Full wwPDB EM Validation Report ⓘ

Oct 15, 2024 – 03:49 AM JST

PDB ID	:	8I5G
EMDB ID	:	EMD-35194
Title	:	Structure of human Nav1.7 in complex with PF-05089771
Authors	:	Wu, Q.R.; Yan, N.
Deposited on	:	2023-01-25
Resolution	:	2.70 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:

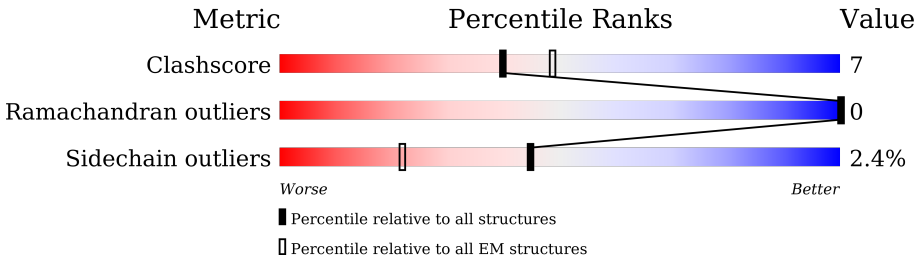
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance

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

The reported resolution of this entry is 2.70 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	B	192	77% 14% 10%
2	C	215	48% 47% 8% 45%
3	A	1988	8% 51% 13% 36%
4	D	2	50% 50%
4	E	2	50% 100%
4	F	2	100%

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 13389 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 Sodium channel subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	173	1416	902	232	272	10	0	0

- Molecule 2 is a protein called Sodium channel subunit beta-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	119	980	615	172	183	10	4	0

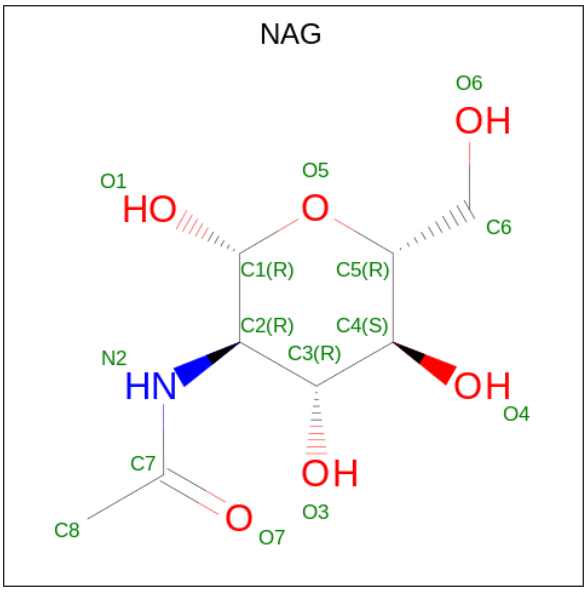
- Molecule 3 is a protein called Sodium channel protein type 9 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	A	1273	10273	6810	1615	1771	77	1	0

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

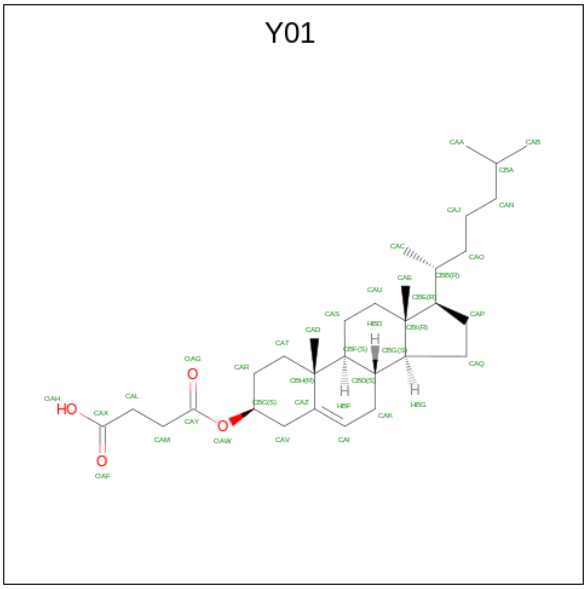
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	2	28	16	2	10	0	0
4	E	2	28	16	2	10	0	0
4	F	2	28	16	2	10	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



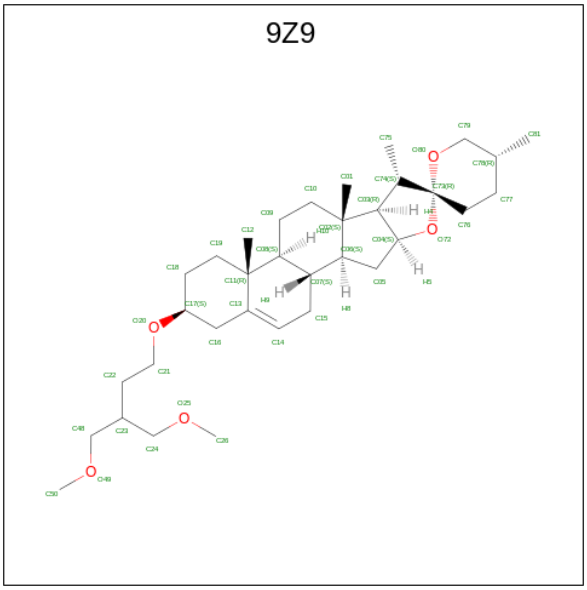
Mol	Chain	Residues	Atoms	AltConf
5	B	1	Total C N O 14 8 1 5	0
5	B	1	Total C N O 14 8 1 5	0
5	B	1	Total C N O 14 8 1 5	0
5	A	1	Total C N O 14 8 1 5	0
5	A	1	Total C N O 14 8 1 5	0

- Molecule 6 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: $C_{31}H_{50}O_4$).



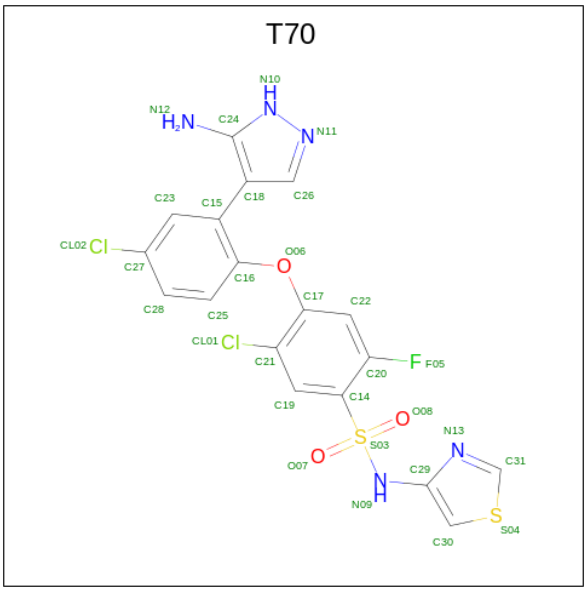
Mol	Chain	Residues	Atoms	AltConf
6	A	1	Total C O 35 31 4	0
6	A	1	Total C O 35 31 4	0

- Molecule 7 is (3beta,14beta,17beta,25R)-3-[4-methoxy-3-(methoxymethyl)butoxy]spirost-5-en (three-letter code: 9Z9) (formula: $C_{34}H_{56}O_5$).



Mol	Chain	Residues	Atoms	AltConf
7	A	1	Total C O 39 34 5	0

- Molecule 8 is PF-05089771 (three-letter code: T70) (formula: $C_{18}H_{12}Cl_2FN_5O_3S_2$) (labeled as "Ligand of Interest" by depositor).

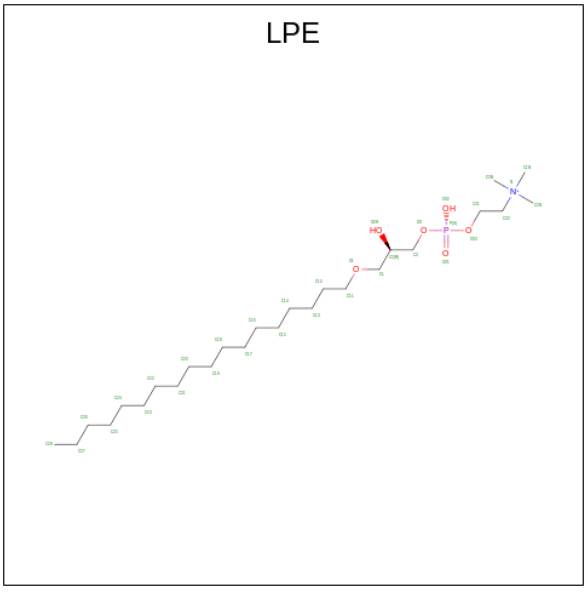


Mol	Chain	Residues	Atoms							AltConf
8	A	1	Total	C	Cl	F	N	O	S	0
			31	18	2	1	5	3	2	

- Molecule 9 is SODIUM ION (three-letter code: NA) (formula: Na).

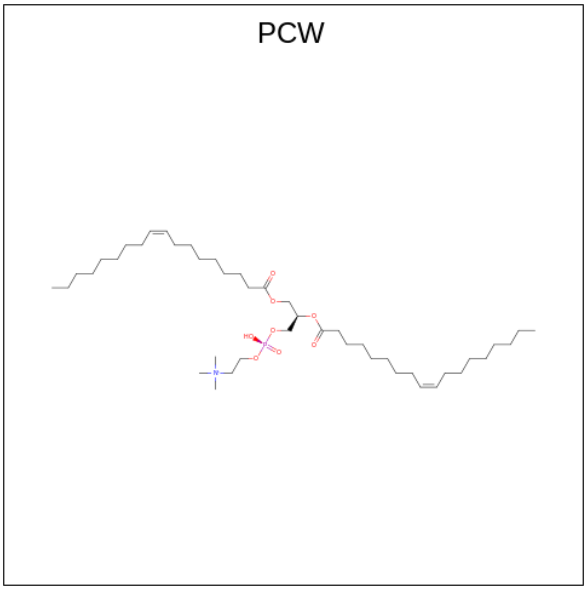
Mol	Chain	Residues	Atoms		AltConf
9	A	1	Total	Na	0
			1	1	

- Molecule 10 is 1-O-OCTADECYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: LPE) (formula: $C_{26}H_{57}NO_6P$).



Mol	Chain	Residues	Atoms					AltConf
10	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
10	A	1	Total	C	N	O	P	0
			18	10	1	6	1	
10	A	1	Total	C	N	O	P	0
			28	20	1	6	1	
10	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
10	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
10	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
10	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
10	A	1	Total	C	N	O	P	0
			17	9	1	6	1	

- Molecule 11 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: $C_{44}H_{85}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
11	A	1	Total	C	N	O	P	0
			53	43	1	8	1	
11	A	1	Total	C	N	O	P	0
			47	37	1	8	1	
11	A	1	Total	C	N	O	P	0
			44	34	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
11	A	1	Total	C	N	O	P	0
			44	34	1	8	1	
11	A	1	Total	C	N	O	P	0
			44	34	1	8	1	

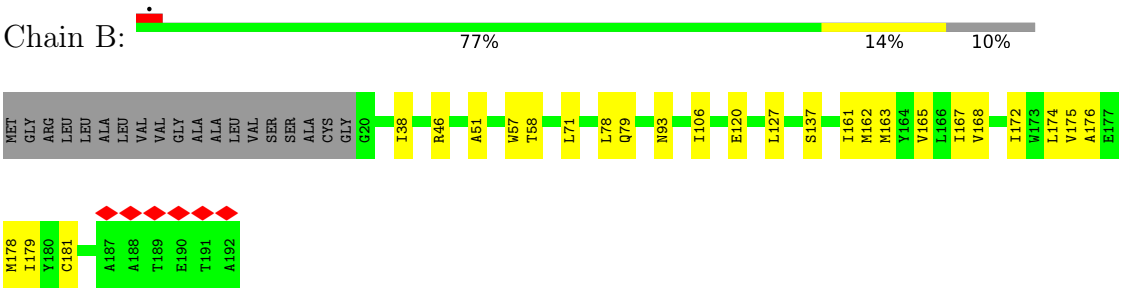
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		AltConf
12	A	5	Total	O	0
			5	5	

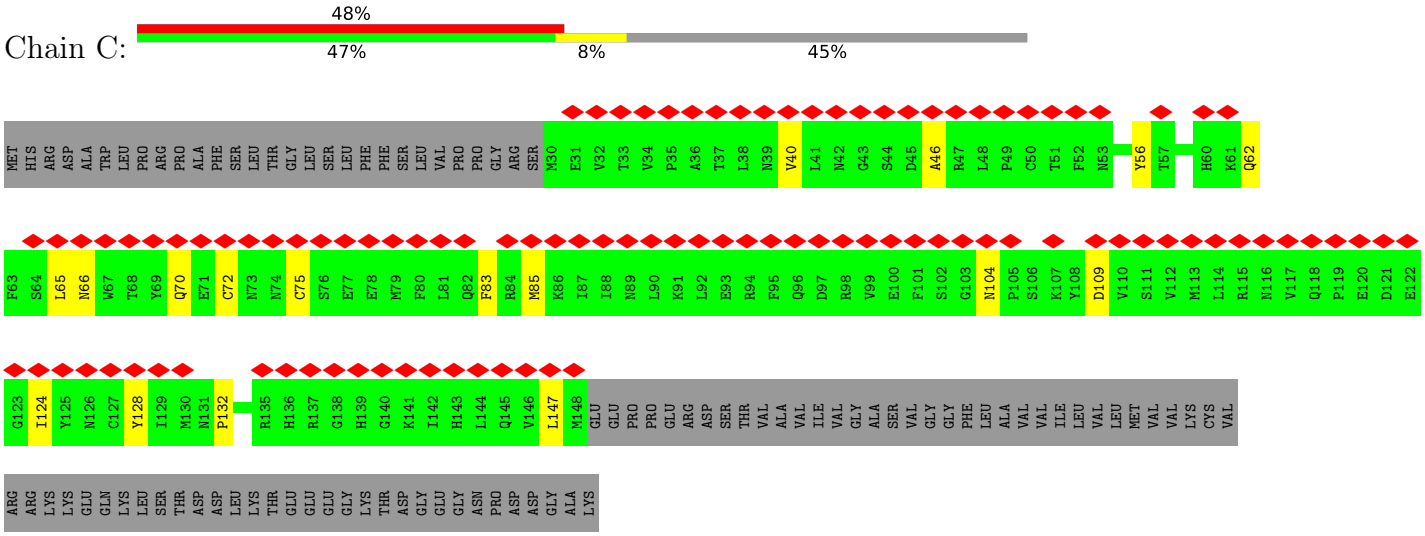
3 Residue-property plots (i)

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.

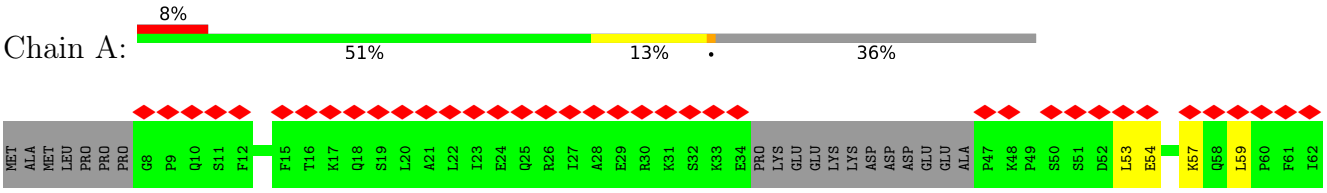
• Molecule 1: Sodium channel subunit beta-1

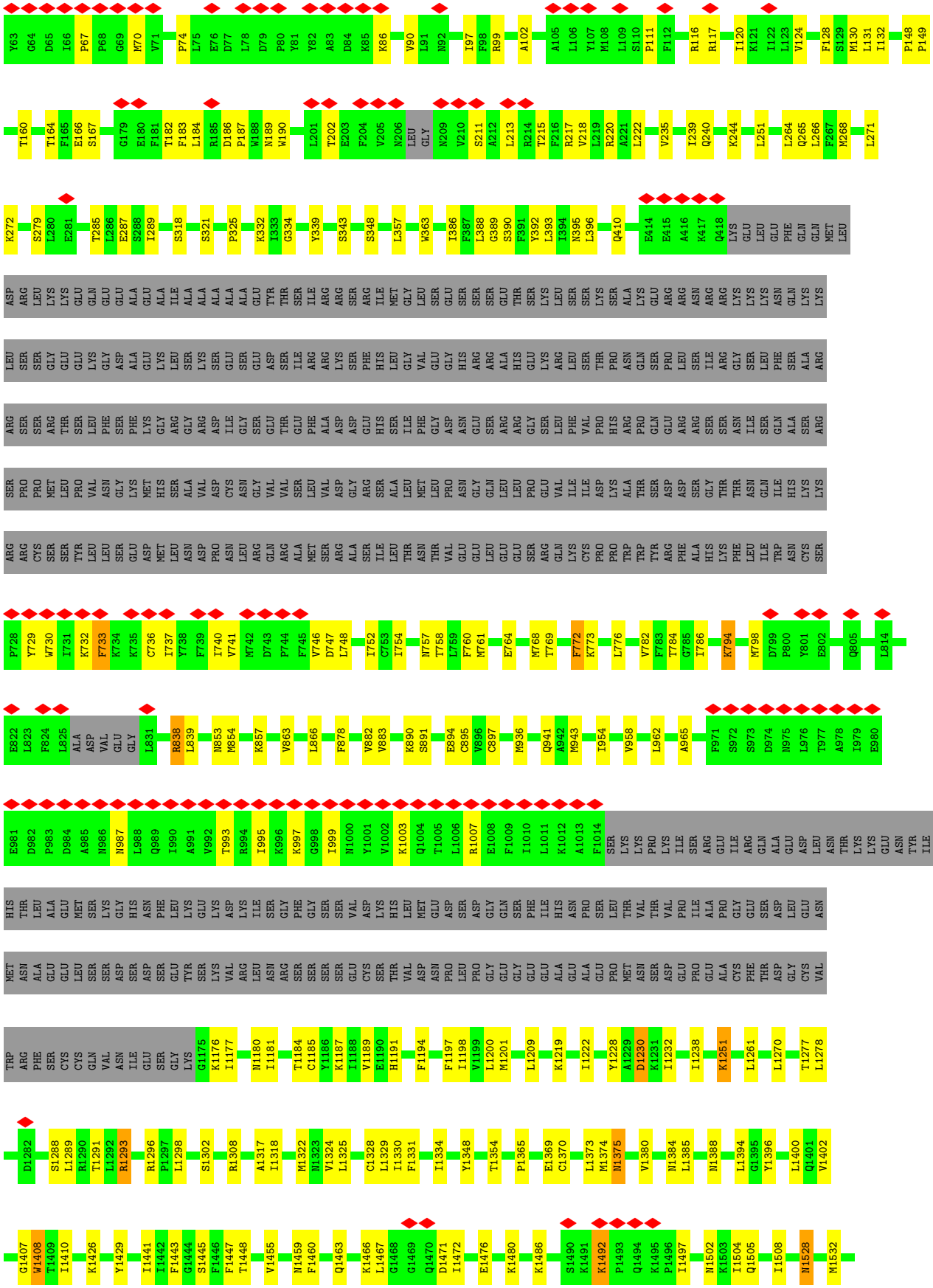


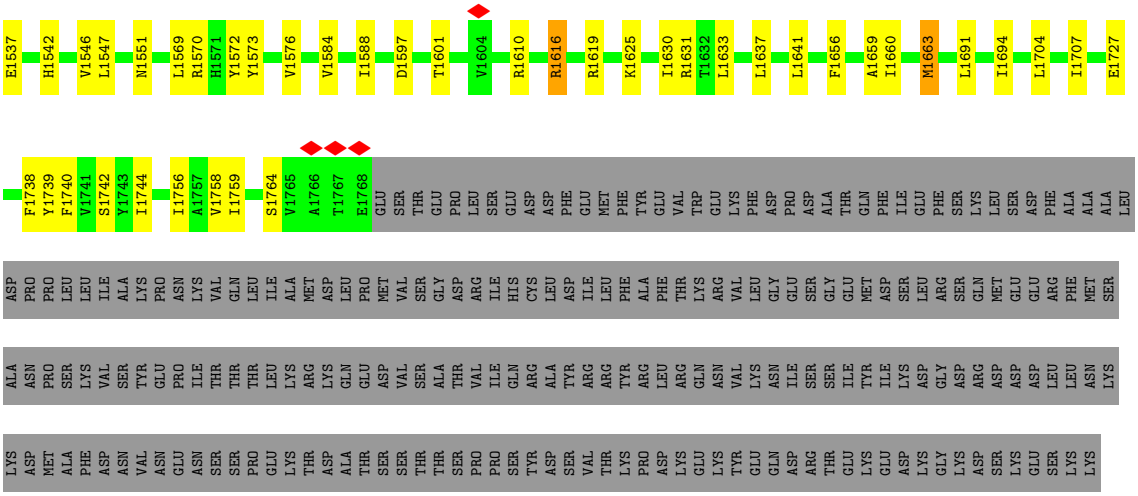
• Molecule 2: Sodium channel subunit beta-2



