Full wwPDB EM Validation Report ⓘ

Feb 28, 2024 – 02:15 PM JST

PDB ID	:	8XMO
EMDB ID	:	EMD-38484
Title	:	Voltage-gated sodium channel Nav1.7 variant M4
Authors	:	Yan, N.; Li, Z.; Wu, Q.; Huang, G.
Deposited on	:	2023-12-27
Resolution	:	3.39 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:

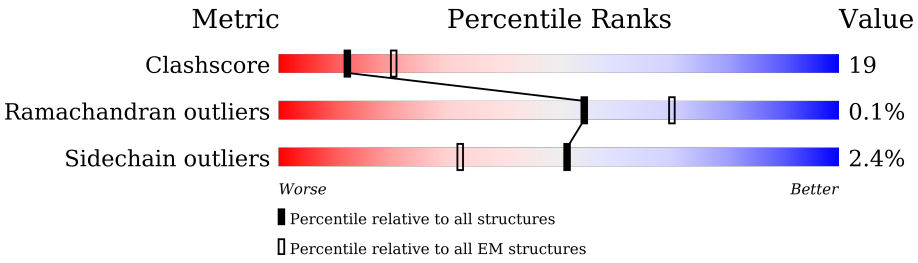
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.39 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	C	227	11% 29% 24% 48%
2	A	2031	39% 23% 37%
3	B	230	45% 28% 25%
4	D	2	50% 50%
4	E	2	50% 50%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13323 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-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	119	Total	C	N	O	S	3	0
			980	615	172	183	10		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	216	LEU	-	expression tag	UNP O60939
C	217	GLU	-	expression tag	UNP O60939
C	218	HIS	-	expression tag	UNP O60939
C	219	HIS	-	expression tag	UNP O60939
C	220	HIS	-	expression tag	UNP O60939
C	221	HIS	-	expression tag	UNP O60939
C	222	HIS	-	expression tag	UNP O60939
C	223	HIS	-	expression tag	UNP O60939
C	224	HIS	-	expression tag	UNP O60939
C	225	HIS	-	expression tag	UNP O60939
C	226	HIS	-	expression tag	UNP O60939
C	227	HIS	-	expression tag	UNP O60939

- Molecule 2 is a protein called Sodium channel protein type 9 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	1286	Total	C	N	O	S	0	0
			10387	6882	1637	1789	79		

There are 47 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-42	MET	-	initiating methionine	UNP Q15858
A	-41	ALA	-	expression tag	UNP Q15858
A	-40	SER	-	expression tag	UNP Q15858
A	-39	TRP	-	expression tag	UNP Q15858
A	-38	SER	-	expression tag	UNP Q15858

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-37	HIS	-	expression tag	UNP Q15858
A	-36	PRO	-	expression tag	UNP Q15858
A	-35	GLN	-	expression tag	UNP Q15858
A	-34	PHE	-	expression tag	UNP Q15858
A	-33	GLU	-	expression tag	UNP Q15858
A	-32	LYS	-	expression tag	UNP Q15858
A	-31	GLY	-	expression tag	UNP Q15858
A	-30	GLY	-	expression tag	UNP Q15858
A	-29	GLY	-	expression tag	UNP Q15858
A	-28	ALA	-	expression tag	UNP Q15858
A	-27	ARG	-	expression tag	UNP Q15858
A	-26	GLY	-	expression tag	UNP Q15858
A	-25	GLY	-	expression tag	UNP Q15858
A	-24	SER	-	expression tag	UNP Q15858
A	-23	GLY	-	expression tag	UNP Q15858
A	-22	GLY	-	expression tag	UNP Q15858
A	-21	GLY	-	expression tag	UNP Q15858
A	-20	SER	-	expression tag	UNP Q15858
A	-19	TRP	-	expression tag	UNP Q15858
A	-18	SER	-	expression tag	UNP Q15858
A	-17	HIS	-	expression tag	UNP Q15858
A	-16	PRO	-	expression tag	UNP Q15858
A	-15	GLN	-	expression tag	UNP Q15858
A	-14	PHE	-	expression tag	UNP Q15858
A	-13	GLU	-	expression tag	UNP Q15858
A	-12	LYS	-	expression tag	UNP Q15858
A	-11	GLY	-	expression tag	UNP Q15858
A	-10	PHE	-	expression tag	UNP Q15858
A	-9	ASP	-	expression tag	UNP Q15858
A	-8	TYR	-	expression tag	UNP Q15858
A	-7	LYS	-	expression tag	UNP Q15858
A	-6	ASP	-	expression tag	UNP Q15858
A	-5	ASP	-	expression tag	UNP Q15858
A	-4	ASP	-	expression tag	UNP Q15858
A	-3	ASP	-	expression tag	UNP Q15858
A	-2	LYS	-	expression tag	UNP Q15858
A	-1	GLY	-	expression tag	UNP Q15858
A	0	THR	-	expression tag	UNP Q15858
A	156	LYS	GLU	variant	UNP Q15858
A	779	ARG	GLY	variant	UNP Q15858
A	866	PHE	LEU	variant	UNP Q15858
A	1454	CYS	GLY	variant	UNP Q15858

- Molecule 3 is a protein called Sodium channel subunit beta-1.

