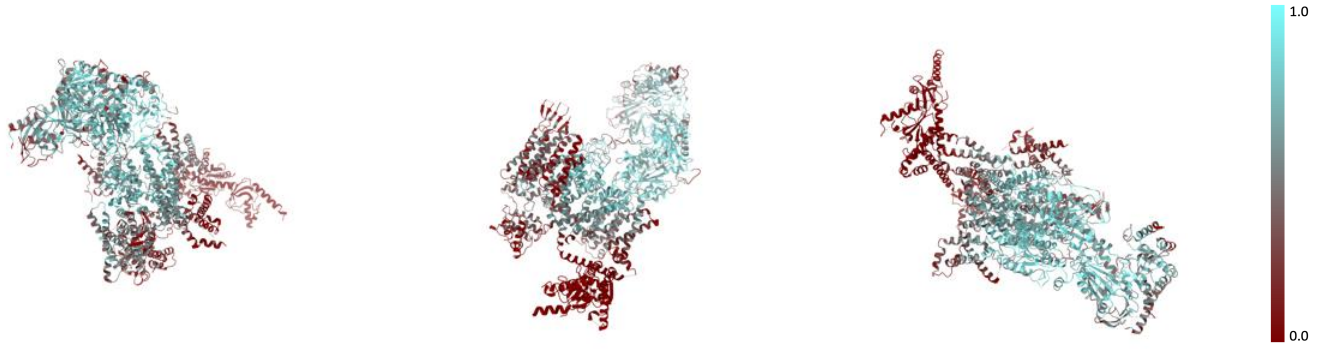
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

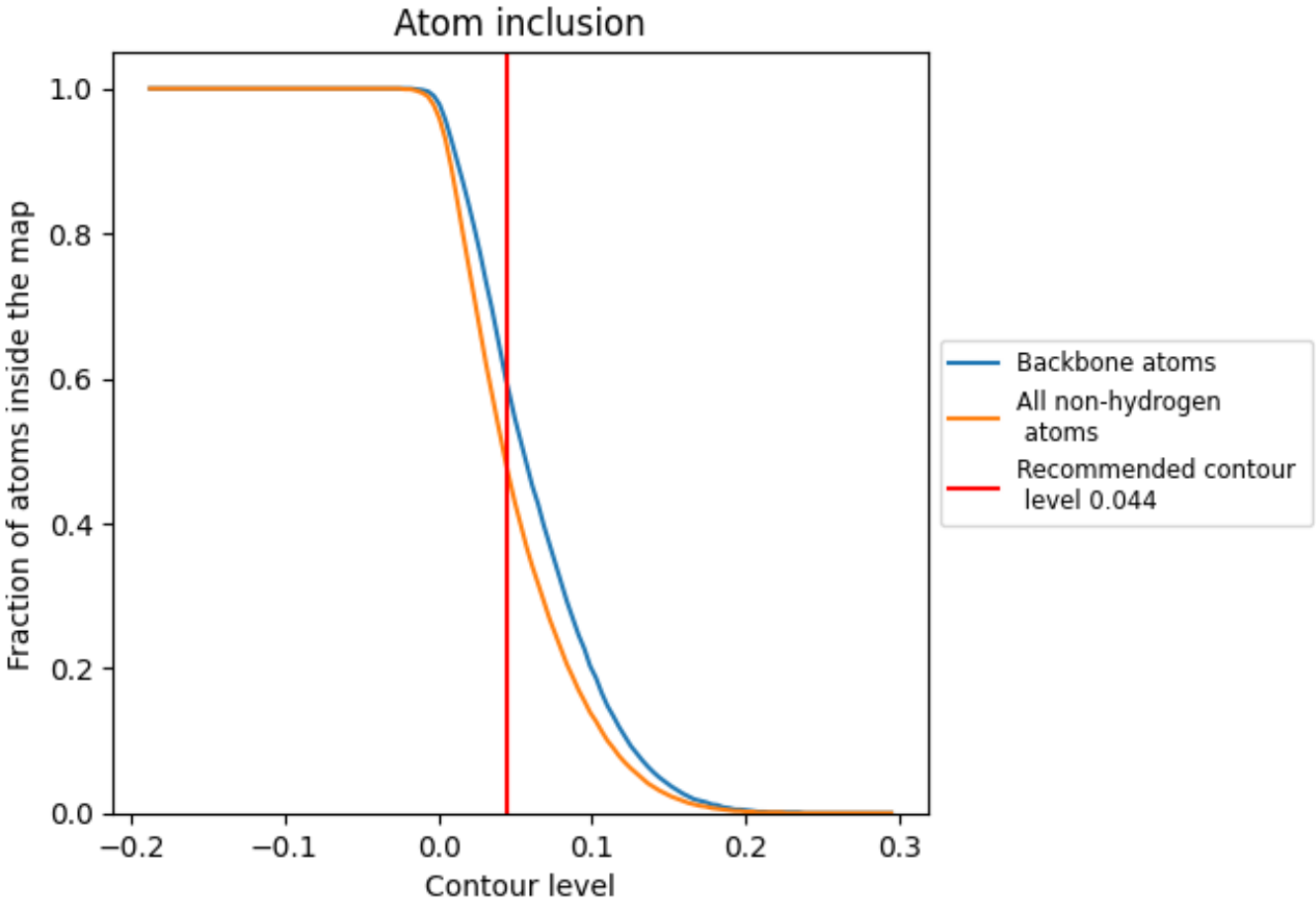
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.044).

9.4 Atom inclusion (i)



At the recommended contour level, 60% of all backbone atoms, 48% 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 (0.044) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4820	0.3850
A	0.4760	0.4090
B	0.0000	0.0240
C	0.0000	0.0110
D	0.0710	0.0690
E	0.3030	0.3460
F	0.6540	0.4590
G	0.1790	0.3640
H	0.3330	0.3700
I	0.6920	0.5200
J	0.5360	0.4920
K	0.2500	0.3890
L	0.2860	0.2870