• Molecule 3: Sodium channel protein type 9 subunit alpha




Y63 G64 D65 I66 P67 P68 G69 M70 V71 P74 L75 E76 D77 L78 D79 P80 Y81 Y82 A83 D84 K85 K86 V90 L91 N92 I97 F98 R99 A102 A105 L106 Y107 M108 L109 S110 P111 F112 R116 R117 I120 K121 I122 L123 V124 F128 S129 M130 L131 I132 P148 P149
T160 T164 F165 E166 S167 G179 E180 F181 T182 F183 L184 R185 D186 P187 W188 N189 W190 L201 T202 E203 F204 V205 N206 LEU GLY N209 V210 S211 A212 L213 R214 T215 F216 R217 V218 L219 R220 A221 L222 V235 I239 Q240 K244 L251 L264 Q265 L266 F267 M268 L271
K272 S279 L280 E281 T285 L286 E287 S288 I289 S318 S321 P325 K332 I333 G334 Y339 S343 S348 L357 W363 I386 F387 L388 G389 S390 F391 Y392 L393 I394 N395 L396 Q410 E414 E415 A416 K417 Q418 LYS GLU LEU GLU PHE GLN GLN MET LEU
ASP ARG LEU LYS LYS GLU GLN GLU GLU ALA GLU ALA ILE ALA ALA ALA ALA ALA GLU TYR THR SER ILE ARG ARG SER ARG ILE MET GLY LEU SER GLU SER SER SER GLU THR SER LYS LEU SER SER LYS SER ALA LYS GLU ARG ARG ASN ARG ARG LYS LYS LYS ASN GLN LYS LYS
LEU SER SER GLY GLU GLU LYS GLY ASP ALA GLU GLU LYS LEU SER LYS SER GLU SER GLU SER GLU ASP SER ILE ARG ARG LYS SER PHE HIS LEU LEU GLY VAL GLU GLU GLY HIS ARG ARG ALA HIS GLU LYS ARG LEU SER THR PRO ASN GLN SER PRO LEU LEU SER ILE ARG GLY SER LEU PHE SER ALA ARG
ARG SER SER ARG THR SER LEU PHE SER PHE LYS GLY ARG GLY ARG ASP ILE GLY SER GLU THR GLY PHE ALA ASP ASP GLU HIS SER ILE PHE GLY GLY ASP ASN GLU GLU SER ARG ARG GLY SER LEU PHE VAL PRO HIS ARG PRO GLN GLU ARG ARG SER SER ASN ILE SER GLN ILE ALA SER ARG
SER PRO PRO MET LEU PRO VAL ASN GLY LYS MET HIS SER ALA VAL ASP CYS ASN GLY VAL VAL SER LEU VAL ASP GLY ARG LEU ALA SER ILE LEU THR ASN THR VAL GLU GLU GLU LEU GLU GLU PRO ASN GLY GLN LEU LEU PRO GLU VAL ILE ILE ASP LYS ALA THR SER ASP ASP SER GLY THR THR ASN GLN ILE HIS LYS LYS
ARG ARG CYS SER SER TYR LEU LEU SER GLU ASP MET LEU ASN ASP PRO ASN LEU ARG GLN ARG GLN ARG ALA MET SER ARG ALA SER ILE LEU THR ASN THR VAL GLU GLU GLU SER ARG GLN LYS CYS PRO PRO TRP TRP TYR ARG PHE ALA ASP PRO TRP ASN CYS SER
P728 Y729 W730 I731 I732 F733 K734 K735 C736 I737 Y738 F739 I740 V741 M742 D743 P744 F745 V746 D747 L748 I752 C753 I754 N757 T758 L759 F760 M761 E764 M768 T769 F772 K773 L776 V782 F783 T784 G785 I786 K794 M798 D799 P800 Y801 E802 Q805 L814
E822 L823 F824 L825 ALA ASP VAL GLU GLY L831 R838 L839 N853 M854 K857 V863 L866 F878 V882 V883 K890 S891 E894 C895 V896 C897 M936 Q941 A942 M943 I954 V958 L962 A965 F971 S972 S973 D974 N975 L976 T977 A978 I979 E980
E981 D982 P983 D984 A985 N986 N987 L988 Q989 I990 A991 V992 T993 R994 I995 K996 K997 G998 I999 N1000 Y1001 V1002 K1003 Q1004 T1005 L1006 R1007 E1008 F1009 I1010 L1011 K1012 A1013 F1014 SER LYS LYS PRO LYS ILE SER ARG GLU ILE ARG GLN ALA GLU ASP LEU ASN THR LYS LYS GLU GLY ASN TYR ILE SER ASN
HIS THR LEU ALA GLU MET SER LYS GLY HIS ASN PHE LEU LYS GLU LYS ASP LYS ILE SER GLY PHE GLY SER SER VAL ASP LYS HIS LEU MET GLU ASP SER ASP GLY GLN SER PHE ILE HIS ASN PRO SER LEU THR VAL THR VAL PRO ILE ALA PRO GLY GLU SER ASP LEU GLU ASN
MET ASN ALA GLU GLU LEU SER SER ASP SER GLU TYR SER LYS VAL ARG LEU ASN ARG SER SER SER GLU CYS SER THR VAL ASP ASN PRO LEU PRO GLY GLU GLY GLU GLU ALA GLU ALA GLU PRO MET ASN SER ASP GLU PRO GLU ALA CYS PHE THR ASP GLY CYS VAL
TRP ARG PHE SER CYS CYS GLN VAL ASN ILE GLU SER GLY LYS G1175 K1176 I1177 N1180 I1181 T1184 C1185 Y1186 K1187 I1188 V1189 E1190 H1191 F1194 F1197 I1198 V1199 L1200 M1201 L1209 K1219 I1222 Y1228 A1229 D1230 K1231 I1232 I1238 K1251 L1261 L1270 T1277 L1278
D1282 S1288 L1289 R1290 T1291 L1292 R1293 R1296 P1297 L1298 S1302 R1308 A1317 I1318 M1322 N1323 V1324 L1325 C1328 L1329 I1330 F1331 I1334 Y1348 T1354 P1365 E1369 C1370 L1373 M1374 N1375 V1380 N1384 L1385 N1388 L1394 G1395 Y1396 L1400 Q1401 V1402
G1407 W1408 T1409 I1410 K1426 Y1429 I1441 I1442 F1443 G1444 S1445 F1446 F1447 T1448 V1455 N1459 F1460 Q1463 K1466 L1467 G1468 G1469 Q1470 D1471 I1472 E1476 K1480 K1486 S1490 K1491 K1492 P1493 Q1494 K1495 P1496 I1497 N1502 K1503 I1504 Q1505 I1508 N1528 M1532

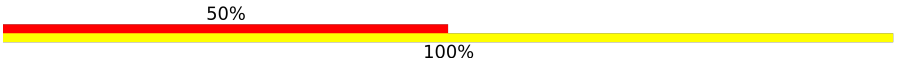


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

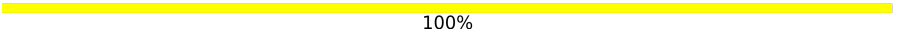
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



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

Chain F:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	297950	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)	1500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.250	Depositor
Minimum map value	-1.973	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.083	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	249.12, 249.12, 249.12	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.865, 0.865, 0.865	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 9Z9, PCW, NA, T70, Y01, NAG, LPE

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	B	0.25	0/1442	0.47	0/1949
2	C	0.24	0/1011	0.51	0/1367
3	A	0.25	0/10524	0.44	0/14258
All	All	0.25	0/12977	0.45	0/17574

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	B	1416	0	1380	14	0
2	C	980	0	935	9	0
3	A	10273	0	10498	159	0
4	D	28	0	25	0	0
4	E	28	0	25	0	0
4	F	28	0	25	0	0
5	A	28	0	26	1	0
5	B	42	0	39	0	0
6	A	70	0	98	2	0
7	A	39	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	31	0	0	1	0
9	A	1	0	0	0	0
10	A	188	0	253	9	0
11	A	232	0	323	13	0
12	A	5	0	0	0	0
All	All	13389	0	13627	185	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 7.

All (185) 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)
3:A:285:THR:O	3:A:289:ILE:HD12	1.80	0.80
3:A:348:SER:HB2	11:A:2011:PCW:H332	1.66	0.76
3:A:67:PRO:HB2	3:A:70:MET:HG3	1.67	0.76
3:A:747:ASP:OD2	3:A:987:ASN:ND2	2.22	0.72
3:A:1324:VAL:HG21	3:A:1455:VAL:HG21	1.73	0.70
1:B:181:CYS:SG	3:A:1187:LYS:NZ	2.64	0.70
3:A:1219:LYS:HB3	3:A:1222:ILE:HD12	1.76	0.66
3:A:1738:PHE:HD1	10:A:2009:LPE:H2N3	1.60	0.65
3:A:1230:ASP:OD1	3:A:1293:ARG:NH2	2.30	0.64
3:A:1467:LEU:HD21	3:A:1472:ILE:HG22	1.81	0.63
3:A:1739:TYR:HD2	10:A:2009:LPE:H3N3	1.63	0.63
1:B:168:VAL:O	1:B:172:ILE:HG23	1.99	0.62
3:A:1502:ASN:HB3	3:A:1505:GLN:HB2	1.81	0.61
3:A:748:LEU:O	3:A:752:ILE:HG12	2.00	0.61
3:A:1277:THR:HG22	3:A:1278:LEU:HD23	1.81	0.60
3:A:1330:ILE:HD12	6:A:2019:Y01:HAA3	1.84	0.60
3:A:265:GLN:NE2	3:A:1610:ARG:O	2.34	0.60
3:A:271:LEU:HD12	3:A:343:SER:HA	1.83	0.59
3:A:1365:PRO:HD2	3:A:1369:GLU:HG3	1.84	0.59
2:C:65:LEU:HB3	2:C:83:PHE:HB3	1.85	0.58
3:A:287:GLU:H	3:A:287:GLU:CD	2.07	0.58
3:A:1003:LYS:HE2	3:A:1007:ARG:HH21	1.68	0.58
3:A:1400:LEU:HD21	3:A:1744:ILE:HD11	1.84	0.58
3:A:1576:VAL:HG13	11:A:2012:PCW:H63	1.85	0.58
3:A:1373:LEU:HG	3:A:1380:VAL:HG21	1.87	0.57
3:A:251:LEU:HD13	3:A:1630:ILE:HB	1.86	0.57
3:A:1400:LEU:HD22	11:A:2008:PCW:H221	1.87	0.57
3:A:124:VAL:HG23	3:A:124:VAL:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:737:ILE:HD13	3:A:740:ILE:HD12	1.87	0.56
3:A:866:LEU:HD21	3:A:965:ALA:HB3	1.87	0.56
1:B:57:TRP:HB2	1:B:71:LEU:HG	1.87	0.56
3:A:1370:CYS:O	3:A:1374:MET:HG3	2.06	0.56
3:A:1659:ALA:O	3:A:1663:MET:HG3	2.06	0.56
2:C:40:VAL:HG11	2:C:46:ALA:HB2	1.87	0.55
3:A:1441:ILE:O	3:A:1445:SER:HB2	2.05	0.55
3:A:993:THR:HG22	3:A:997:LYS:HE3	1.87	0.55
3:A:1497:ILE:HD12	3:A:1572:TYR:HB3	1.89	0.55
2:C:104:ASN:N	2:C:109:ASP:O	2.39	0.55
3:A:1194:PHE:HD1	10:A:2020:LPE:H32	1.71	0.55
3:A:1385:LEU:O	3:A:1388:ASN:ND2	2.39	0.55
3:A:1394:LEU:HG	11:A:2008:PCW:H132	1.89	0.55
3:A:1597:ASP:O	3:A:1601:THR:HG23	2.08	0.54
3:A:936:MET:HG2	3:A:941:GLN:HA	1.90	0.54
3:A:53:LEU:O	3:A:99:ARG:NH2	2.41	0.54
3:A:86:LYS:HB2	3:A:102:ALA:HB3	1.90	0.54
3:A:218:VAL:HG11	3:A:883:VAL:HG23	1.90	0.54
3:A:111:PRO:HA	3:A:116:ARG:HD2	1.89	0.53
1:B:176:ALA:O	1:B:179:ILE:HG13	2.08	0.53
3:A:1288:SER:O	3:A:1291:THR:OG1	2.27	0.53
3:A:754:ILE:O	3:A:758:THR:HG22	2.09	0.52
1:B:71:LEU:HD13	1:B:78:LEU:HD11	1.91	0.52
3:A:1348:TYR:CE1	3:A:1384:ASN:HB2	2.45	0.52
2:C:70:GLN:HG3	2:C:124:ILE:HB	1.93	0.51
3:A:1177:ILE:O	3:A:1181:ILE:HG12	2.09	0.51
3:A:1588:ILE:HG22	11:A:2018:PCW:H232	1.92	0.51
3:A:202:THR:HB	3:A:213:LEU:HD13	1.92	0.51
3:A:757:ASN:O	3:A:761:MET:HG3	2.10	0.51
3:A:268:MET:HG2	3:A:1537:GLU:HG2	1.92	0.51
3:A:272:LYS:NZ	3:A:334:GLY:O	2.36	0.51
3:A:863:VAL:HG22	3:A:863:VAL:O	2.10	0.51
3:A:1691:LEU:HD23	3:A:1694:ILE:HD11	1.93	0.51
3:A:1396:TYR:HB3	11:A:2008:PCW:H211	1.93	0.51
3:A:1707:ILE:HD12	3:A:1740:PHE:HE2	1.76	0.51
3:A:318:SER:OG	3:A:321:SER:OG	2.28	0.50
3:A:211:SER:O	3:A:215:THR:OG1	2.27	0.50
3:A:782:VAL:O	3:A:786:ILE:HG13	2.11	0.50
3:A:1185:CYS:O	3:A:1189:VAL:HG22	2.12	0.50
3:A:217:ARG:O	3:A:220:ARG:HD3	2.12	0.50
3:A:160:THR:O	3:A:164:THR:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:62:GLN:HB3	2:C:132:PRO:HG2	1.93	0.49
3:A:90:VAL:HG21	3:A:120:ILE:HG21	1.93	0.49
3:A:1547:LEU:O	3:A:1551:ASN:ND2	2.43	0.49
3:A:784:THR:OG1	3:A:838:ARG:NH2	2.46	0.49
3:A:187:PRO:HA	3:A:190[B]:TRP:HD1	1.77	0.49
3:A:54:GLU:HB3	3:A:57:LYS:HE3	1.95	0.49
3:A:392:TYR:CZ	3:A:1637:LEU:HB2	2.48	0.48
3:A:1228:TYR:O	3:A:1232:ILE:HG13	2.13	0.48
3:A:266:LEU:O	3:A:1610:ARG:NH1	2.46	0.48
3:A:866:LEU:HD23	3:A:962:LEU:HD12	1.94	0.48
3:A:1191:HIS:CG	10:A:2020:LPE:H322	2.48	0.48
3:A:878:PHE:O	3:A:882:VAL:HG12	2.13	0.48
3:A:184:LEU:O	3:A:190[A]:TRP:NE1	2.42	0.48
3:A:1200:LEU:HD23	3:A:1201:MET:CE	2.44	0.48
3:A:1200:LEU:HD23	3:A:1201:MET:HE1	1.95	0.48
3:A:1325:LEU:O	3:A:1329:LEU:HG	2.14	0.47
3:A:1302:SER:O	3:A:1308:ARG:NH1	2.47	0.47
3:A:395:ASN:HD22	3:A:1758:VAL:HG11	1.79	0.47
3:A:760:PHE:HE1	3:A:776:LEU:HA	1.80	0.47
3:A:1528:ASN:O	3:A:1532:MET:HG3	2.15	0.47
3:A:1759:ILE:HG21	7:A:2003:9Z9:C10	2.45	0.46
3:A:357:LEU:HD23	3:A:363:TRP:HB2	1.97	0.46
1:B:163:MET:O	1:B:167:ILE:HG13	2.16	0.46
3:A:268:MET:CG	3:A:1537:GLU:HG2	2.46	0.46
3:A:392:TYR:CZ	3:A:396:LEU:HD11	2.51	0.46
3:A:235:VAL:O	3:A:239:ILE:HG12	2.14	0.46
3:A:1180:ASN:O	3:A:1184:THR:HG22	2.16	0.46
1:B:175:VAL:O	1:B:179:ILE:HG23	2.16	0.46
1:B:46:ARG:HD3	3:A:325:PRO:HG3	1.98	0.46
3:A:866:LEU:HD21	3:A:965:ALA:CB	2.45	0.46
3:A:1656:PHE:O	3:A:1660:ILE:HG12	2.15	0.46
3:A:1251:LYS:H	3:A:1251:LYS:CD	2.28	0.45
3:A:386:ILE:O	3:A:390:SER:HB3	2.16	0.45
3:A:1630:ILE:HA	3:A:1633:LEU:HD12	1.98	0.45
3:A:730:TRP:CD1	3:A:733:PHE:HE1	2.34	0.45
2:C:147:LEU:HD23	2:C:147:LEU:H	1.81	0.45
3:A:285:THR:C	3:A:289:ILE:HD12	2.37	0.45
3:A:995:ILE:HG23	3:A:999:ILE:HD12	1.98	0.45
3:A:1375:ASN:OD1	5:A:2004:NAG:H2	2.16	0.45
3:A:1443:PHE:HA	3:A:1447:PHE:HD2	1.81	0.45
3:A:244:LYS:HB3	3:A:244:LYS:NZ	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1261:LEU:HD21	3:A:1298:LEU:HB3	1.99	0.45
3:A:1328:CYS:HB2	11:A:2008:PCW:H281	1.99	0.45
1:B:38:ILE:HD12	1:B:106:ILE:HD11	2.00	0.44
1:B:58:THR:OG1	1:B:120:GLU:HB2	2.17	0.44
3:A:128:PHE:O	3:A:132:ILE:HG12	2.17	0.44
1:B:51:ALA:HB2	1:B:127:LEU:HD23	2.00	0.44
2:C:72:CYS:H	2:C:75:CYS:HB2	1.82	0.44
3:A:890:LYS:O	3:A:894:GLU:HG2	2.17	0.44
3:A:1426:LYS:HB2	3:A:1429:TYR:HB2	1.99	0.44
3:A:839:LEU:HB3	3:A:1334:ILE:HG23	1.99	0.44
3:A:1476:GLU:O	3:A:1480:LYS:HG2	2.17	0.44
3:A:1542:HIS:O	3:A:1546:VAL:HG23	2.18	0.44
2:C:66:ASN:HB2	2:C:128:TYR:HB2	1.99	0.44
3:A:240:GLN:HA	3:A:240:GLN:OE1	2.17	0.44
3:A:265:GLN:OE1	3:A:1616:ARG:NH1	2.50	0.44
3:A:396:LEU:HD22	3:A:1633:LEU:HD22	2.00	0.44
3:A:1375:ASN:HD22	3:A:1375:ASN:HA	1.54	0.44
1:B:162:MET:HA	1:B:165:VAL:HG22	1.99	0.43
2:C:56:TYR:CE1	3:A:897:CYS:HB2	2.53	0.43
11:A:2017:PCW:H182	11:A:2018:PCW:H181	2.00	0.43
3:A:1569:LEU:HD12	3:A:1573:TYR:HD1	1.83	0.43
3:A:1209:LEU:HD11	3:A:1296:ARG:HG2	2.00	0.43
3:A:1492:LYS:HB3	3:A:1492:LYS:HE3	1.88	0.43
10:A:2007:LPE:H121	11:A:2008:PCW:H172	2.01	0.43
1:B:174:LEU:O	1:B:178:MET:HG3	2.19	0.43
3:A:761:MET:SD	3:A:838:ARG:HD2	2.59	0.43
3:A:1318:ILE:HD13	3:A:1318:ILE:HA	1.85	0.43
3:A:1317:ALA:HA	3:A:1459:ASN:OD1	2.19	0.42
3:A:794:LYS:HB3	3:A:794:LYS:HE2	1.80	0.42
3:A:1194:PHE:O	3:A:1198:ILE:HG12	2.19	0.42
3:A:339:TYR:O	11:A:2011:PCW:H61	2.20	0.42
3:A:1407:GLY:O	3:A:1410:ILE:HG22	2.18	0.42
3:A:1476:GLU:OE1	3:A:1476:GLU:N	2.51	0.42
3:A:1504:ILE:O	3:A:1508:ILE:HG13	2.19	0.42
3:A:264:LEU:O	3:A:268:MET:HB2	2.19	0.42
3:A:760:PHE:CE1	3:A:776:LEU:HA	2.54	0.42
3:A:1402:VAL:HA	3:A:1408:TRP:HB3	2.02	0.42
10:A:2014:LPE:H12	10:A:2014:LPE:H122	1.78	0.42
3:A:768:MET:HG2	3:A:772:PHE:HB3	2.01	0.42
3:A:729:TYR:HA	3:A:732:LYS:HD3	2.02	0.42
3:A:854:MET:SD	3:A:857:LYS:NZ	2.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1238:ILE:HD11	3:A:1270:LEU:HD13	2.01	0.42
3:A:74:PRO:HG2	3:A:117:ARG:HH21	1.84	0.41
3:A:1197:PHE:O	3:A:1201:MET:HG2	2.20	0.41
3:A:1328:CYS:SG	3:A:1448:THR:HG23	2.60	0.41
3:A:1742:SER:HA	10:A:2007:LPE:H212	2.02	0.41
3:A:769:THR:O	3:A:773:LYS:HG3	2.21	0.41
3:A:1460:PHE:CD2	3:A:1756:ILE:HD13	2.55	0.41
3:A:891:SER:O	3:A:895:CYS:HB2	2.20	0.41
3:A:1194:PHE:HB2	10:A:2020:LPE:O31	2.19	0.41
3:A:166:GLU:HG3	3:A:167:SER:N	2.36	0.41
3:A:1625:LYS:O	3:A:1631:ARG:NH1	2.53	0.41
6:A:2019:Y01:HAO2	6:A:2019:Y01:HAP1	1.37	0.41
11:A:2012:PCW:H2	11:A:2012:PCW:O2P	2.21	0.41
3:A:1619:ARG:HH12	8:A:2005:T70:C30	2.32	0.41
3:A:59:LEU:HA	3:A:97:ILE:HD11	2.03	0.41
3:A:222:LEU:HD23	3:A:222:LEU:HA	1.84	0.41
3:A:388:LEU:O	3:A:392:TYR:HB3	2.21	0.41
3:A:741:VAL:HA	3:A:746:VAL:HG21	2.02	0.41
11:A:2012:PCW:H382	11:A:2017:PCW:H382	2.03	0.41
3:A:1463:GLN:HA	3:A:1466:LYS:HE3	2.03	0.41
3:A:853:ASN:O	3:A:857:LYS:HG3	2.21	0.40
3:A:1663:MET:HG3	3:A:1663:MET:H	1.76	0.40
1:B:161:ILE:HD13	1:B:161:ILE:HA	1.85	0.40
3:A:1176:LYS:H	3:A:1176:LYS:HG2	1.67	0.40
3:A:1584:VAL:HG11	11:A:2012:PCW:H161	2.04	0.40
3:A:332:LYS:HB3	3:A:332:LYS:HE3	1.89	0.40
3:A:954:ILE:O	3:A:958:VAL:HG23	2.21	0.40
3:A:182:THR:OG1	3:A:183:PHE:N	2.55	0.40
3:A:410:GLN:OE1	3:A:410:GLN:HA	2.21	0.40
3:A:1584:VAL:O	3:A:1588:ILE:HG23	2.22	0.40
3:A:148:PRO:HA	3:A:149:PRO:HD3	1.96	0.40
3:A:186:ASP:HB3	3:A:189:ASN:HD22	1.87	0.40
3:A:389:GLY:O	3:A:393:LEU:HB2	2.22	0.40
3:A:1641:LEU:HB3	10:A:2013:LPE:H11	2.03	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	B	171/192 (89%)	171 (100%)	0	0	100	100
2	C	120/215 (56%)	117 (98%)	3 (2%)	0	100	100
3	A	1262/1988 (64%)	1241 (98%)	21 (2%)	0	100	100
All	All	1553/2395 (65%)	1529 (98%)	24 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	157/169 (93%)	154 (98%)	3 (2%)	52	79
2	C	114/193 (59%)	113 (99%)	1 (1%)	75	90
3	A	1136/1778 (64%)	1106 (97%)	30 (3%)	41	70
All	All	1407/2140 (66%)	1373 (98%)	34 (2%)	45	73