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

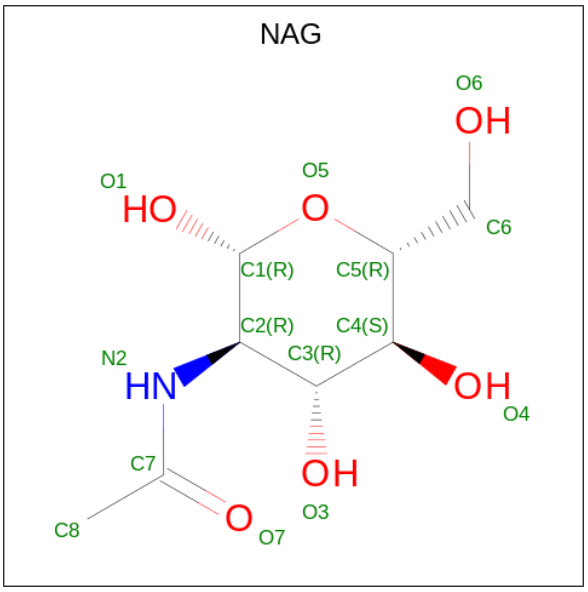
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	219	LEU	-	expression tag	UNP Q07699
B	220	GLU	-	expression tag	UNP Q07699
B	221	HIS	-	expression tag	UNP Q07699
B	222	HIS	-	expression tag	UNP Q07699
B	223	HIS	-	expression tag	UNP Q07699
B	224	HIS	-	expression tag	UNP Q07699
B	225	HIS	-	expression tag	UNP Q07699
B	226	HIS	-	expression tag	UNP Q07699
B	227	HIS	-	expression tag	UNP Q07699
B	228	HIS	-	expression tag	UNP Q07699
B	229	HIS	-	expression tag	UNP Q07699
B	230	HIS	-	expression tag	UNP Q07699

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

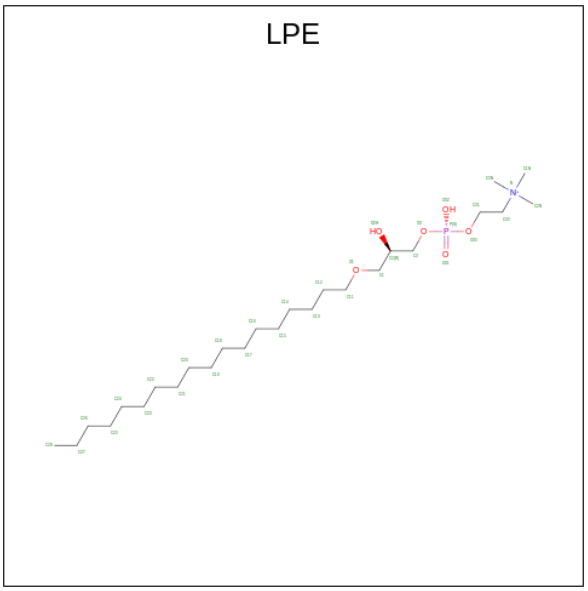
Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		

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



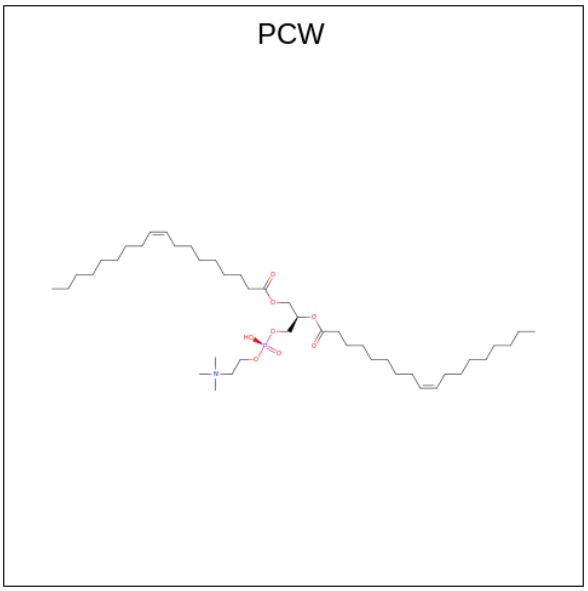
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 6 is 1-O-OCTADECYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: LPE) (formula: $C_{26}H_{57}NO_6P$).



Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
6	A	1	Total	C	N	O	P	0
			20	12	1	6	1	
6	A	1	Total	C	N	O	P	0
			28	20	1	6	1	
6	A	1	Total	C	N	O	P	0
			28	20	1	6	1	
6	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
6	A	1	Total	C	N	O	P	0
			25	17	1	6	1	
6	A	1	Total	C	N	O	P	0
			17	9	1	6	1	

- Molecule 7 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: $C_{44}H_{85}NO_8P$).

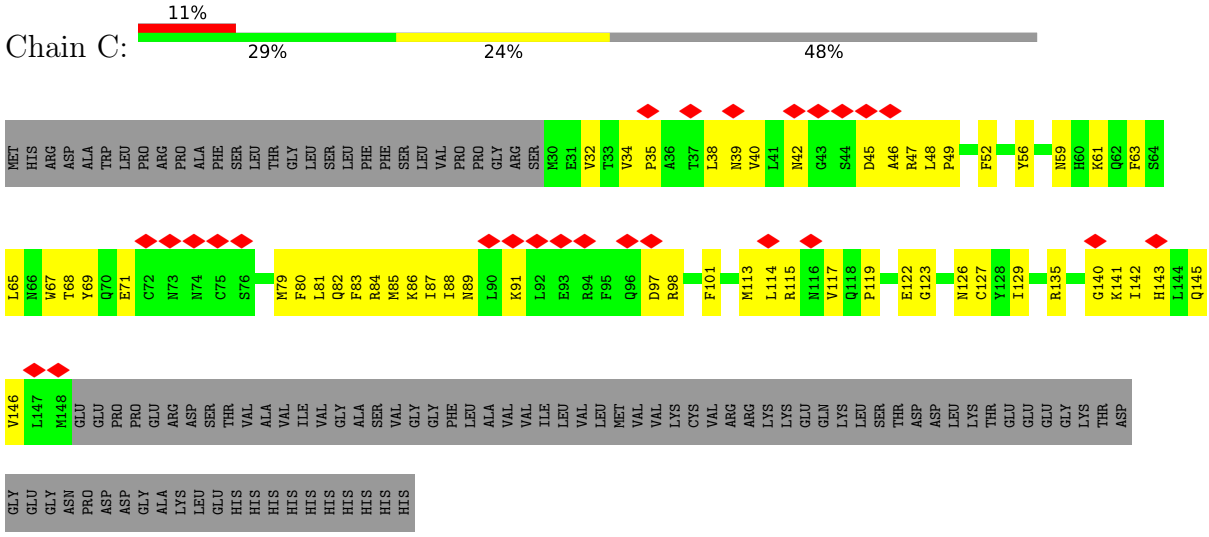


Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	N	O	P	0
			53	43	1	8	1	
7	A	1	Total	C	N	O	P	0
			47	37	1	8	1	
7	A	1	Total	C	N	O	P	0
			44	34	1	8	1	
7	A	1	Total	C	N	O	P	0
			44	34	1	8	1	
7	A	1	Total	C	N	O	P	0
			44	34	1	8	1	

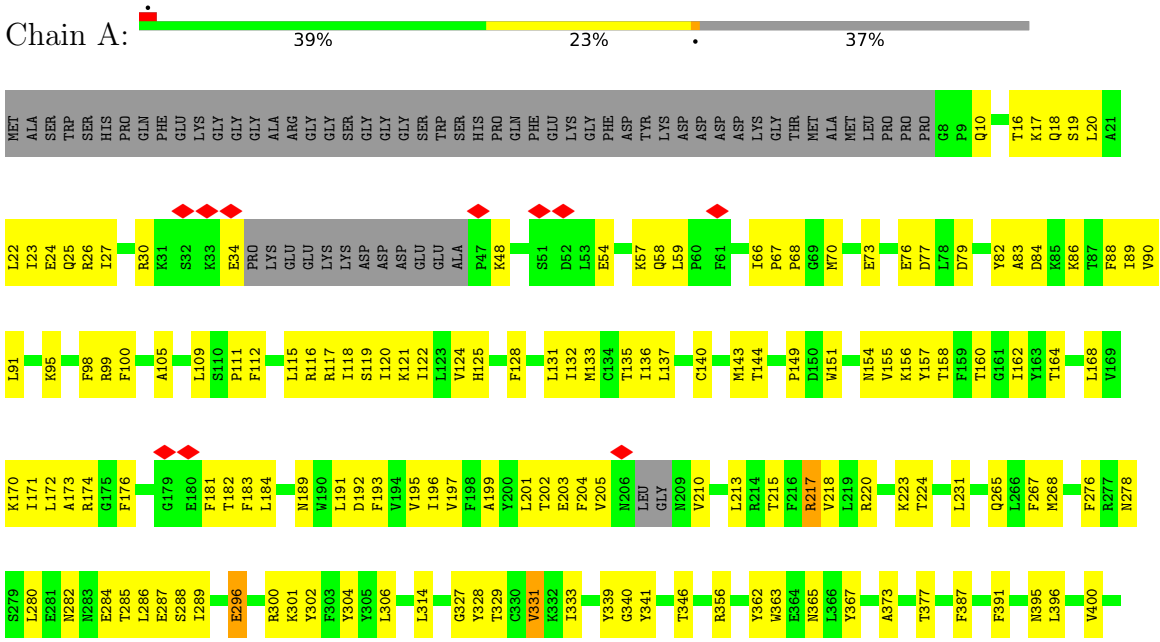
3 Residue-property plots (i)