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	79	GLN
1	B	93	ASN
1	B	137	SER
2	C	85	MET
3	A	130	MET

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Mol	Chain	Res	Type
3	A	131	LEU
3	A	279	SER
3	A	733	PHE
3	A	736	CYS
3	A	764	GLU
3	A	772	PHE
3	A	794	LYS
3	A	798	MET
3	A	838	ARG
3	A	943	MET
3	A	1230	ASP
3	A	1251	LYS
3	A	1289	LEU
3	A	1293	ARG
3	A	1322	MET
3	A	1331	PHE
3	A	1354	THR
3	A	1375	ASN
3	A	1408	TRP
3	A	1471	ASP
3	A	1486	LYS
3	A	1492	LYS
3	A	1528	ASN
3	A	1570	ARG
3	A	1616	ARG
3	A	1663	MET
3	A	1704	LEU
3	A	1727	GLU
3	A	1764	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	941	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

6 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	$\#\|Z\| > 2$
4	NAG	D	1	4,1	14,14,15	0.31	0	17,19,21	0.79	1 (5%)
4	NAG	D	2	4	14,14,15	0.31	0	17,19,21	0.78	0
4	NAG	E	1	4,3	14,14,15	0.34	0	17,19,21	0.91	1 (5%)
4	NAG	E	2	4	14,14,15	0.33	0	17,19,21	0.78	1 (5%)
4	NAG	F	1	4,3	14,14,15	0.45	0	17,19,21	1.77	4 (23%)
4	NAG	F	2	4	14,14,15	0.30	0	17,19,21	0.83	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
4	NAG	D	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	NAG	E	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	NAG	F	1	4,3	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	1	NAG	C1-O5-C5	4.80	118.69	112.19
4	F	1	NAG	C4-C3-C2	-2.76	106.98	111.02
4	D	1	NAG	C1-O5-C5	2.63	115.75	112.19
4	F	1	NAG	O5-C1-C2	2.55	115.31	111.29
4	F	2	NAG	C1-O5-C5	2.42	115.47	112.19
4	E	1	NAG	C4-C3-C2	2.29	114.37	111.02
4	F	1	NAG	O4-C4-C3	2.19	115.40	110.35
4	E	2	NAG	O5-C1-C2	-2.11	107.95	111.29

There are no chirality outliers.

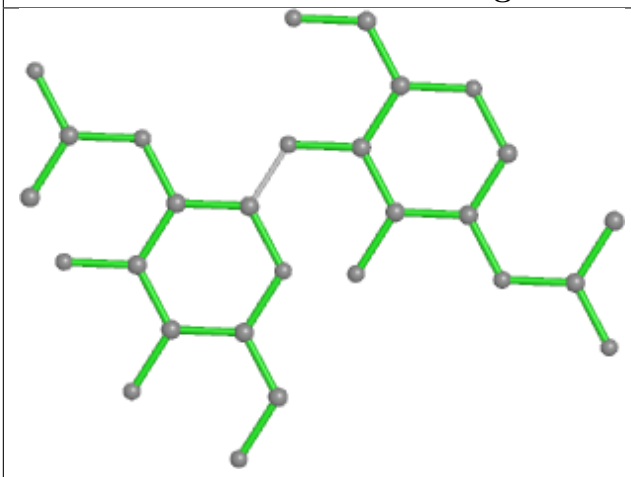
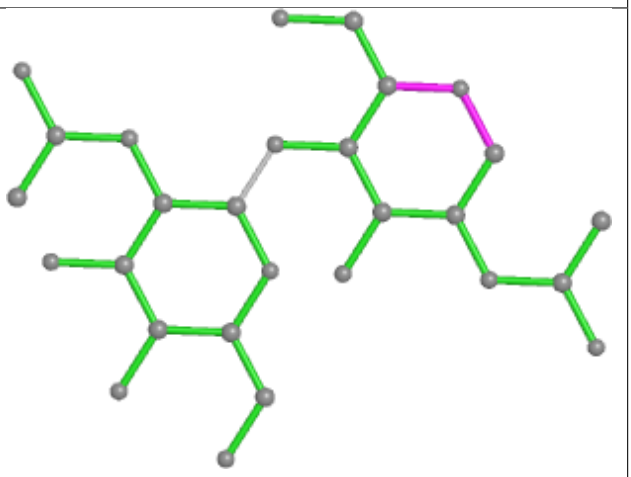
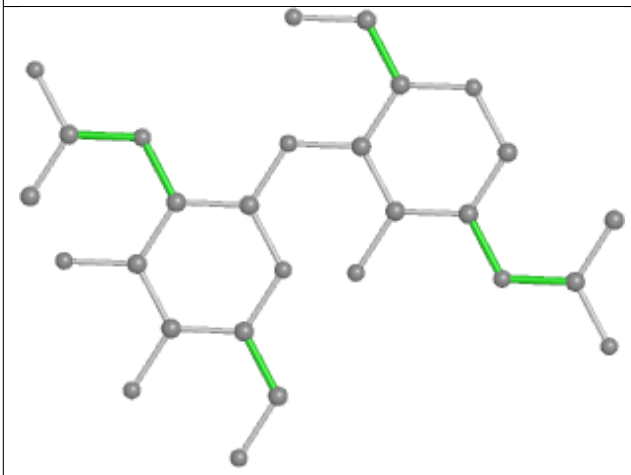
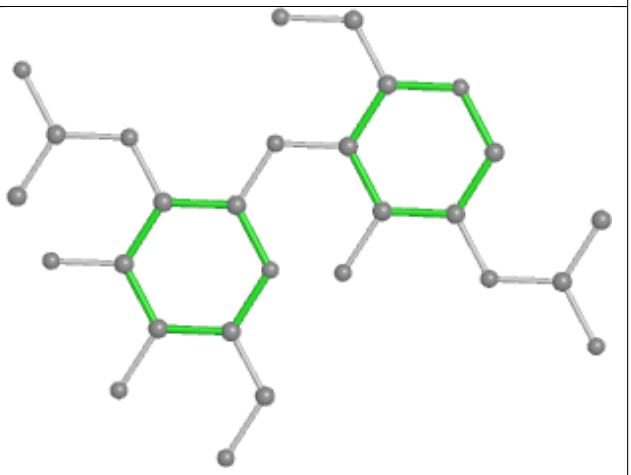
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	2	NAG	C8-C7-N2-C2
4	E	2	NAG	O7-C7-N2-C2
4	F	1	NAG	O5-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6

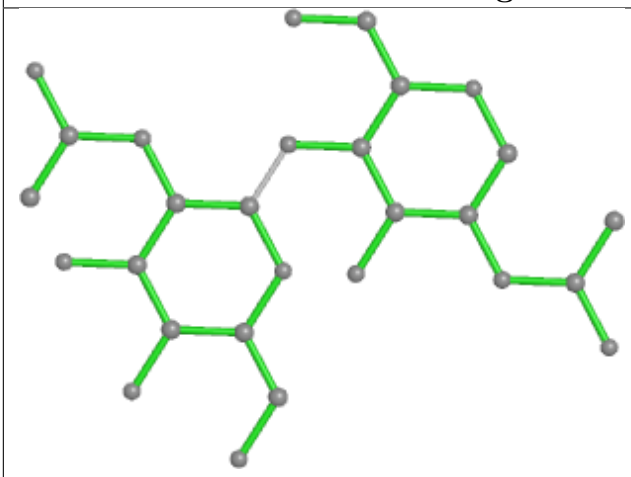
There are no ring outliers.

No monomer is involved in short contacts.

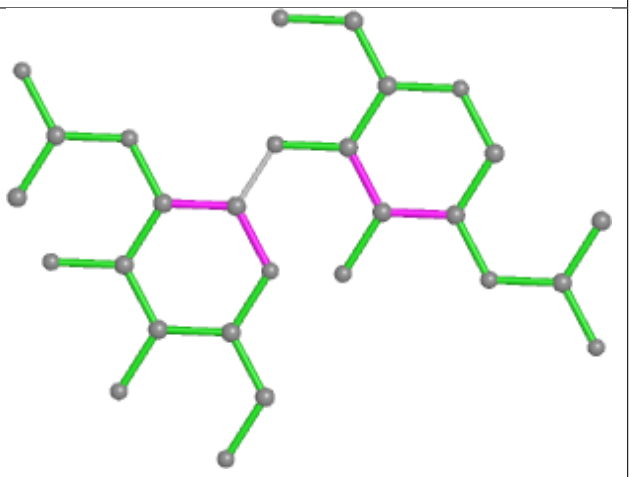
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain D	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

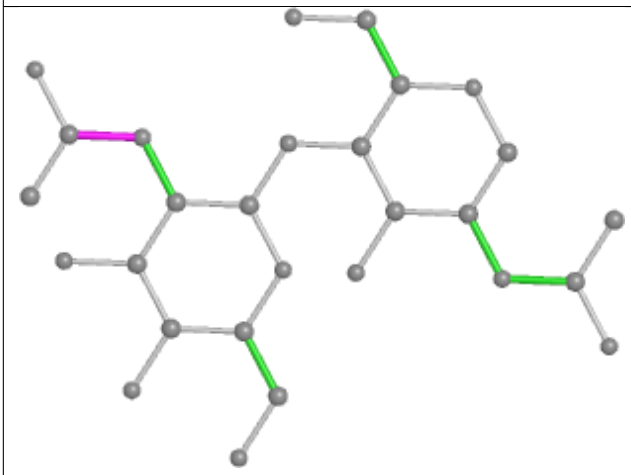
Oligosaccharide Chain E



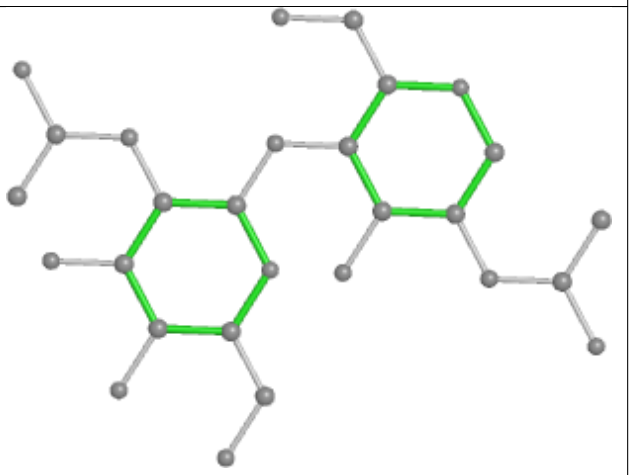
Bond lengths



Bond angles

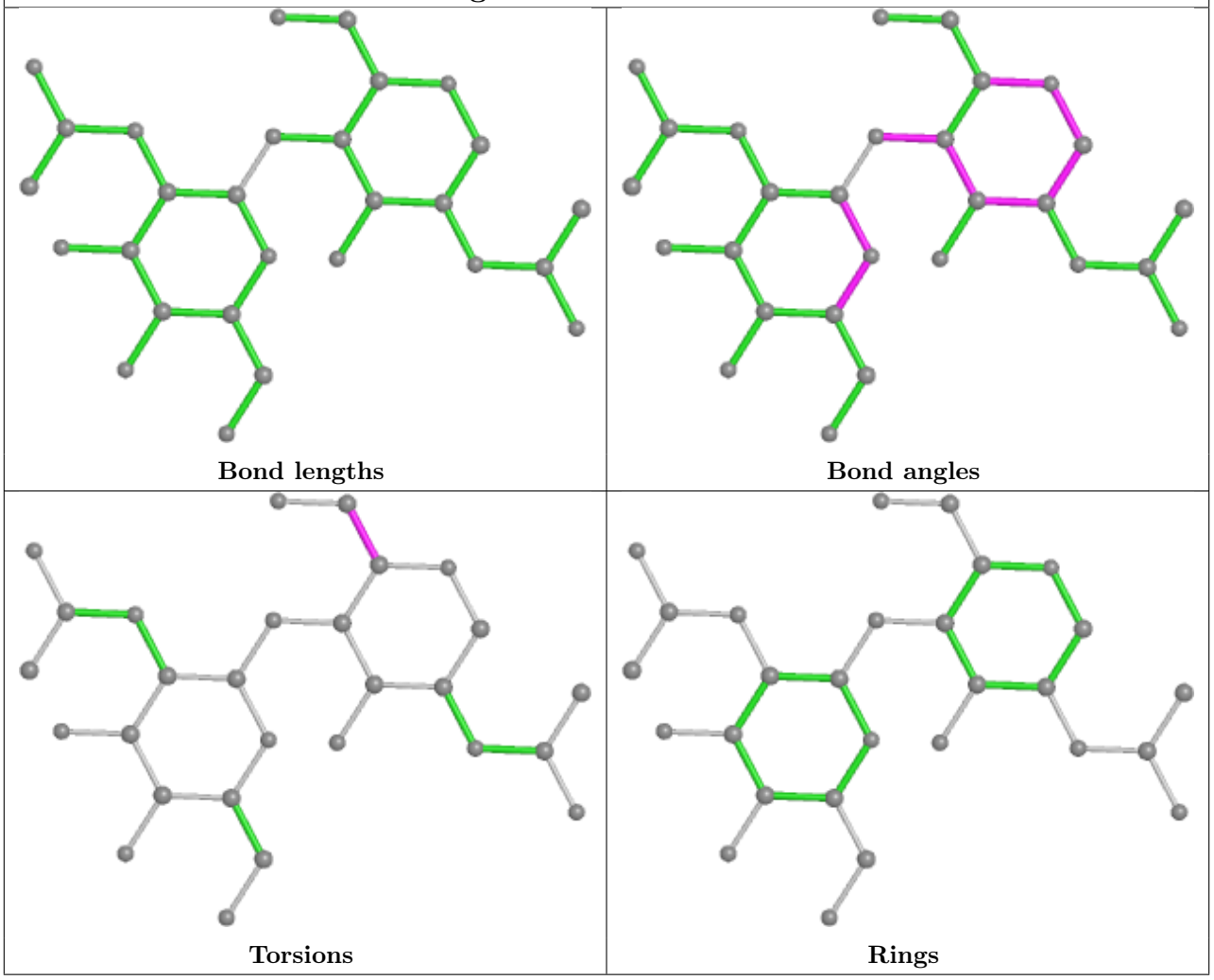


Torsions



Rings

Oligosaccharide Chain F



5.6 Ligand geometry (i)

Of 23 ligands modelled in this entry, 1 is 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	LPE	A	2013	-	24,24,33	0.28	0	28,30,39	0.41	0
10	LPE	A	2015	-	24,24,33	0.28	0	28,30,39	0.32	0
10	LPE	A	2009	-	17,17,33	0.35	0	21,23,39	0.39	0
10	LPE	A	2016	-	24,24,33	0.28	0	28,30,39	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	9Z9	A	2003	-	44,44,44	0.26	0	66,68,68	0.47	0
11	PCW	A	2018	-	43,43,53	0.31	0	49,51,61	0.32	0
11	PCW	A	2011	-	46,46,53	0.31	0	52,54,61	0.37	0
8	T70	A	2005	-	29,34,34	5.29	7 (24%)	33,50,50	2.15	5 (15%)
5	NAG	A	2001	3	14,14,15	0.37	0	17,19,21	0.61	0
11	PCW	A	2012	-	43,43,53	0.32	0	49,51,61	0.36	0
10	LPE	A	2007	-	24,24,33	0.31	0	25,27,39	0.43	0
5	NAG	B	303	1	14,14,15	0.29	0	17,19,21	0.65	0
5	NAG	B	301	1	14,14,15	0.29	0	17,19,21	0.60	0
11	PCW	A	2008	-	52,52,53	0.31	0	58,60,61	0.32	0
6	Y01	A	2019	-	38,38,38	0.44	0	57,57,57	0.52	0
5	NAG	B	302	1	14,14,15	0.32	0	17,19,21	0.77	1 (5%)
10	LPE	A	2020	-	16,16,33	0.34	0	20,22,39	0.42	0
5	NAG	A	2004	3	14,14,15	0.52	0	17,19,21	1.44	2 (11%)
10	LPE	A	2014	-	24,24,33	0.28	0	28,30,39	0.35	0
11	PCW	A	2017	-	43,43,53	0.31	0	49,51,61	0.32	0
6	Y01	A	2002	-	38,38,38	0.44	0	57,57,57	0.49	0
10	LPE	A	2010	-	27,27,33	0.26	0	31,33,39	0.34	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	LPE	A	2013	-	-	7/25/25/34	-
10	LPE	A	2015	-	-	4/25/25/34	-
10	LPE	A	2009	-	-	5/18/18/34	-
10	LPE	A	2016	-	-	8/25/25/34	-
7	9Z9	A	2003	-	-	0/12/100/100	0/6/6/6
11	PCW	A	2018	-	-	5/47/47/57	-
11	PCW	A	2011	-	-	9/50/50/57	-
8	T70	A	2005	-	-	2/17/19/19	0/4/4/4
5	NAG	A	2001	3	-	2/6/23/26	0/1/1/1
11	PCW	A	2012	-	-	4/47/47/57	-
10	LPE	A	2007	-	-	3/25/25/34	-
5	NAG	B	303	1	-	2/6/23/26	0/1/1/1
5	NAG	B	301	1	-	0/6/23/26	0/1/1/1
11	PCW	A	2008	-	-	15/56/56/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	Y01	A	2019	-	-	7/19/77/77	0/4/4/4
5	NAG	B	302	1	-	2/6/23/26	0/1/1/1
10	LPE	A	2020	-	-	6/17/17/34	-
5	NAG	A	2004	3	-	4/6/23/26	0/1/1/1
10	LPE	A	2014	-	-	5/25/25/34	-
11	PCW	A	2017	-	-	8/47/47/57	-
6	Y01	A	2002	-	-	7/19/77/77	0/4/4/4
10	LPE	A	2010	-	-	5/28/28/34	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	2005	T70	O07-S03	19.27	1.65	1.43
8	A	2005	T70	O08-S03	19.08	1.65	1.43
8	A	2005	T70	S03-N09	4.66	1.71	1.63
8	A	2005	T70	C24-N12	4.53	1.45	1.34
8	A	2005	T70	C14-S03	3.22	1.82	1.77
8	A	2005	T70	C21-CL01	2.25	1.79	1.73
8	A	2005	T70	C27-CL02	2.01	1.78	1.74

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	2005	T70	O08-S03-O07	-9.38	108.01	119.55
8	A	2005	T70	C22-C20-C14	-5.18	120.10	123.10
5	A	2004	NAG	C1-O5-C5	4.85	118.76	112.19
8	A	2005	T70	C14-S03-N09	2.76	110.50	107.27
8	A	2005	T70	C30-S04-C31	2.52	97.51	92.37
8	A	2005	T70	C29-N09-S03	-2.16	120.34	124.97
5	B	302	NAG	C1-O5-C5	2.16	115.11	112.19
5	A	2004	NAG	O5-C1-C2	2.05	114.52	111.29

There are no chirality outliers.