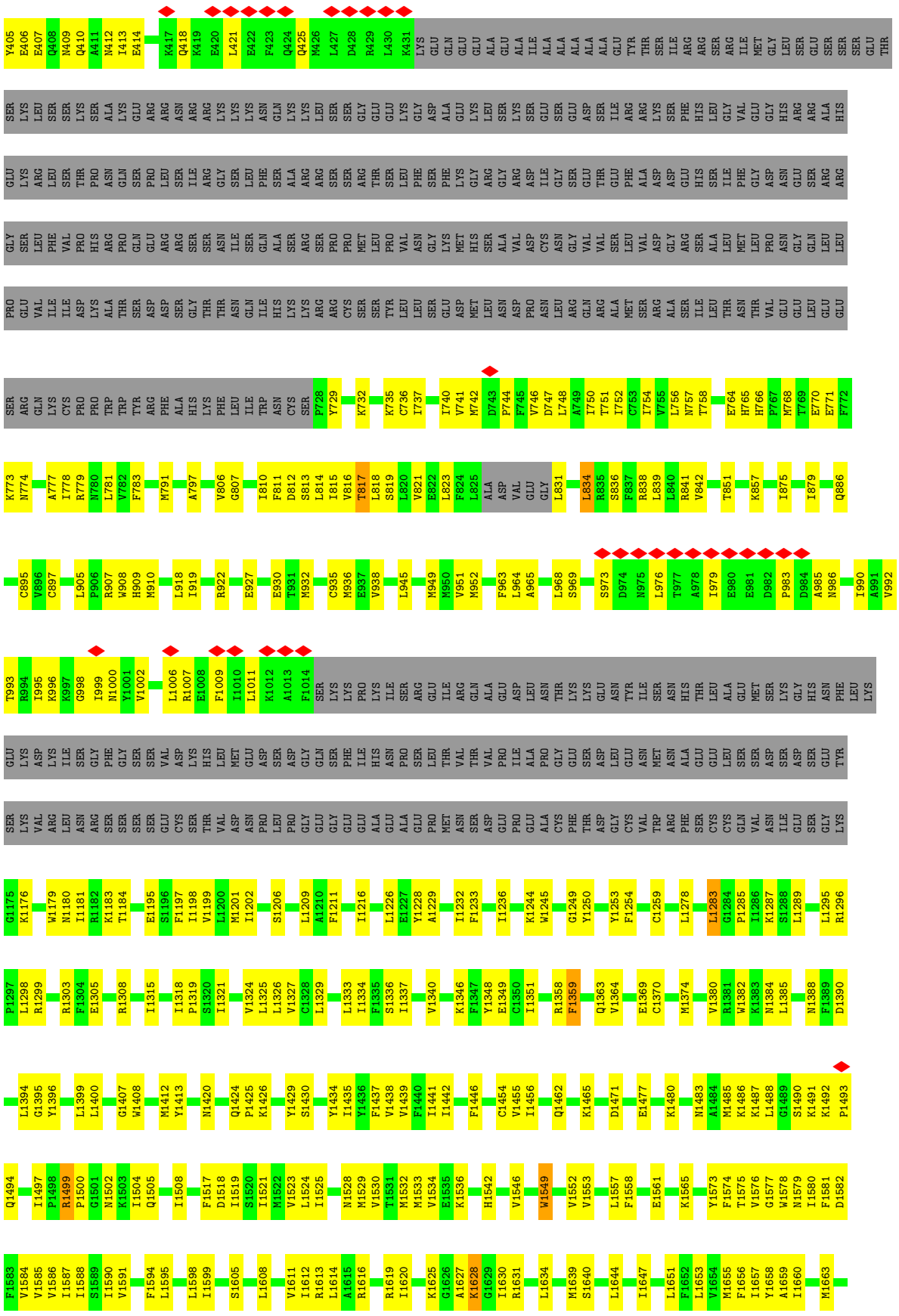
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

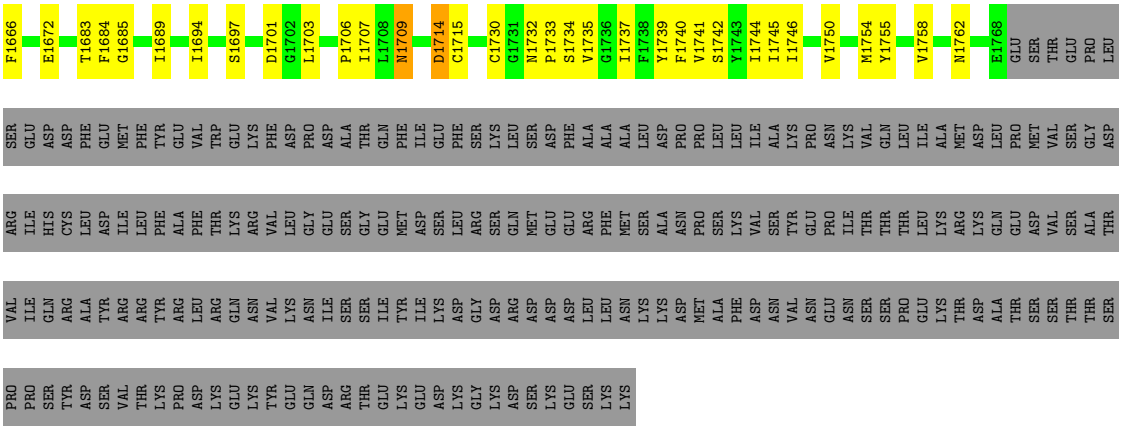
• Molecule 1: Sodium channel subunit beta-2



• Molecule 2: Sodium channel protein type 9 subunit alpha

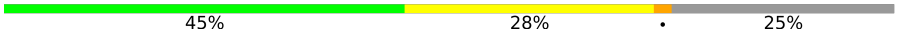


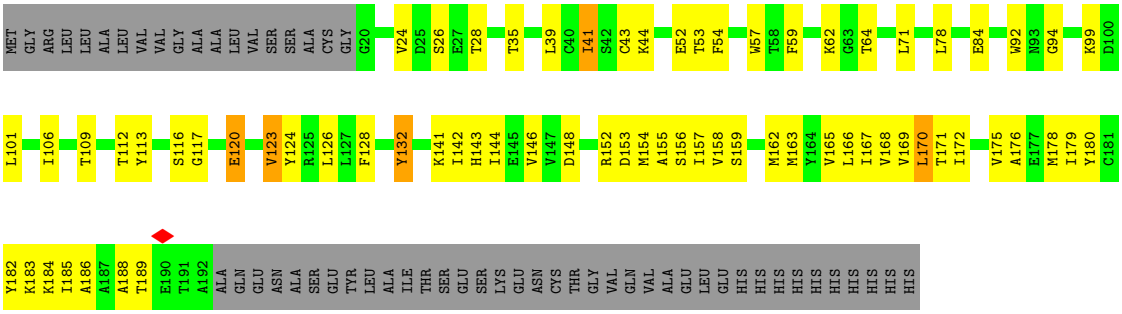




• Molecule 3: Sodium channel subunit beta-1

Chain B:





• 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:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	181009	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	2.459	Depositor
Minimum map value	-1.193	Depositor
Average map value	0.010	Depositor
Map value standard deviation	0.063	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	281.0624, 281.0624, 281.0624	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0979, 1.0979, 1.0979	Depositor

5 Model quality

5.1 Standard geometry

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

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	C	0.35	0/1011	0.60	0/1367
2	A	0.70	0/10638	0.71	0/14405
3	B	0.96	0/1442	0.94	0/1949
All	All	0.71	0/13091	0.73	0/17721

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	C	980	0	945	45	0
2	A	10387	0	10628	410	0
3	B	1416	0	1379	58	0
4	D	28	0	25	1	0
4	E	28	0	25	0	0
5	A	28	0	26	0	0
5	B	56	0	52	0	0
6	A	168	0	228	6	0
7	A	232	0	323	18	0
All	All	13323	0	13631	516	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 19.