All (110) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2004	NAG	C8-C7-N2-C2
5	A	2004	NAG	O7-C7-N2-C2
8	A	2005	T70	C16-C15-C18-C24

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Mol	Chain	Res	Type	Atoms
10	A	2007	LPE	C31-O33-P-O3
10	A	2007	LPE	C31-O33-P-O31
10	A	2007	LPE	C32-C31-O33-P
10	A	2009	LPE	C31-O33-P-O31
10	A	2013	LPE	C3-O3-P-O31
10	A	2014	LPE	C31-O33-P-O31
10	A	2015	LPE	C31-O33-P-O31
10	A	2016	LPE	C31-O33-P-O3
10	A	2016	LPE	C31-O33-P-O31
10	A	2016	LPE	C31-O33-P-O32
10	A	2016	LPE	C32-C31-O33-P
10	A	2020	LPE	C32-C31-O33-P
10	A	2020	LPE	O33-C31-C32-N
11	A	2008	PCW	C4-O4P-P-O2P
11	A	2011	PCW	O4P-C4-C5-N
11	A	2011	PCW	C1-O3P-P-O2P
11	A	2017	PCW	C4-O4P-P-O2P
11	A	2018	PCW	C1-O3P-P-O2P
6	A	2019	Y01	CAJ-CAO-CBB-CAC
6	A	2019	Y01	CAC-CBB-CBE-CAP
6	A	2002	Y01	CAJ-CAO-CBB-CBE
5	B	303	NAG	C8-C7-N2-C2
5	B	303	NAG	O7-C7-N2-C2
6	A	2019	Y01	CAC-CBB-CBE-CBI
6	A	2002	Y01	CAJ-CAO-CBB-CAC
6	A	2019	Y01	CAO-CBB-CBE-CBI
5	A	2004	NAG	O5-C5-C6-O6
6	A	2019	Y01	CAJ-CAO-CBB-CBE
11	A	2012	PCW	C2-C1-O3P-P
11	A	2017	PCW	C11-C12-C13-C14
6	A	2019	Y01	CAO-CBB-CBE-CAP
10	A	2020	LPE	C31-O33-P-O3
11	A	2011	PCW	C4-O4P-P-O3P
11	A	2017	PCW	C1-O3P-P-O4P
5	B	302	NAG	C8-C7-N2-C2
5	A	2004	NAG	C4-C5-C6-O6
10	A	2016	LPE	O1-C1-C2-O2H
11	A	2008	PCW	O3P-C1-C2-C3
11	A	2011	PCW	C35-C36-C37-C38
10	A	2016	LPE	C2-C1-O1-C11
5	A	2001	NAG	C8-C7-N2-C2
5	B	302	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
6	A	2019	Y01	CAN-CAJ-CAO-CBB
10	A	2013	LPE	C3-O3-P-O33
11	A	2018	PCW	O2-C2-C3-O3
10	A	2015	LPE	C2-C3-O3-P
11	A	2008	PCW	C32-C33-C34-C35
11	A	2011	PCW	C1-O3P-P-O4P
10	A	2020	LPE	C31-O33-P-O31
11	A	2011	PCW	C4-O4P-P-O2P
11	A	2017	PCW	C1-O3P-P-O2P
10	A	2009	LPE	C32-C31-O33-P
10	A	2014	LPE	C32-C31-O33-P
11	A	2008	PCW	C5-C4-O4P-P
11	A	2008	PCW	C31-C32-C33-C34
5	A	2001	NAG	O7-C7-N2-C2
10	A	2009	LPE	O33-C31-C32-N
10	A	2013	LPE	O33-C31-C32-N
10	A	2014	LPE	O33-C31-C32-N
10	A	2015	LPE	O33-C31-C32-N
10	A	2016	LPE	O33-C31-C32-N
11	A	2008	PCW	O4P-C4-C5-N
11	A	2017	PCW	O4P-C4-C5-N
11	A	2018	PCW	O4P-C4-C5-N
11	A	2008	PCW	O3P-C1-C2-O2
10	A	2009	LPE	C3-O3-P-O33
10	A	2009	LPE	C31-O33-P-O3
10	A	2010	LPE	C3-O3-P-O33
10	A	2010	LPE	C31-O33-P-O3
10	A	2013	LPE	C31-O33-P-O3
10	A	2014	LPE	C31-O33-P-O3
10	A	2015	LPE	C31-O33-P-O3
10	A	2020	LPE	C3-O3-P-O33
11	A	2008	PCW	C1-O3P-P-O4P
11	A	2008	PCW	C4-O4P-P-O3P
11	A	2012	PCW	C1-O3P-P-O4P
11	A	2017	PCW	C4-O4P-P-O3P
11	A	2018	PCW	C1-O3P-P-O4P
10	A	2014	LPE	C12-C11-O1-C1
11	A	2011	PCW	C17-C18-C19-C20
6	A	2002	Y01	CAO-CBB-CBE-CBI
10	A	2010	LPE	C2-C3-O3-P
8	A	2005	T70	C20-C14-S03-O07
11	A	2017	PCW	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
6	A	2002	Y01	CAO-CBB-CBE-CAP
6	A	2002	Y01	CAR-CBC-OAW-CAY
11	A	2011	PCW	C39-C40-C41-C42
6	A	2002	Y01	CAC-CBB-CBE-CBI
11	A	2008	PCW	O31-C31-O2-C2
11	A	2008	PCW	O2-C2-C3-O3
11	A	2017	PCW	C2-C1-O3P-P
11	A	2018	PCW	C1-C2-C3-O3
11	A	2008	PCW	C17-C18-C19-C20
11	A	2008	PCW	C37-C38-C39-C40
11	A	2011	PCW	C37-C38-C39-C40
11	A	2008	PCW	C39-C40-C41-C42
6	A	2002	Y01	CAV-CBC-OAW-CAY
11	A	2008	PCW	C32-C31-O2-C2
10	A	2013	LPE	C2-C1-O1-C11
10	A	2010	LPE	C3-O3-P-O31
10	A	2010	LPE	C31-O33-P-O31
10	A	2013	LPE	C31-O33-P-O31
10	A	2016	LPE	C3-O3-P-O31
10	A	2020	LPE	C3-O3-P-O31
11	A	2012	PCW	O2-C31-C32-C33
10	A	2013	LPE	C32-C31-O33-P
11	A	2012	PCW	O31-C31-C32-C33

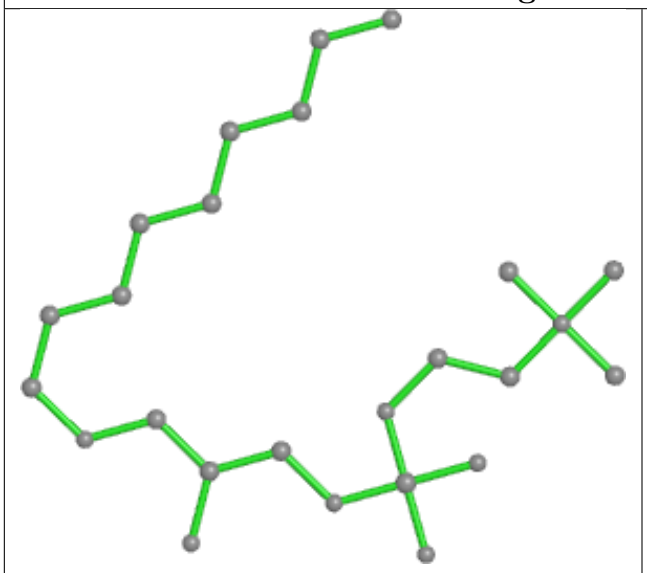
There are no ring outliers.

14 monomers are involved in 26 short contacts:

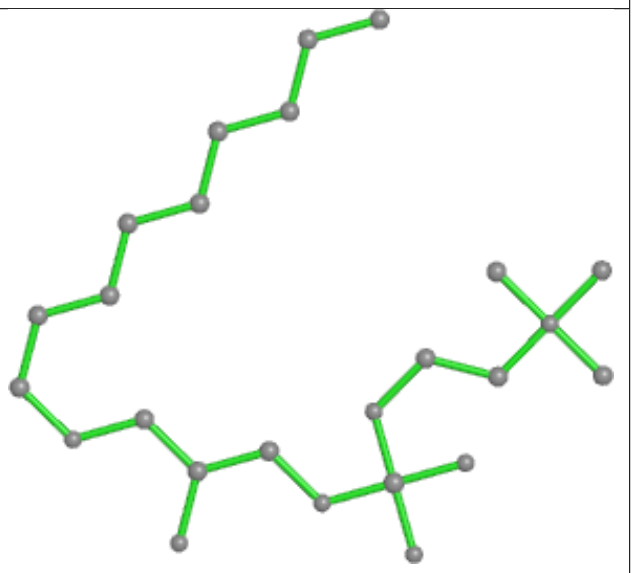
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	2013	LPE	1	0
10	A	2009	LPE	2	0
7	A	2003	9Z9	1	0
11	A	2018	PCW	2	0
11	A	2011	PCW	2	0
8	A	2005	T70	1	0
11	A	2012	PCW	4	0
10	A	2007	LPE	2	0
11	A	2008	PCW	5	0
6	A	2019	Y01	2	0
10	A	2020	LPE	3	0
5	A	2004	NAG	1	0
10	A	2014	LPE	1	0
11	A	2017	PCW	2	0

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.