All (516) 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)
2:A:1283:LEU:CD1	2:A:1285:PRO:HD2	1.69	1.21
2:A:1283:LEU:HD13	2:A:1285:PRO:CD	1.83	1.08
2:A:199:ALA:HA	2:A:217:ARG:NH2	1.69	1.07
2:A:1283:LEU:HD13	2:A:1285:PRO:HD2	1.01	0.99
3:B:120:GLU:HB3	3:B:141:LYS:HA	1.44	0.99
3:B:172:ILE:HA	3:B:175:VAL:HG22	1.46	0.96
2:A:328:TYR:HE1	3:B:132:TYR:HE1	1.11	0.95
2:A:729:TYR:HA	2:A:732:LYS:HE2	1.50	0.94
2:A:1494:GLN:N	2:A:1494:GLN:OE1	2.04	0.90
3:B:113:TYR:HA	3:B:146:VAL:HG11	1.55	0.88
2:A:1250:TYR:O	2:A:1254:PHE:HB2	1.75	0.87
2:A:20:LEU:HA	2:A:23:ILE:HG12	1.59	0.85
2:A:1549:TRP:HA	2:A:1552:VAL:HG12	1.59	0.82
2:A:908:TRP:CZ3	2:A:922:ARG:HD3	2.16	0.81
2:A:199:ALA:HA	2:A:217:ARG:HH22	1.44	0.79
1:C:80:PHE:HD1	1:C:81:LEU:HD23	1.48	0.78
2:A:57:LYS:HG2	2:A:58:GLN:H	1.47	0.78
2:A:410:GLN:HA	2:A:413:ILE:HG12	1.64	0.77
2:A:20:LEU:HD11	2:A:112:PHE:HE1	1.49	0.77
2:A:111:PRO:HA	2:A:116:ARG:HD3	1.66	0.76
2:A:217:ARG:O	2:A:220:ARG:HG3	1.85	0.76
2:A:1228:TYR:HD2	3:B:159:SER:HB2	1.51	0.75
2:A:1437:PHE:O	2:A:1441:ILE:HG12	1.86	0.75
3:B:162:MET:HA	3:B:165:VAL:HG12	1.69	0.75
2:A:1732:ASN:HB3	2:A:1735:VAL:HG12	1.69	0.74
1:C:45:ASP:OD2	1:C:115:ARG:NE	2.20	0.74
1:C:98:ARG:HH21	1:C:114:LEU:HG	1.54	0.73
1:C:68:THR:OG1	1:C:126:ASN:ND2	2.21	0.73
2:A:109:LEU:HD21	2:A:116:ARG:HB2	1.72	0.71
2:A:1283:LEU:CD1	2:A:1285:PRO:CD	2.56	0.71
2:A:770:GLU:HA	2:A:773:LYS:NZ	2.06	0.71
2:A:1584:VAL:O	2:A:1588:ILE:HG13	1.90	0.71
2:A:1348:TYR:HD2	2:A:1382:TRP:NE1	1.89	0.70
2:A:992:VAL:O	2:A:996:LYS:N	2.23	0.70
2:A:131:LEU:O	2:A:135:THR:HG23	1.92	0.70
2:A:771:GLU:OE1	2:A:771:GLU:N	2.22	0.70
2:A:1253:TYR:CE1	2:A:1259:CYS:HB3	2.28	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:314:LEU:HD23	2:A:373:ALA:HB2	1.75	0.69
2:A:286:LEU:HD21	2:A:333:ILE:HG21	1.75	0.69
3:B:175:VAL:O	3:B:178:MET:HG3	1.95	0.67
2:A:199:ALA:HA	2:A:217:ARG:HH21	1.57	0.67
2:A:737:ILE:HG13	2:A:797:ALA:HB2	1.76	0.67
1:C:119:PRO:HA	1:C:146:VAL:HG21	1.77	0.66
2:A:1336:SER:O	2:A:1340:VAL:HG23	1.95	0.66
2:A:1658:TYR:HD2	2:A:1739:TYR:CE1	2.14	0.66
2:A:327:GLY:O	2:A:328:TYR:HD1	1.79	0.66
2:A:1741:VAL:O	2:A:1745:ILE:HG13	1.96	0.65
1:C:68:THR:HG22	1:C:79:MET:HG2	1.78	0.65
2:A:1485:MET:HE3	2:A:1639:MET:HA	1.77	0.65
3:B:159:SER:HA	3:B:162:MET:HB2	1.77	0.65
2:A:1573:TYR:CE1	2:A:1579:ASN:HB3	2.31	0.65
3:B:53:THR:CG2	3:B:123:VAL:HG12	2.27	0.65
2:A:1672:GLU:HB2	2:A:1706:PRO:HB3	1.78	0.65