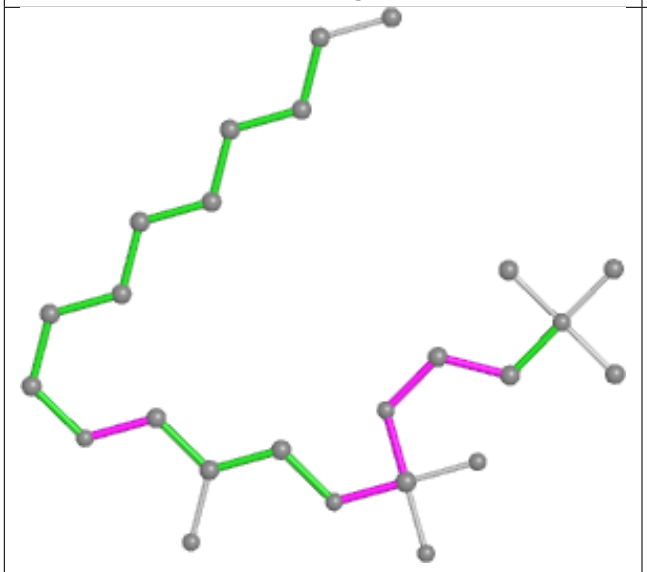
Ligand LPE A 2013



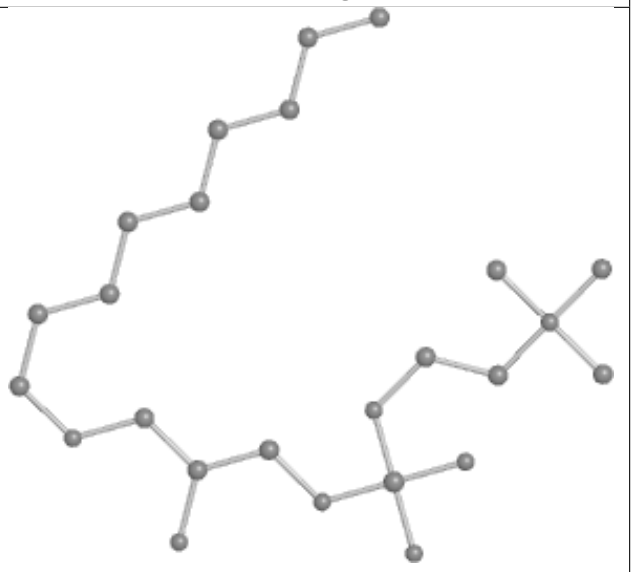
Bond lengths



Bond angles

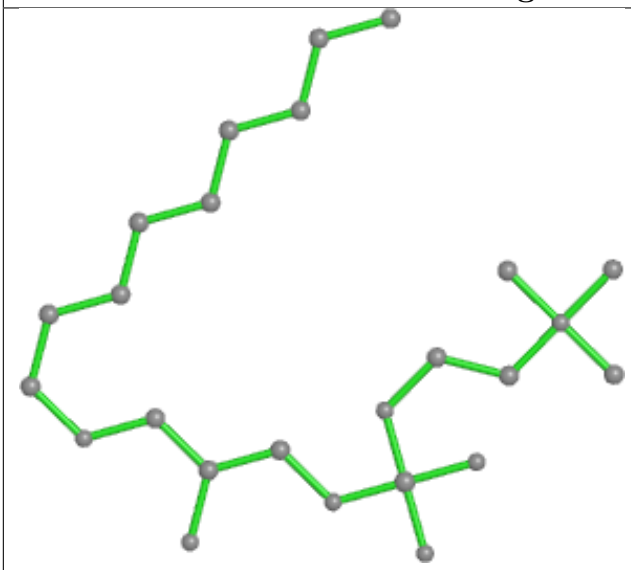


Torsions

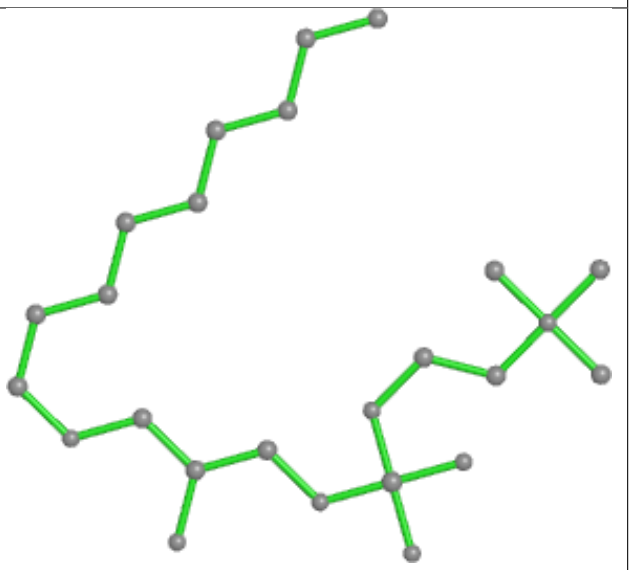


Rings

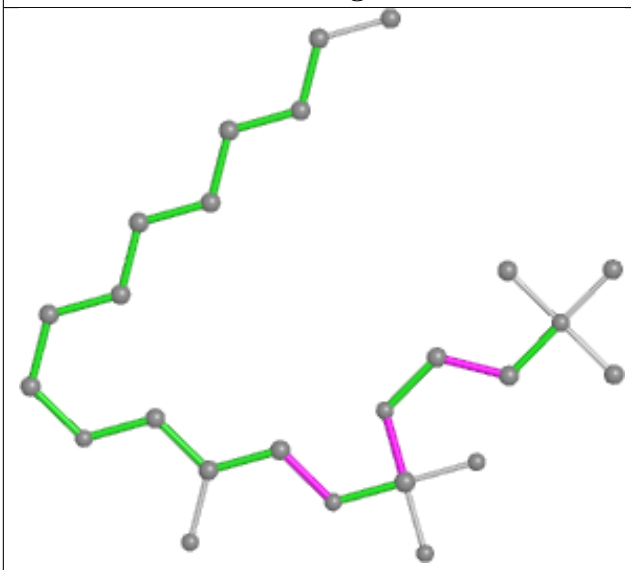
Ligand LPE A 2015



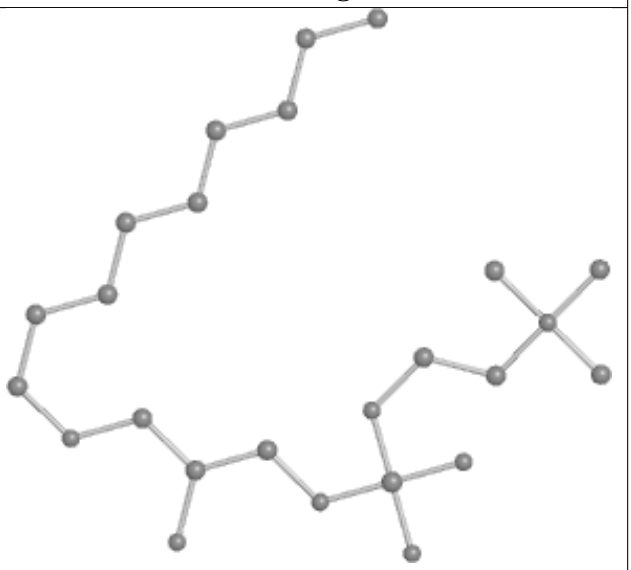
Bond lengths



Bond angles

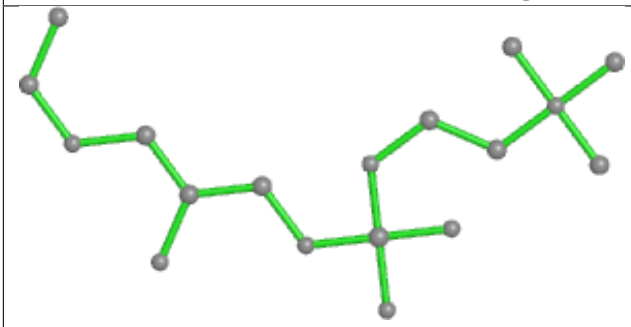


Torsions

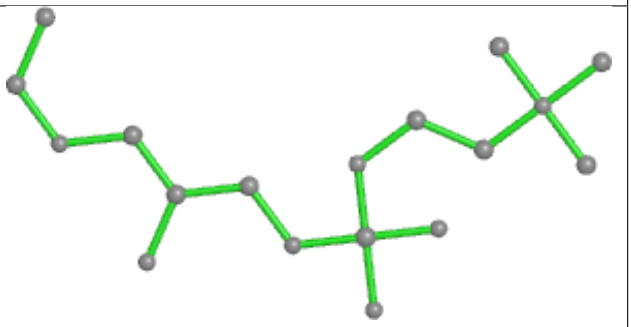


Rings

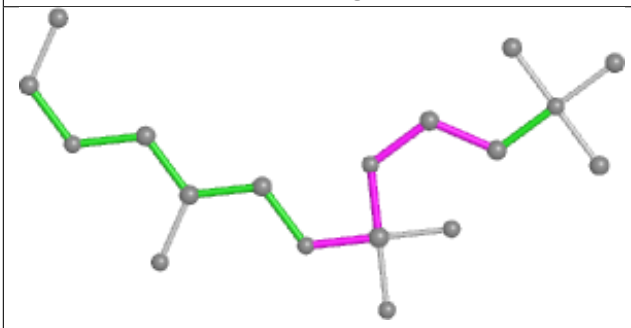
Ligand LPE A 2009



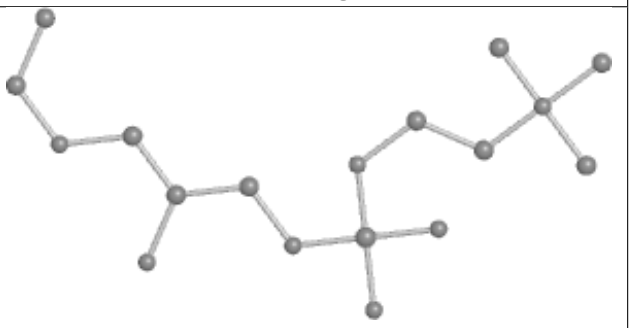
Bond lengths



Bond angles

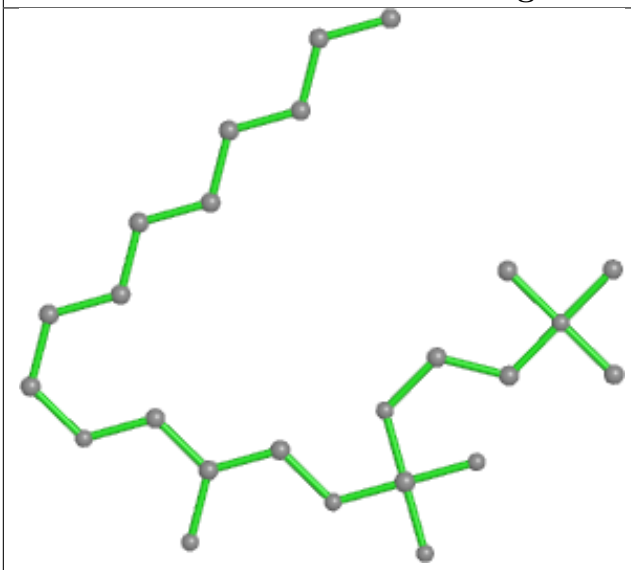


Torsions

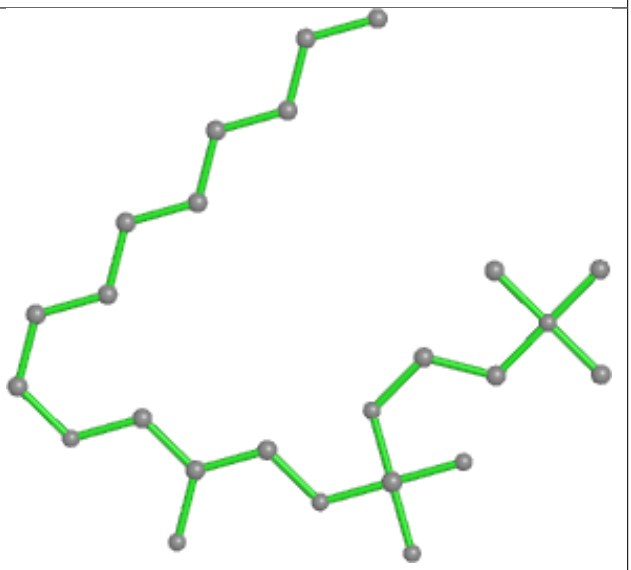


Rings

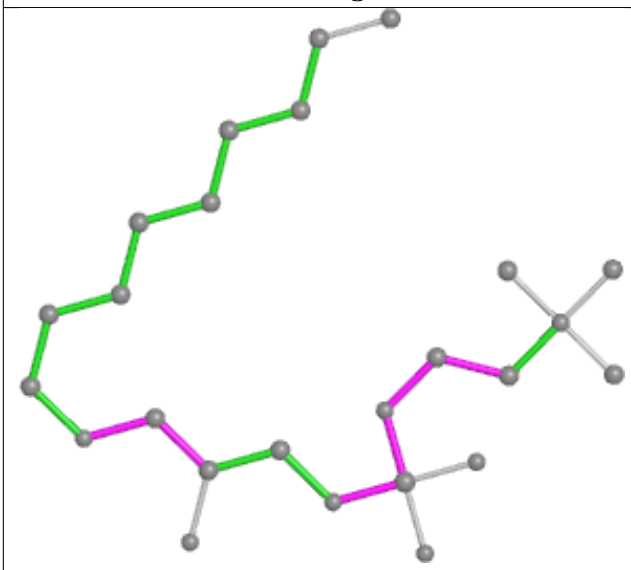
Ligand LPE A 2016



Bond lengths



Bond angles



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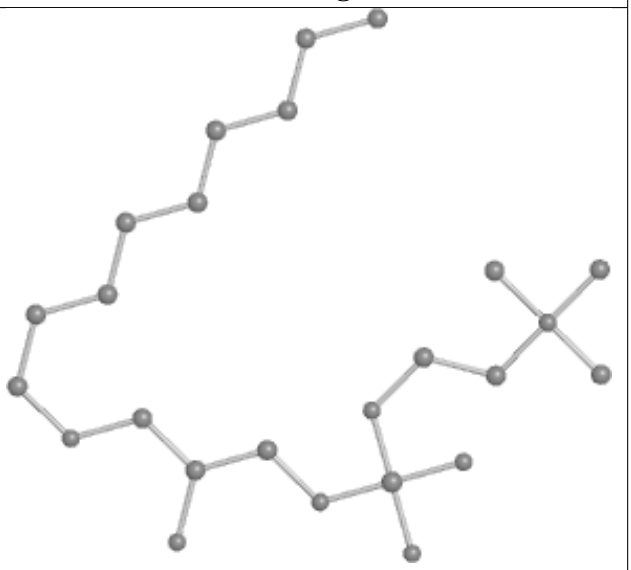
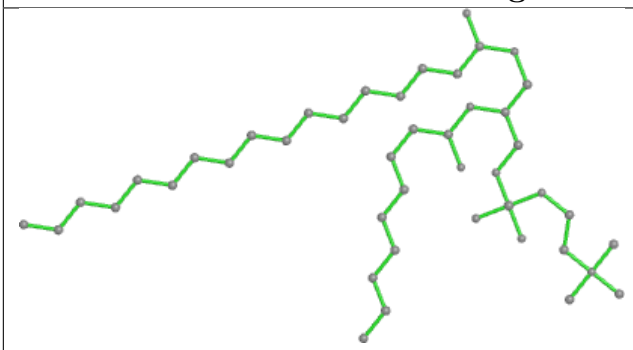
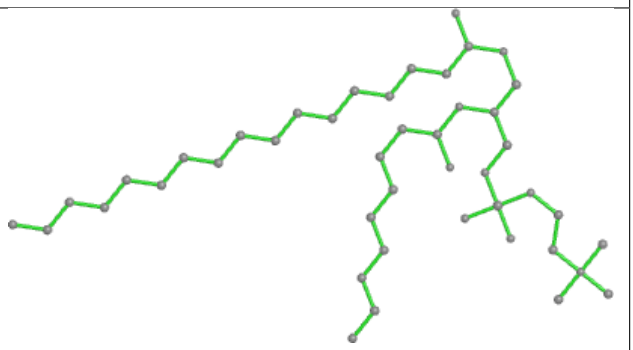


Rings

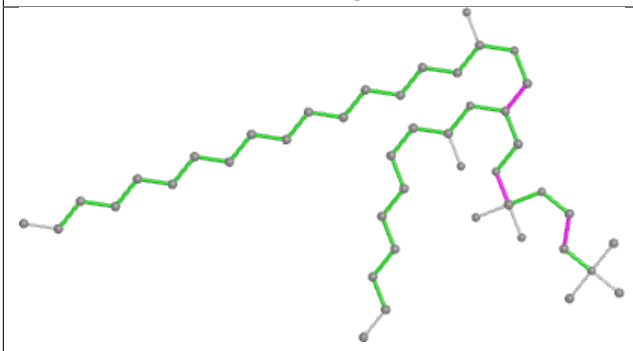
Ligand PCW A 2018



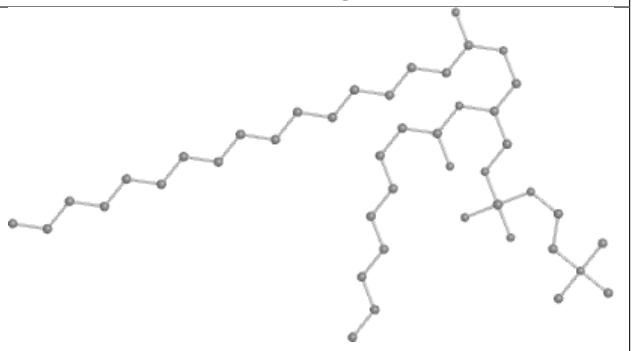
Bond lengths



Bond angles

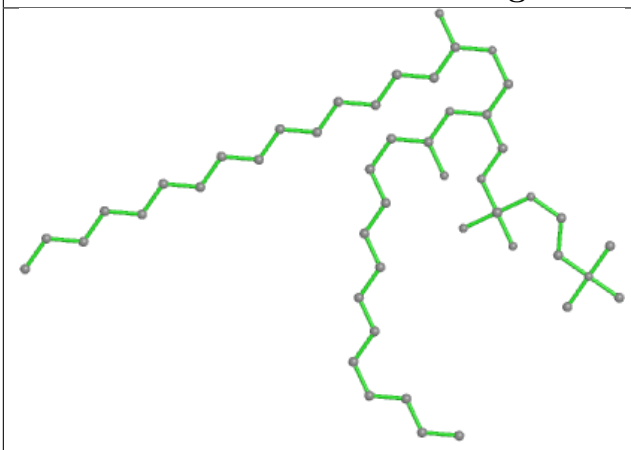


Torsions

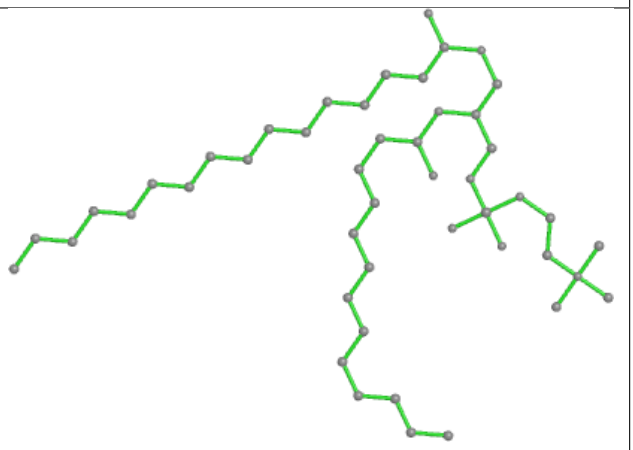


Rings

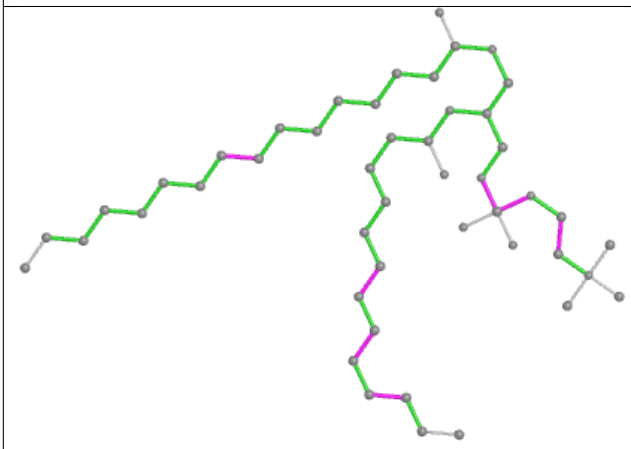
Ligand PCW A 2011



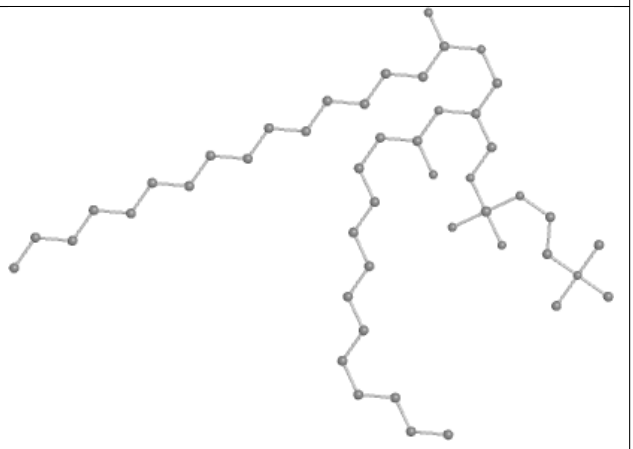
Bond lengths



Bond angles

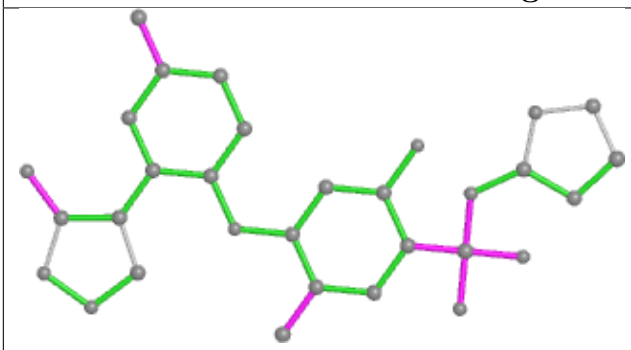


Torsions

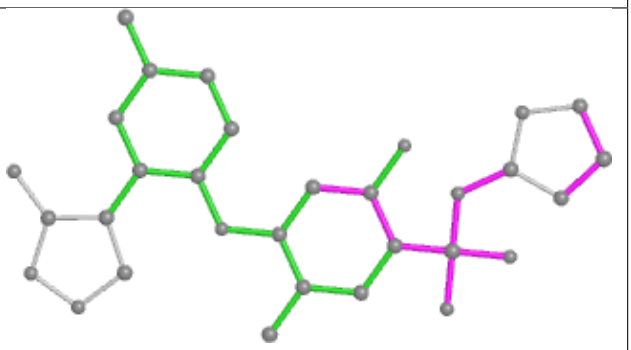


Rings

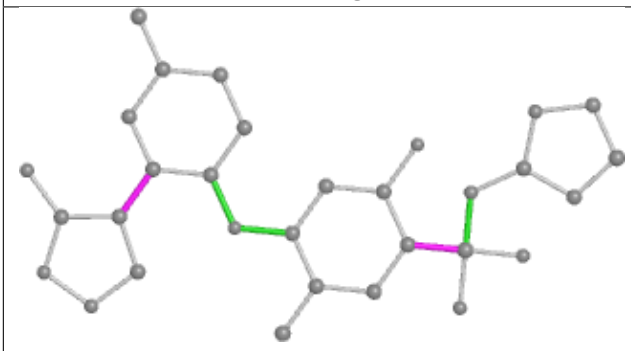
Ligand T70 A 2005



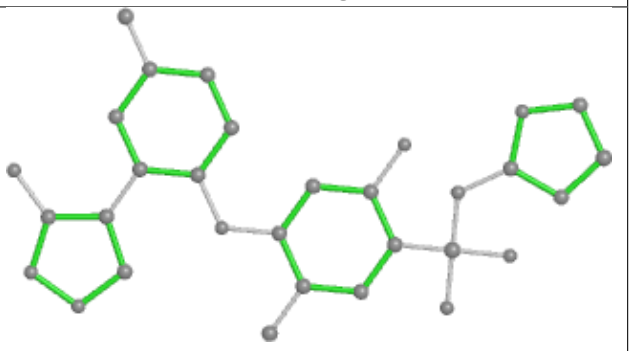
Bond lengths



Bond angles

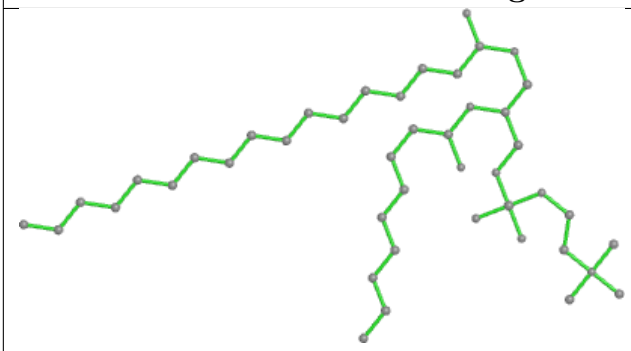


Torsions

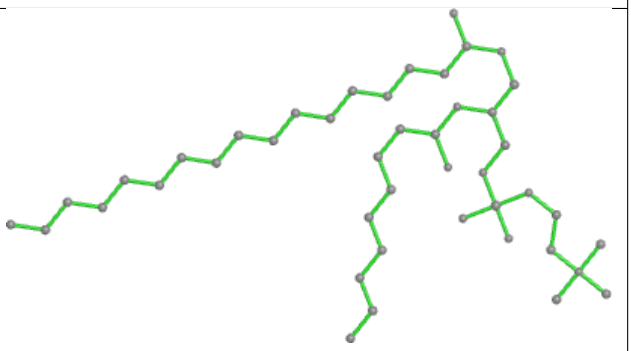


Rings

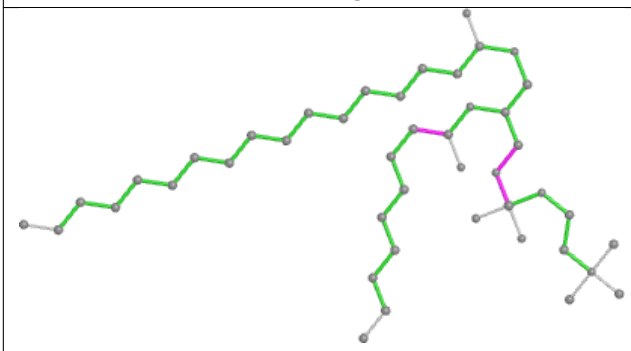
Ligand PCW A 2012



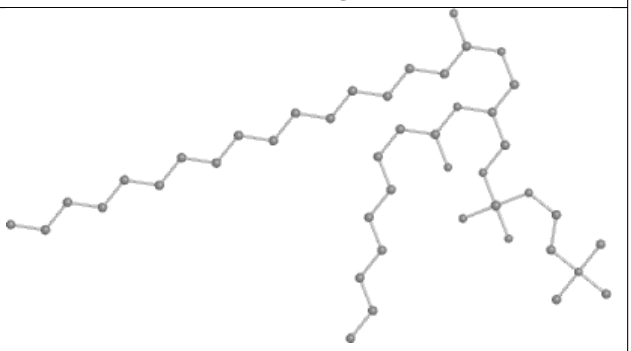
Bond lengths



Bond angles

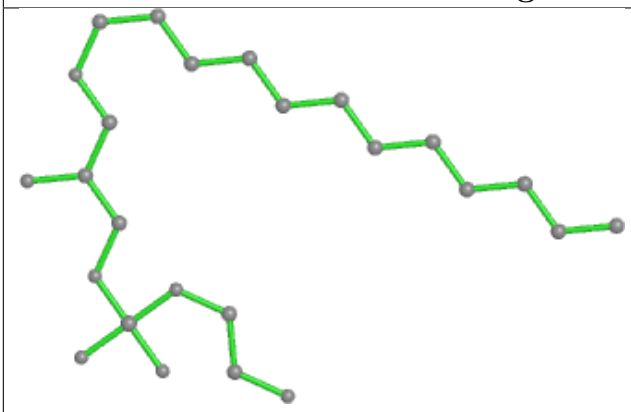


Torsions



Rings

Ligand LPE A 2007



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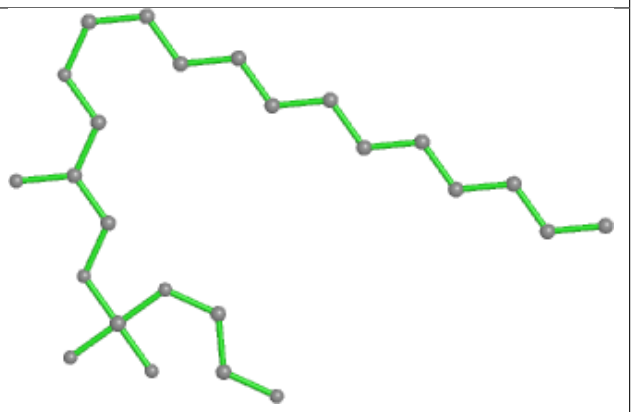
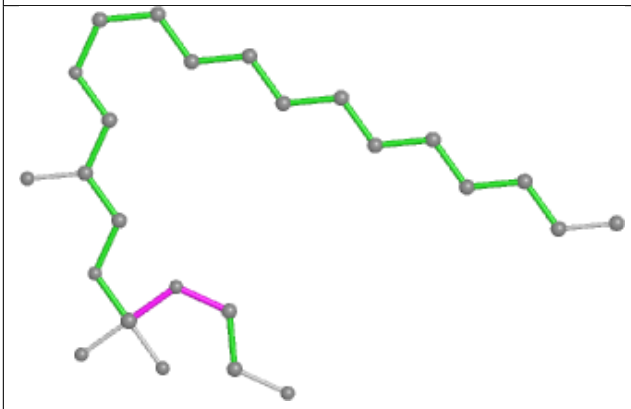
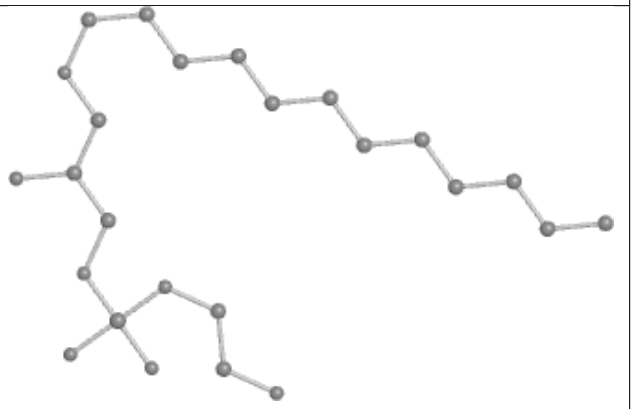


Bond angles

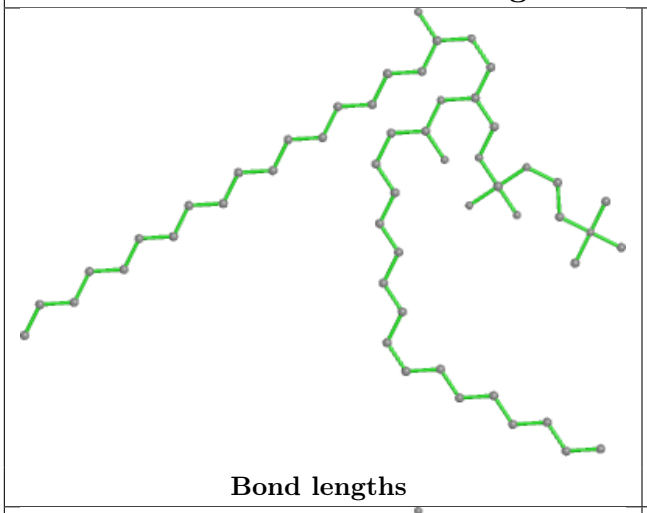


Torsions



Rings

Ligand PCW A 2008



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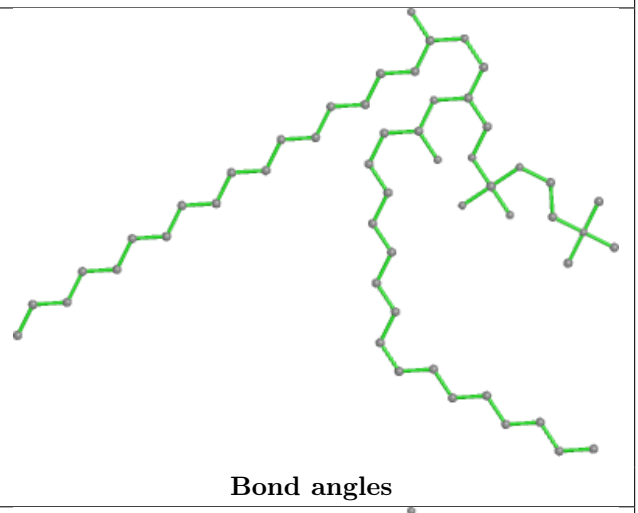
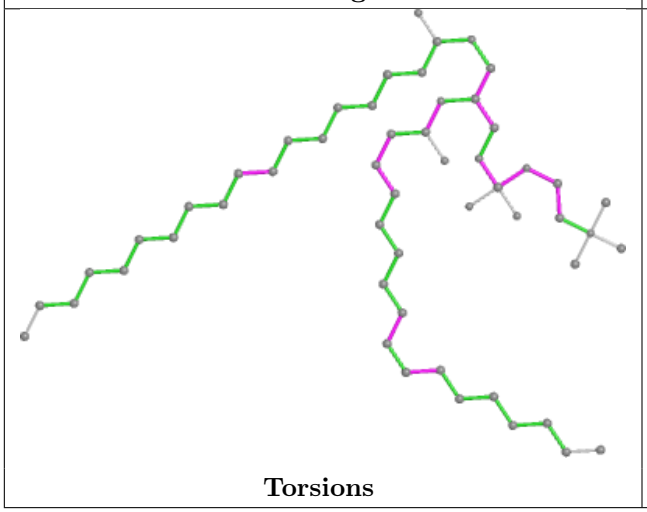
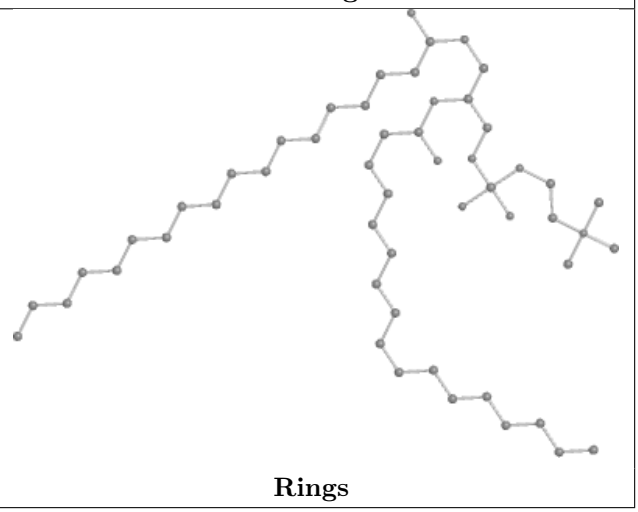


Bond angles

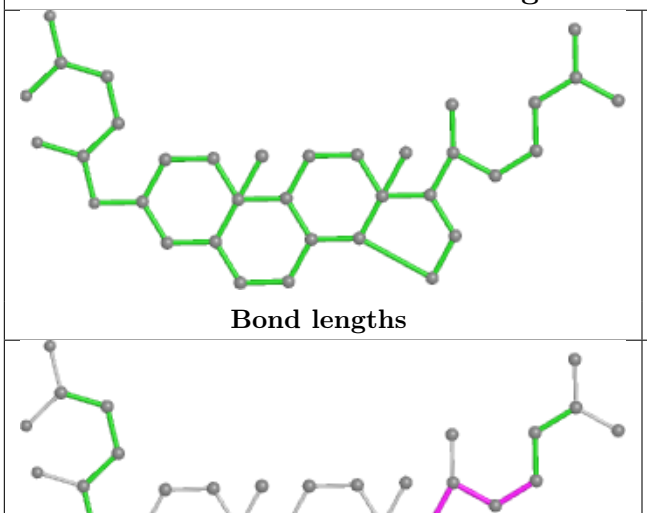


Torsions

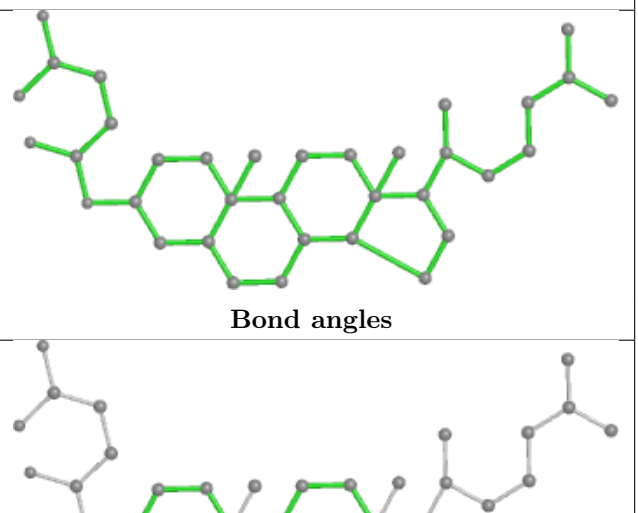


Rings

Ligand Y01 A 2019



Bond lengths

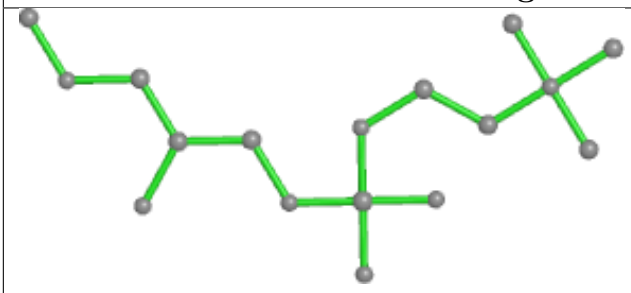


Bond angles

Torsions

Rings

Ligand LPE A 2020



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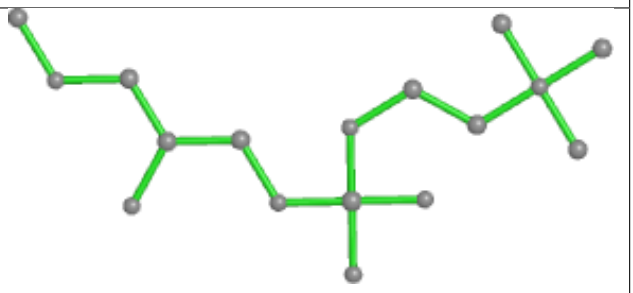
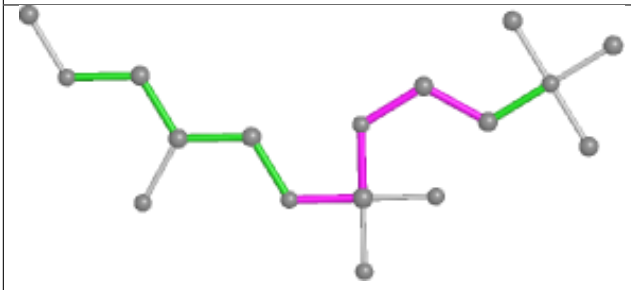
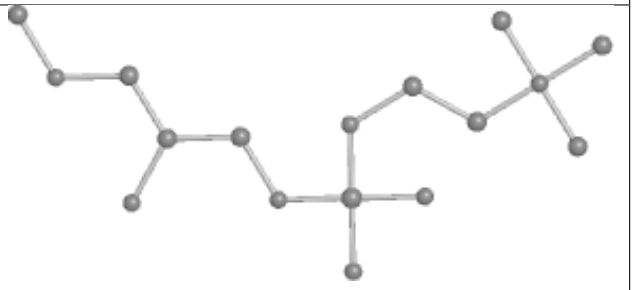


Bond angles

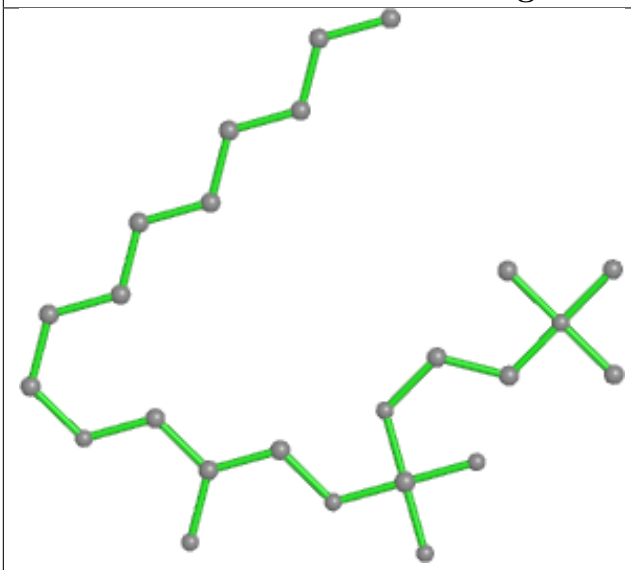


Torsions

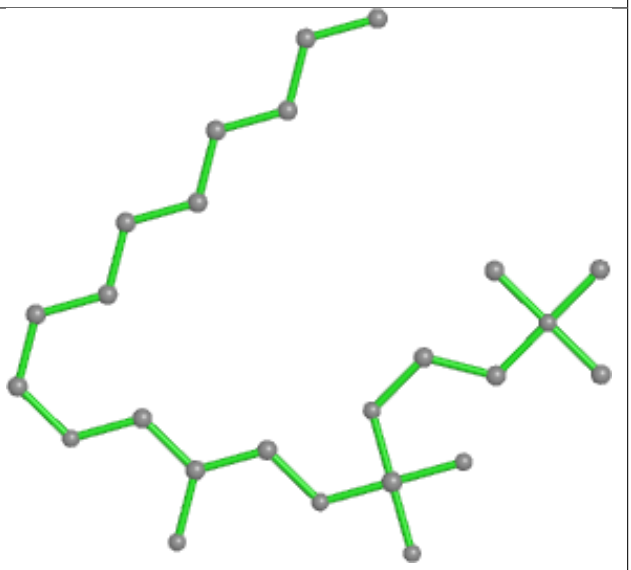


Rings

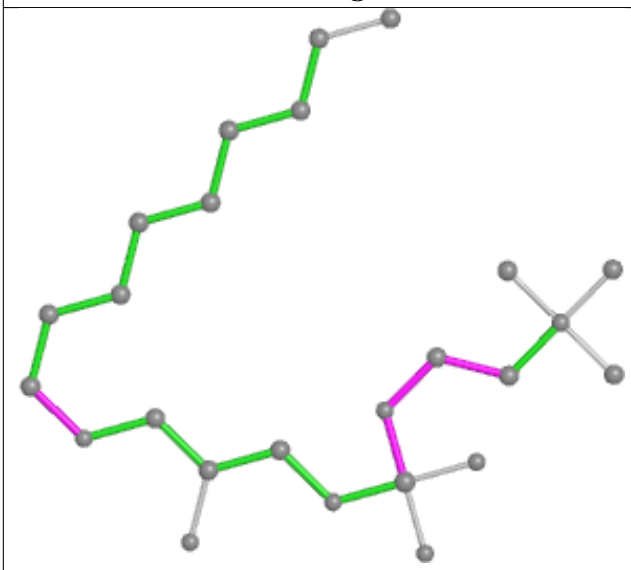
Ligand LPE A 2014



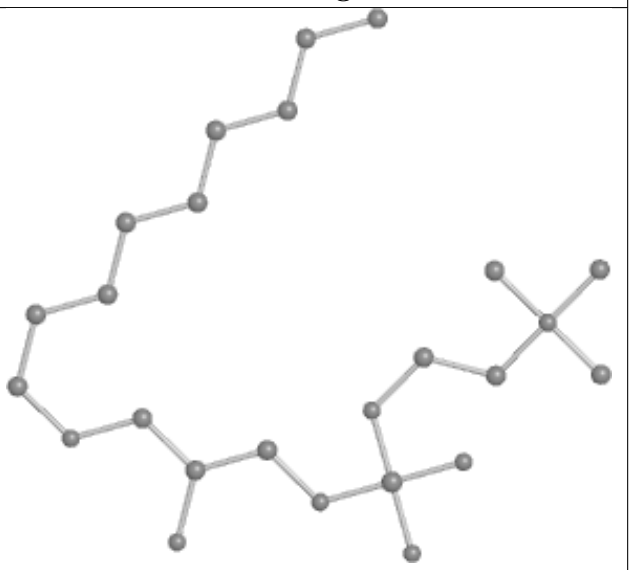
Bond lengths



Bond angles

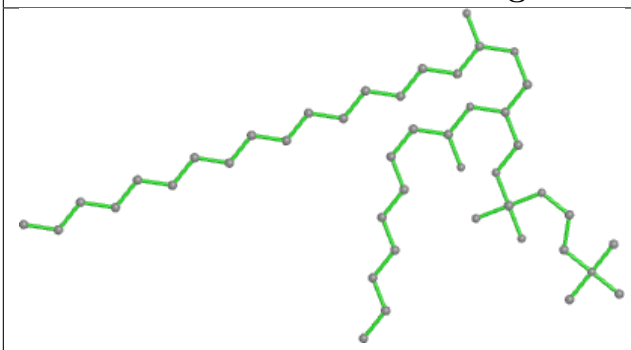


Torsions

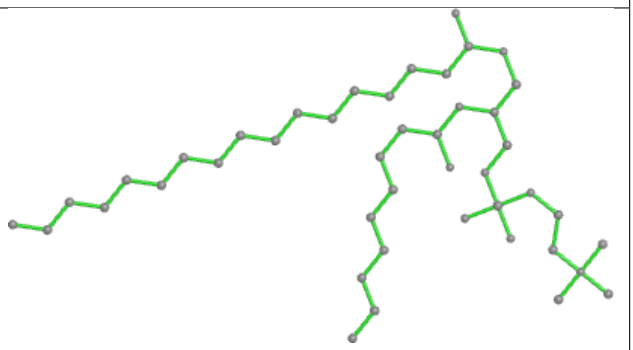


Rings

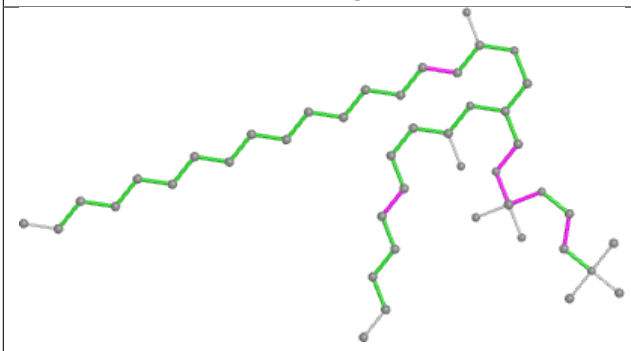
Ligand PCW A 2017



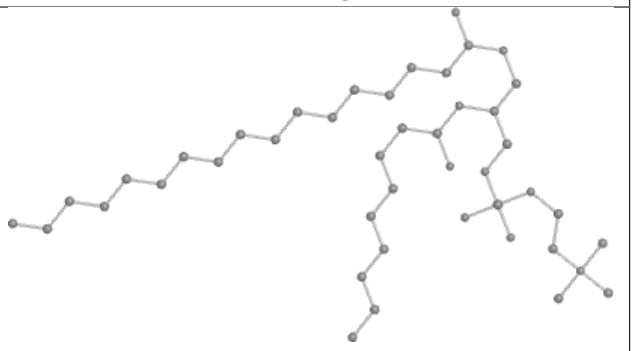
Bond lengths



Bond angles

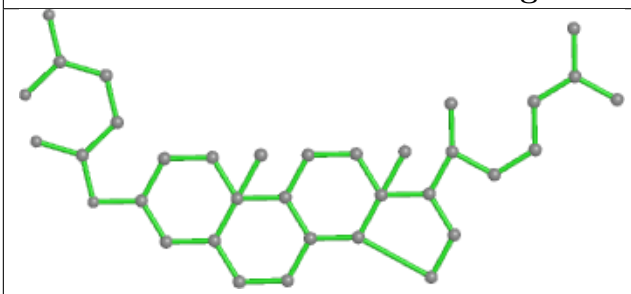


Torsions



Rings

Ligand Y01 A 2002



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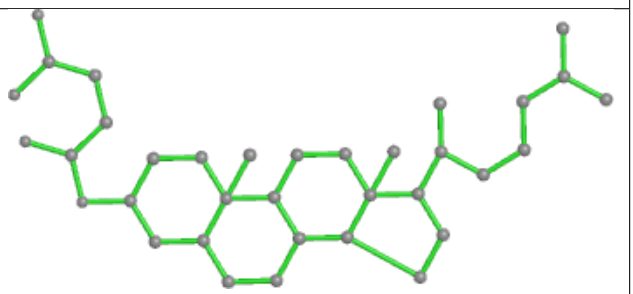
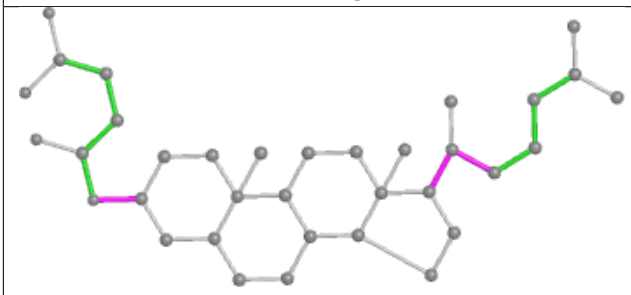
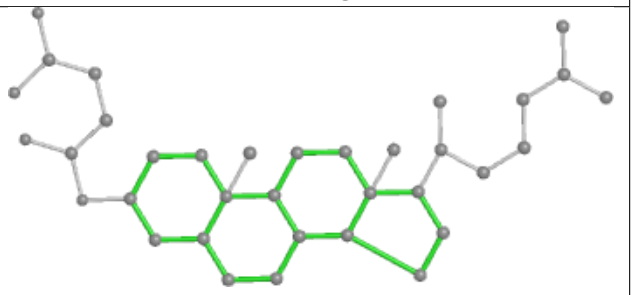


Bond angles

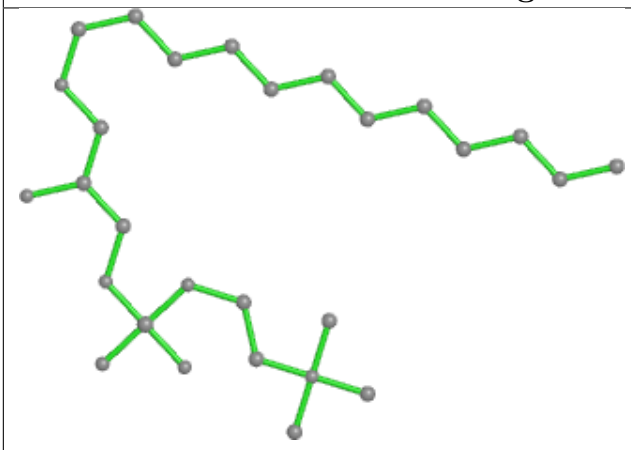


Torsions

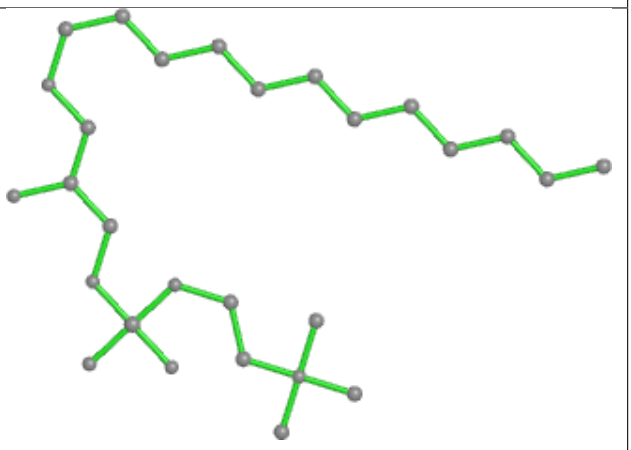


Rings

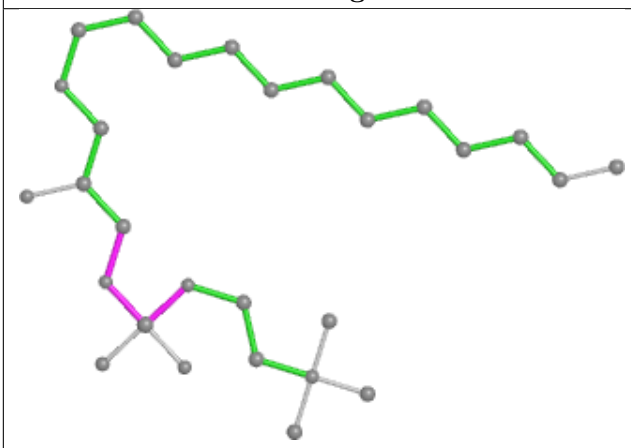
Ligand LPE A 2010



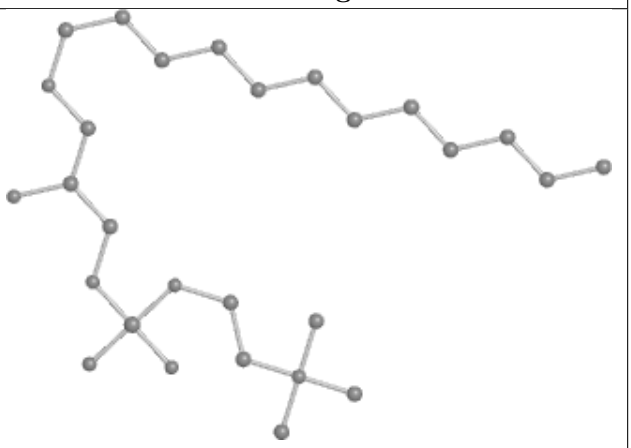
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

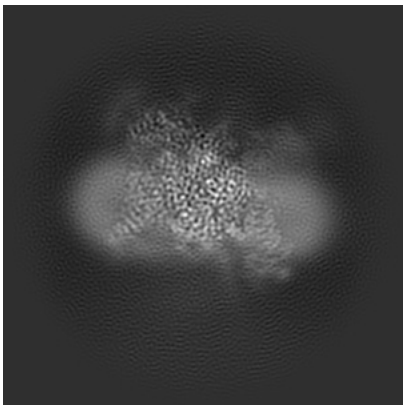
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-35194. These allow visual inspection of the internal detail of the map and identification of artifacts.