2:A:1734:SER:HA	6:A:2003:LPE:H11	1.79	0.65
2:A:328:TYR:CE1	3:B:132:TYR:HE1	2.04	0.65
2:A:328:TYR:HE1	3:B:132:TYR:CE1	2.04	0.64
2:A:48:LYS:HE3	2:A:48:LYS:HA	1.79	0.64
2:A:340:GLY:HA3	7:A:2008:PCW:H82	1.78	0.64
2:A:387:PHE:O	2:A:391:PHE:HB3	1.98	0.64
2:A:1521:ILE:O	2:A:1525:ILE:HG13	1.97	0.64
2:A:737:ILE:HA	2:A:740:ILE:HD12	1.80	0.64
3:B:176:ALA:O	3:B:179:ILE:HG12	1.98	0.63
2:A:1346:LYS:NZ	2:A:1420:ASN:HA	2.13	0.63
2:A:770:GLU:HA	2:A:773:LYS:HZ3	1.61	0.63
2:A:814:LEU:O	2:A:818:LEU:HG	1.99	0.63
2:A:195:VAL:HG11	2:A:220:ARG:HG2	1.80	0.63
3:B:167:ILE:O	3:B:171:THR:HG23	1.99	0.63
2:A:1733:PRO:O	2:A:1737:ILE:HG13	1.98	0.62
2:A:736:CYS:O	2:A:740:ILE:HG13	2.00	0.62
2:A:197:VAL:O	2:A:201:LEU:HG	2.00	0.62
2:A:304:TYR:HB2	2:A:328:TYR:CE2	2.35	0.62
2:A:831:LEU:N	2:A:834:LEU:HB2	2.15	0.62
2:A:1580:ILE:H	2:A:1580:ILE:HD12	1.65	0.62
3:B:172:ILE:HA	3:B:175:VAL:CG2	2.25	0.62
2:A:875:ILE:O	2:A:879:ILE:HG12	2.00	0.62
2:A:1236:ILE:HD11	3:B:170:LEU:HD13	1.81	0.61
2:A:174:ARG:HH22	2:A:181:PHE:HB3	1.65	0.61
2:A:115:LEU:HD13	2:A:118:ILE:HD11	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1634:LEU:HB3	7:A:2009:PCW:H332	1.83	0.61
1:C:56:TYR:CE1	2:A:897:CYS:HB2	2.36	0.60
2:A:59:LEU:HD12	2:A:91:LEU:HG	1.84	0.60
2:A:406:GLU:O	2:A:410:GLN:HG2	2.02	0.60
2:A:88:PHE:CZ	2:A:100:PHE:HB2	2.37	0.59
2:A:168:LEU:HA	2:A:171:ILE:HG22	1.84	0.59
2:A:1659:ALA:O	2:A:1663:MET:HG3	2.02	0.59
2:A:409:ASN:HA	2:A:412:ASN:ND2	2.17	0.59
3:B:35:THR:HG22	3:B:109:THR:O	2.01	0.59
1:C:135:ARG:HA	1:C:135:ARG:CZ	2.32	0.59
2:A:1651:LEU:O	2:A:1655:MET:HG3	2.01	0.59
1:C:122:GLU:HG2	1:C:145:GLN:HA	1.85	0.59
2:A:747:ASP:O	2:A:751:THR:HG23	2.02	0.59
2:A:66:ILE:HD12	2:A:67:PRO:HD2	1.85	0.59
2:A:1346:LYS:HZ3	2:A:1420:ASN:HA	1.66	0.59
2:A:26:ARG:O	2:A:30:ARG:HG3	2.02	0.59
2:A:57:LYS:HG2	2:A:58:GLN:N	2.17	0.58
2:A:1006:LEU:HA	2:A:1009:PHE:HB2	1.84	0.58
2:A:1176:LYS:HE3	2:A:1176:LYS:HA	1.84	0.58
2:A:1180:ASN:O	2:A:1184:THR:HG23	2.04	0.58
2:A:199:ALA:CA	2:A:217:ARG:NH2	2.57	0.58
2:A:1384:ASN:OD1	2:A:1388:ASN:ND2	2.36	0.58
2:A:1707:ILE:HD12	2:A:1740:PHE:HE2	1.69	0.58
2:A:54:GLU:HA	2:A:99:ARG:HH22	1.67	0.58
2:A:1348:TYR:CD2	2:A:1382:TRP:NE1	2.72	0.57
2:A:1530:VAL:O	2:A:1534:VAL:HG23	2.04	0.57
2:A:171:ILE:HD11	2:A:176:PHE:HB3	1.86	0.57
2:A:1283:LEU:HD12	2:A:1285:PRO:HD2	1.80	0.57
2:A:90:VAL:HB	2:A:98:PHE:HB2	1.87	0.57
2:A:90:VAL:N	2:A:98:PHE:O	2.32	0.57
2:A:758:THR:HG21	2:A:842:VAL:HG22	1.87	0.57