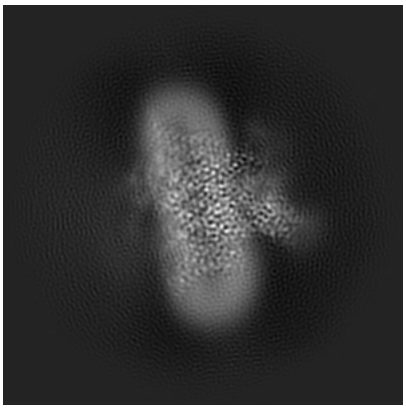
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

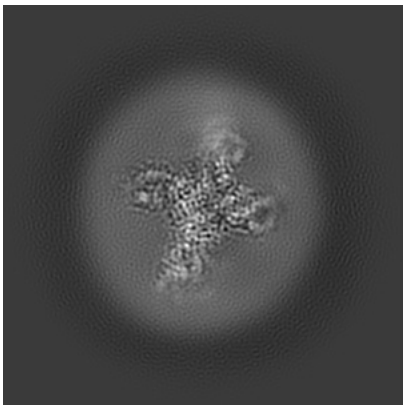
6.1.1 Primary map



X

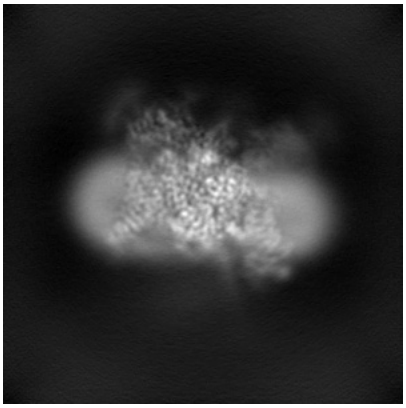


Y

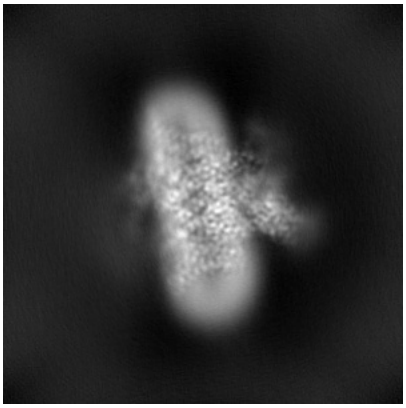


Z

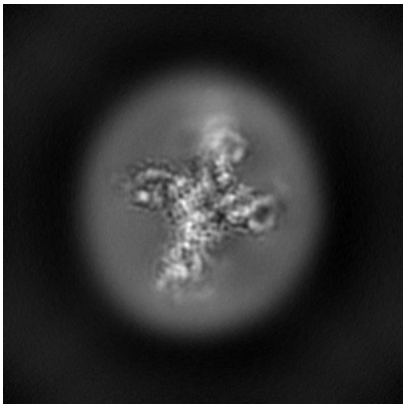
6.1.2 Raw map



X



Y

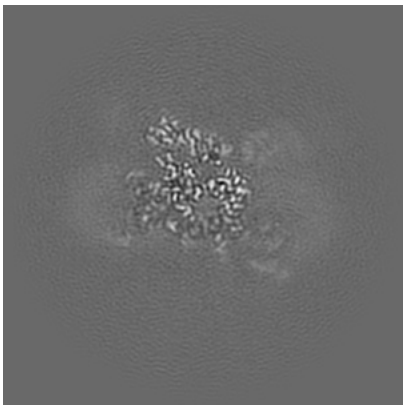


Z

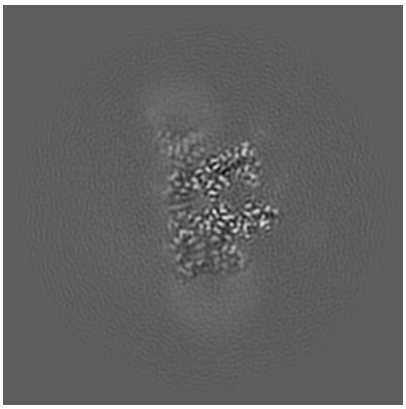
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

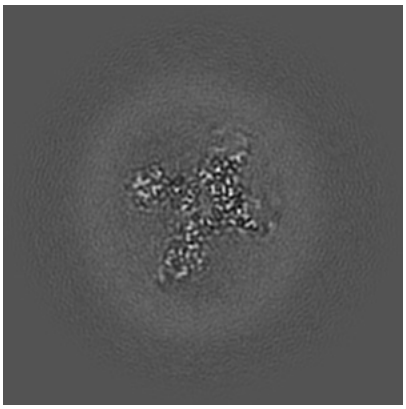
6.2.1 Primary map



X Index: 144

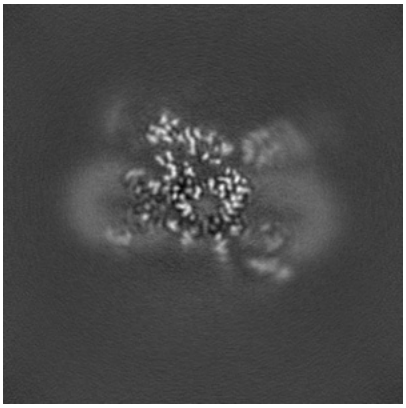


Y Index: 144

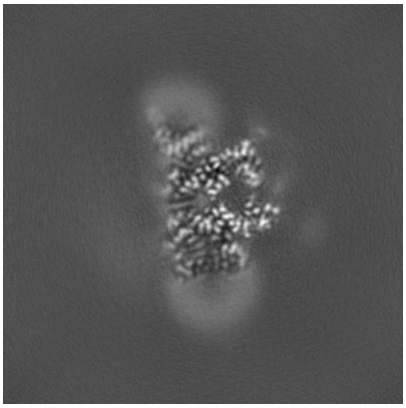


Z Index: 144

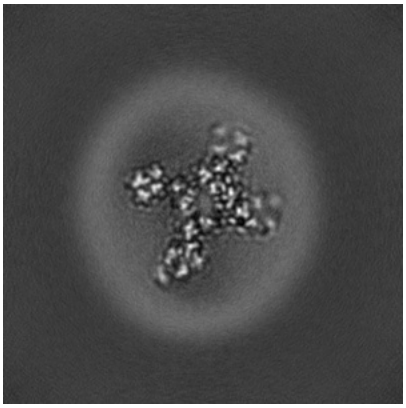
6.2.2 Raw map



X Index: 144



Y Index: 144

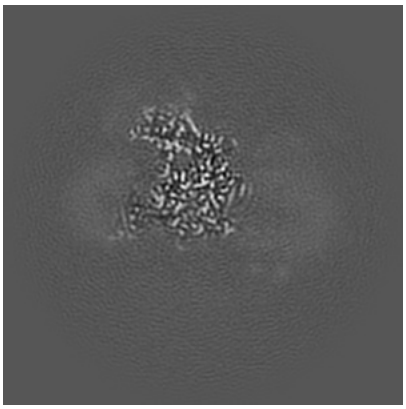


Z Index: 144

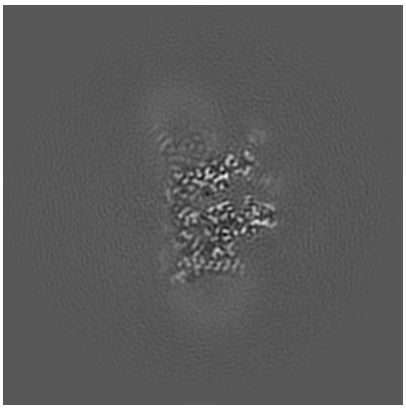
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

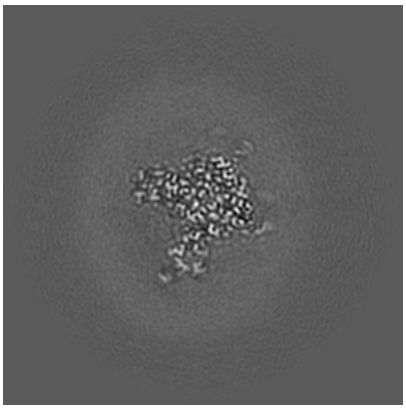
6.3.1 Primary map



X Index: 134

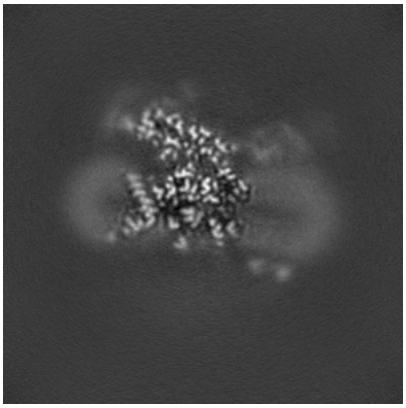


Y Index: 149

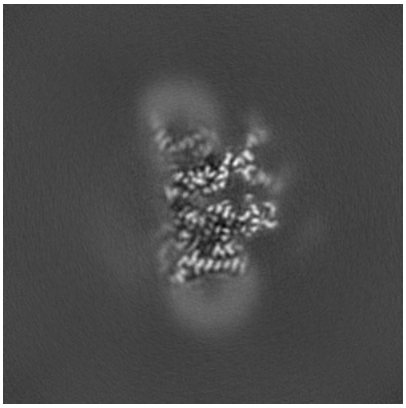


Z Index: 152

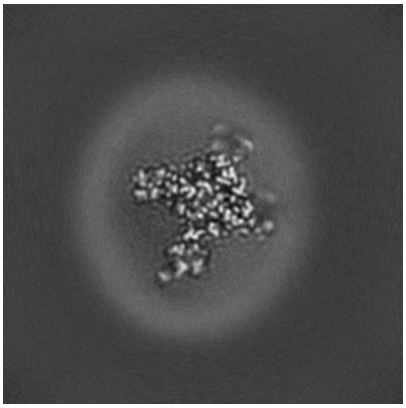
6.3.2 Raw map



X Index: 139



Y Index: 148

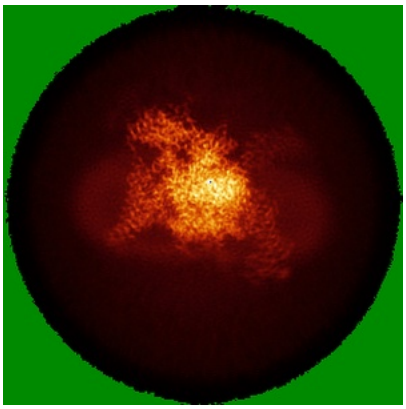


Z Index: 151

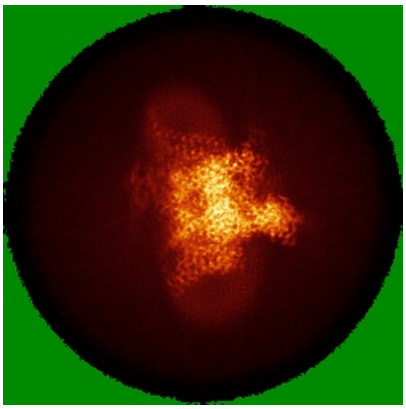
The images above show the largest variance slices of the map in three orthogonal directions.

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

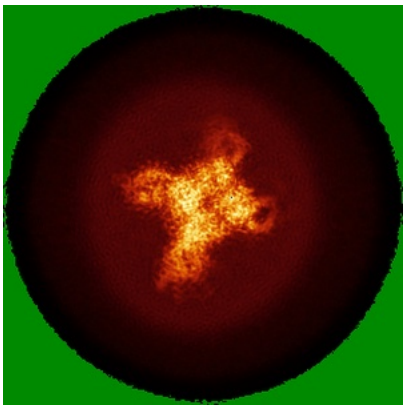
6.4.1 Primary map



X

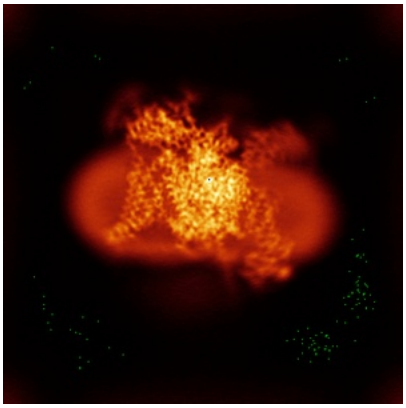


Y

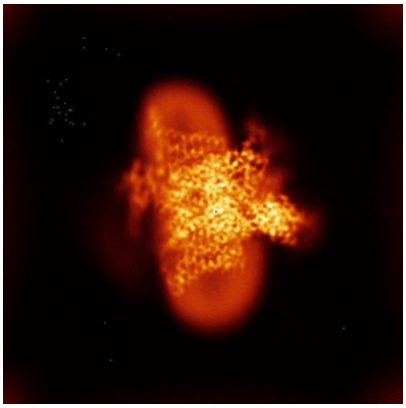


Z

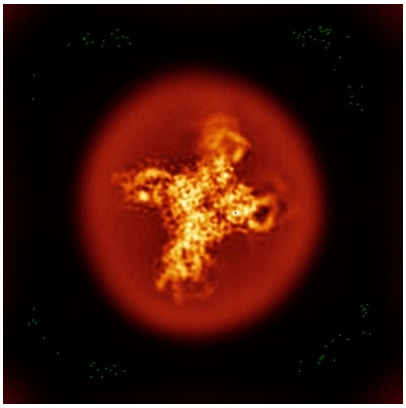
6.4.2 Raw map



X



Y



Z

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

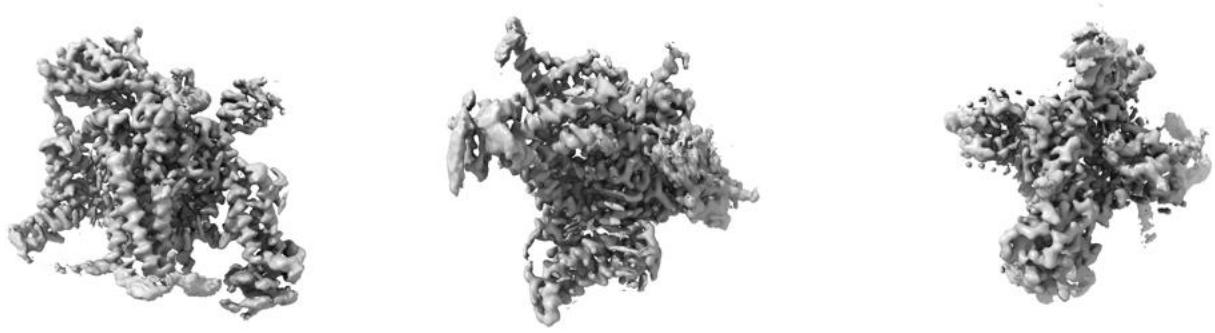
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.35. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

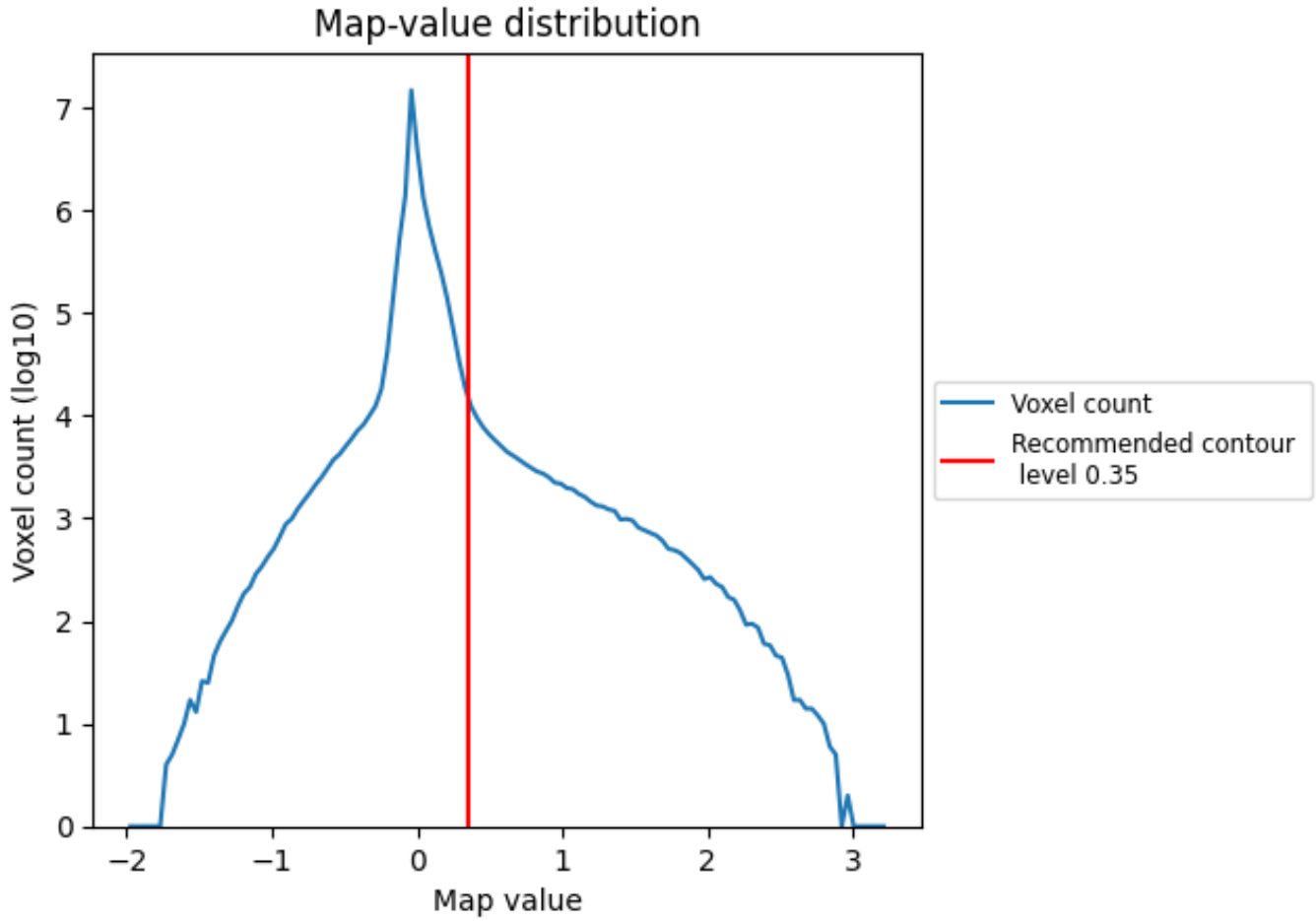
6.6 Mask visualisation (i)

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

7 Map analysis

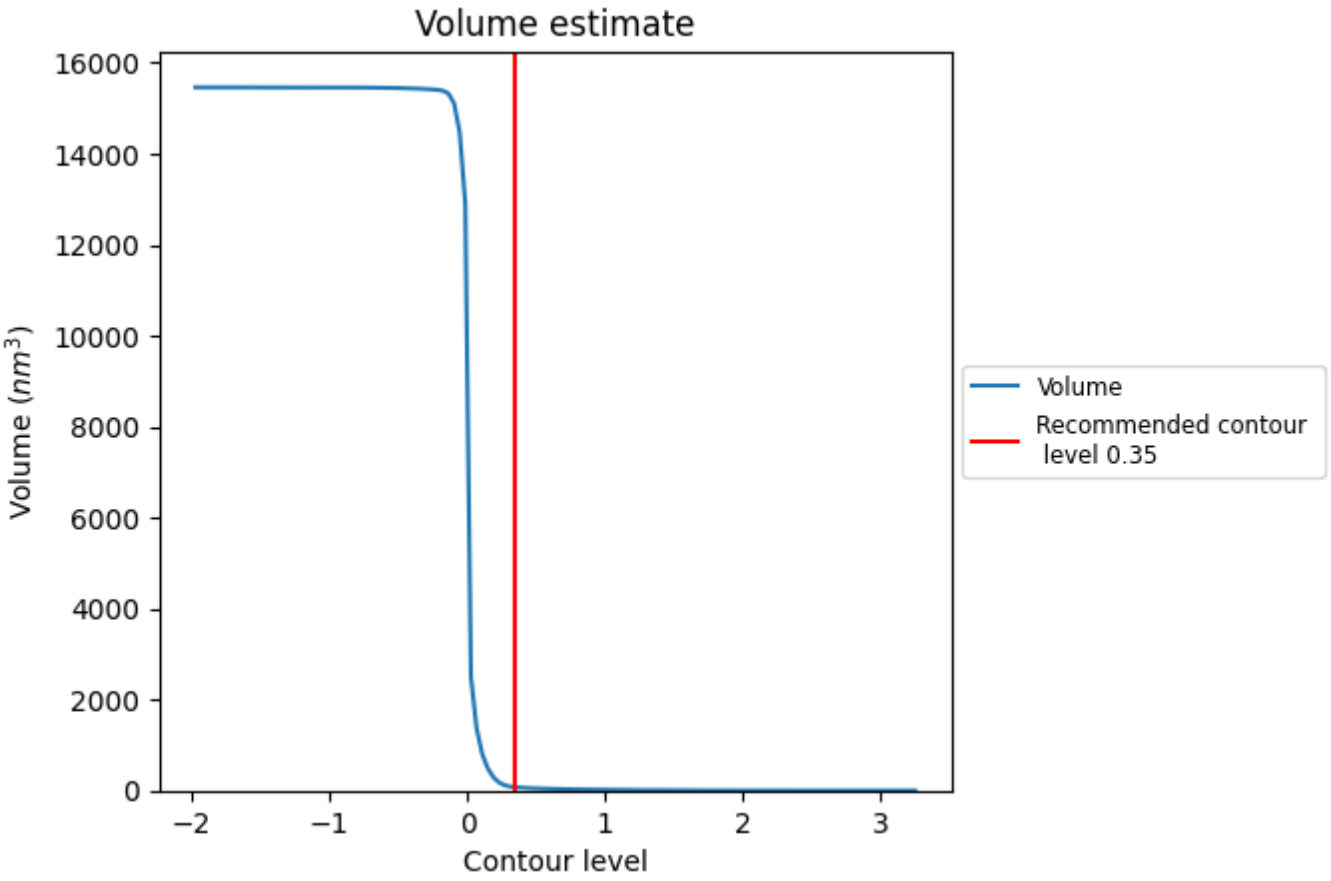
This section contains the results of statistical analysis of the map.

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.

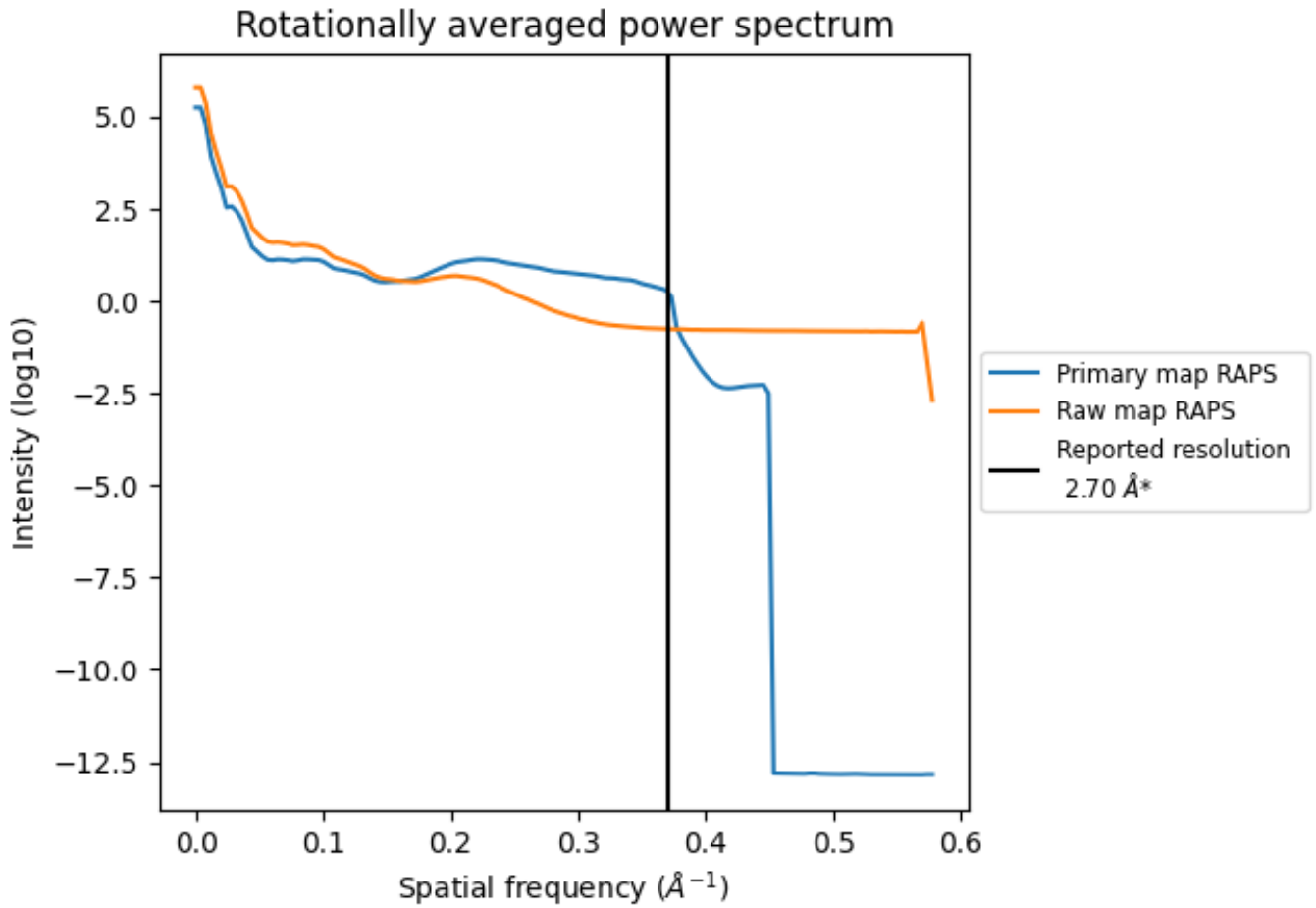
7.2 Volume estimate



The volume at the recommended contour level is 73 nm^3; this corresponds to an approximate mass of 66 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)

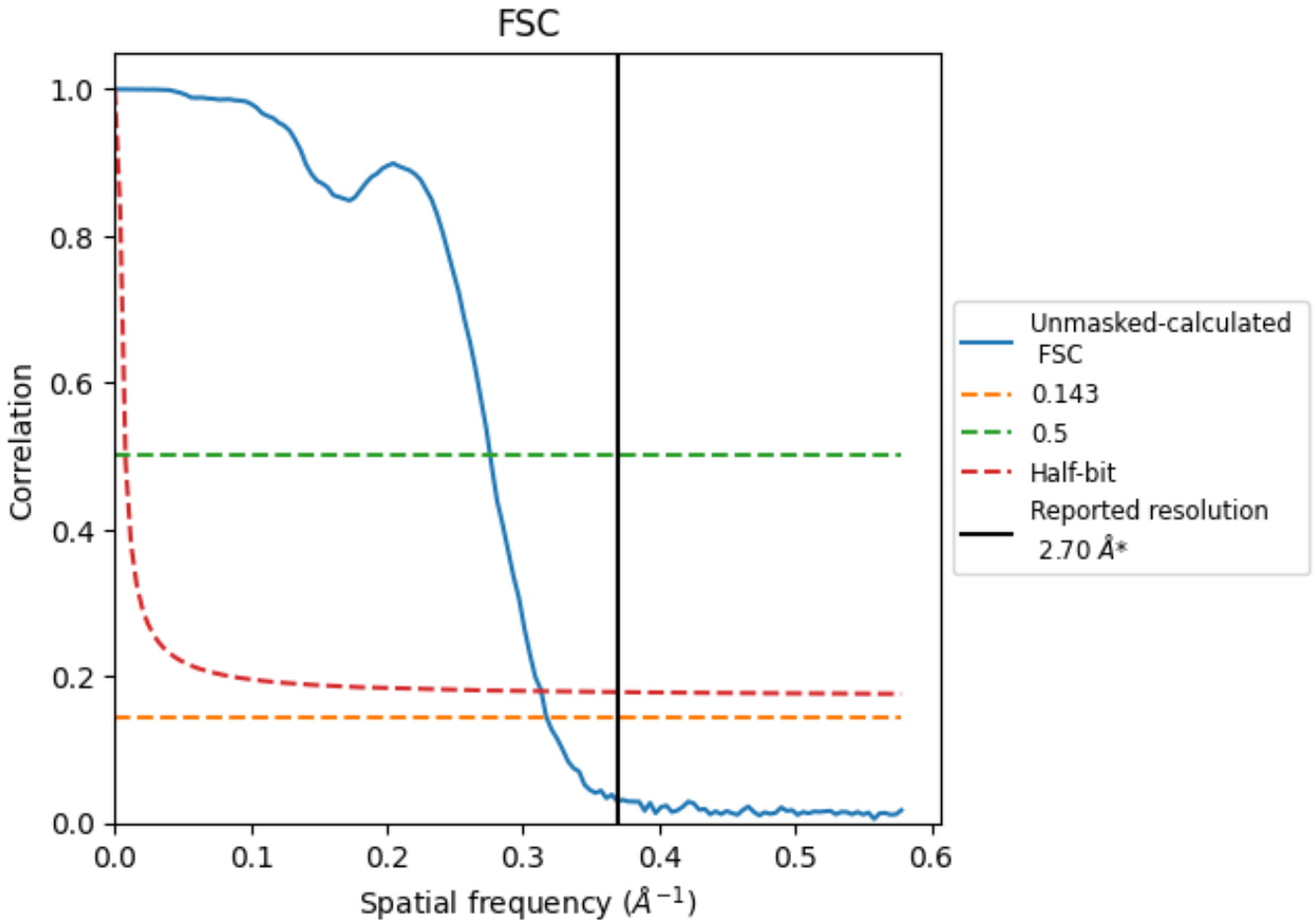


*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.370 $Å^{-1}$

8.2 Resolution estimates (i)

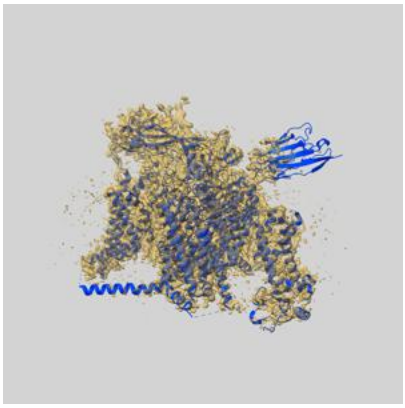
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.15	3.62	3.19

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.15 differs from the reported value 2.7 by more than 10 %

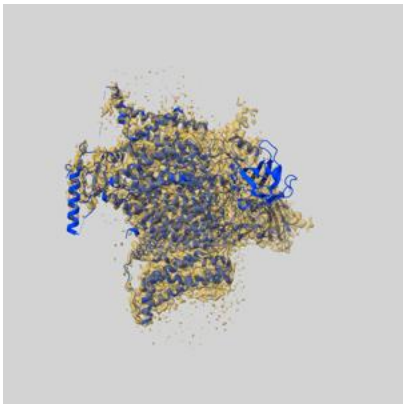
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-35194 and PDB model 8I5G. Per-residue inclusion information can be found in section 3 on page 9.

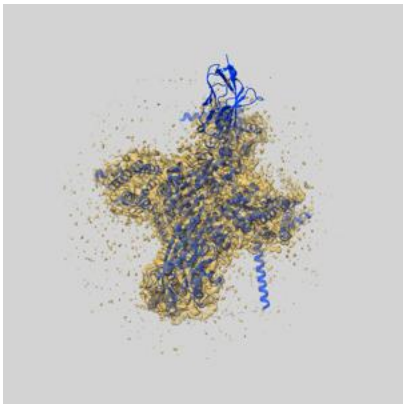
9.1 Map-model overlay



X



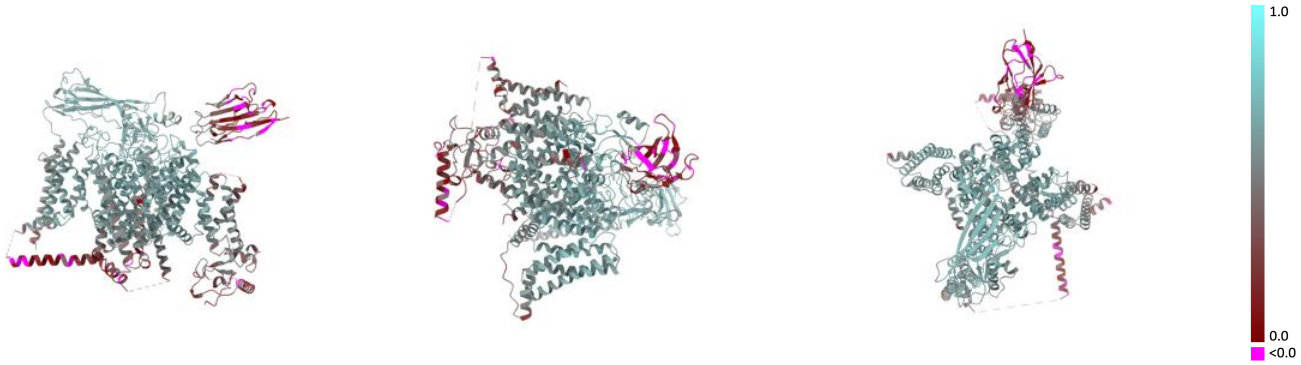
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.35 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.

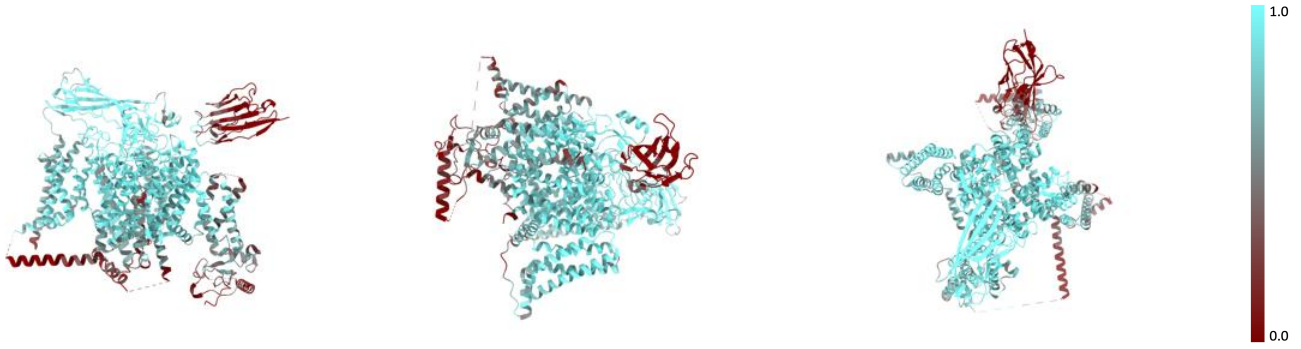
9.2 Q-score mapped to coordinate model (i)



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.

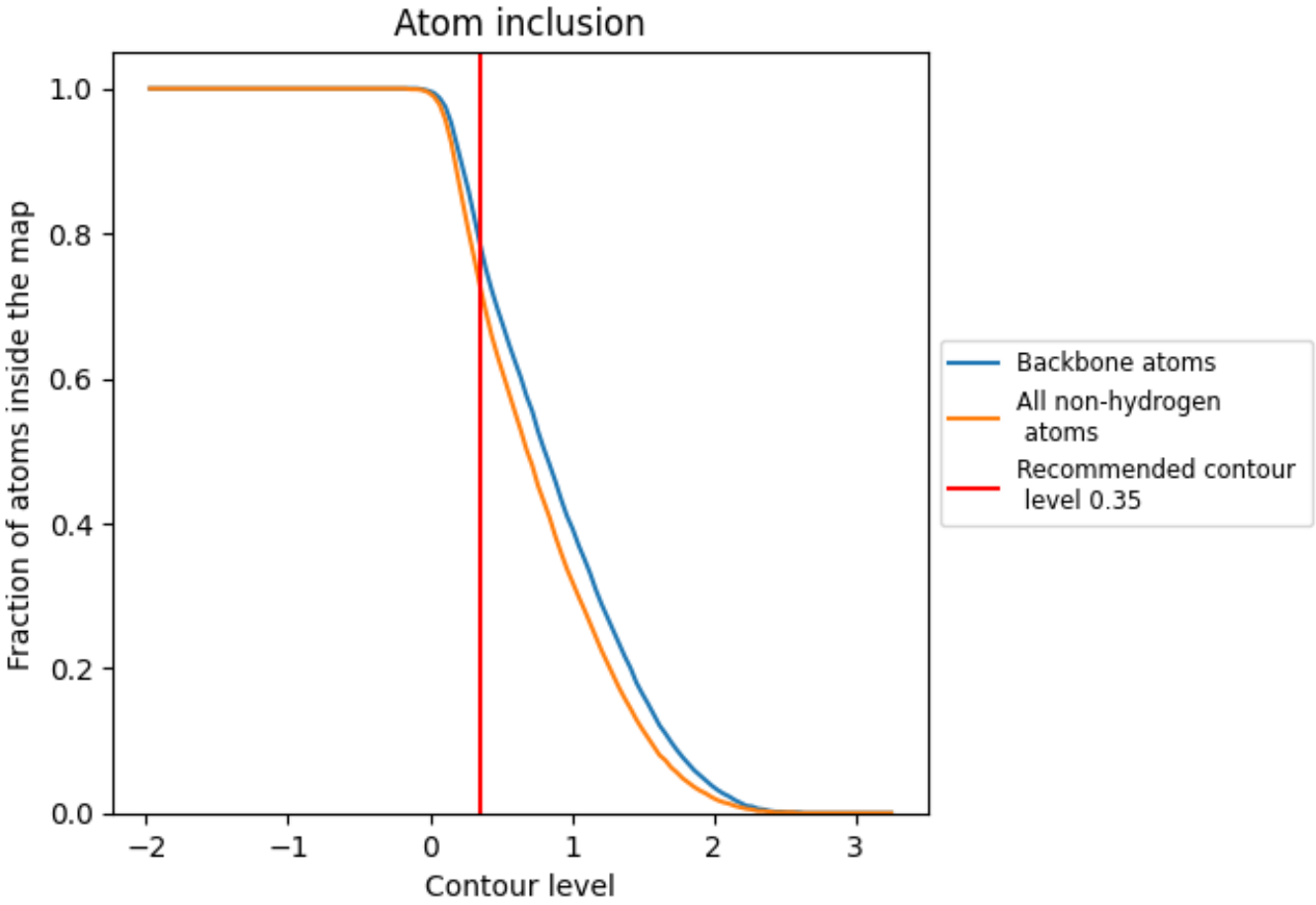
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.35).

9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 73% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7290	0.5160
A	0.7640	0.5360
B	0.8470	0.5850
C	0.1510	0.1900
D	0.9640	0.6110
E	0.5710	0.4120
F	0.8210	0.5170