2:A:1578:TRP:CD2	2:A:1625:LYS:HG3	2.39	0.57
2:A:105:ALA:HB3	2:A:109:LEU:HB3	1.87	0.57
2:A:1709:ASN:HB2	2:A:1714:ASP:HB3	1.87	0.57
2:A:895:CYS:O	2:A:938:VAL:HG23	2.05	0.56
3:B:172:ILE:CA	3:B:175:VAL:HG22	2.27	0.56
2:A:1408:TRP:O	2:A:1412:MET:HG3	2.04	0.56
2:A:754:ILE:O	2:A:758:THR:HG23	2.05	0.56
2:A:1517:PHE:CE2	2:A:1521:ILE:HD11	2.40	0.56
2:A:1666:PHE:HE2	2:A:1739:TYR:CD2	2.23	0.56
7:A:2010:PCW:H71	7:A:2014:PCW:H62	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:185:ILE:O	3:B:189:THR:HG23	2.06	0.56
2:A:737:ILE:O	2:A:741:VAL:HG23	2.06	0.56
2:A:744:PRO:HG3	2:A:990:ILE:HD12	1.87	0.56
2:A:815:ILE:HG22	2:A:841:ARG:HH21	1.70	0.56
2:A:752:ILE:O	2:A:756:LEU:HG	2.05	0.56
2:A:304:TYR:HB2	2:A:328:TYR:CD2	2.41	0.56
2:A:811:PHE:CE2	2:A:815:ILE:HD11	2.40	0.56
2:A:1577:GLY:HA2	2:A:1580:ILE:HD13	1.87	0.56
2:A:409:ASN:HA	2:A:412:ASN:HD22	1.71	0.56
2:A:1348:TYR:HE1	2:A:1384:ASN:ND2	2.03	0.56
2:A:1181:ILE:HB	3:B:182:TYR:HE1	1.71	0.55
2:A:1348:TYR:CE1	2:A:1384:ASN:ND2	2.74	0.55
2:A:836:SER:O	2:A:839:LEU:HD12	2.05	0.55
1:C:84:ARG:HH21	1:C:88:ILE:HG13	1.71	0.55
2:A:116:ARG:O	2:A:120:ILE:HG12	2.06	0.55
2:A:1582:ASP:O	2:A:1586:VAL:HG23	2.06	0.55
2:A:1581:PHE:O	2:A:1585:VAL:HG23	2.07	0.55
2:A:79:ASP:OD1	2:A:82:TYR:N	2.32	0.55
2:A:19:SER:O	2:A:23:ILE:HG23	2.07	0.55
2:A:979:ILE:HD11	2:A:983:PRO:HG3	1.89	0.55
2:A:1430:SER:O	2:A:1430:SER:OG	2.15	0.54
2:A:1493:PRO:C	2:A:1494:GLN:OE1	2.45	0.54
2:A:1518:ASP:HA	2:A:1521:ILE:HD12	1.89	0.54
2:A:1594:PHE:O	2:A:1598:LEU:HG	2.06	0.54
2:A:1656:PHE:O	2:A:1660:ILE:HG12	2.07	0.54
3:B:53:THR:HG23	3:B:123:VAL:HG12	1.90	0.54
2:A:851:THR:HG22	2:A:1327:VAL:HG21	1.89	0.54
3:B:54:PHE:CZ	3:B:124:TYR:HD2	2.26	0.54
2:A:777:ALA:O	2:A:781:LEU:HG	2.08	0.54
2:A:1517:PHE:O	2:A:1521:ILE:HG13	2.08	0.54
2:A:1578:TRP:CE2	2:A:1625:LYS:HG3	2.42	0.54
2:A:1500:PRO:HB2	2:A:1505:GLN:HE22	1.73	0.54
2:A:819:SER:O	2:A:823:LEU:HD23	2.08	0.54
1:C:63:PHE:HE1	1:C:129:ILE:HG23	1.72	0.54
2:A:1370:CYS:SG	2:A:1382:TRP:HB2	2.47	0.54
1:C:87:ILE:HG13	1:C:101:PHE:HD1	1.73	0.53
1:C:98:ARG:HH22	1:C:117:VAL:HA	1.72	0.53
2:A:189:ASN:O	2:A:193:PHE:HD1	1.92	0.53
2:A:1492:LYS:HD3	2:A:1492:LYS:N	2.23	0.53
3:B:153:ASP:OD2	3:B:156:SER:HB2	2.07	0.53
2:A:128:PHE:O	2:A:132:ILE:HG12	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:183:PHE:CE2	2:A:189:ASN:HB3	2.43	0.53
2:A:1333:LEU:O	2:A:1337:ILE:HG13	2.07	0.53
2:A:1480:LYS:HA	2:A:1483:ASN:ND2	2.23	0.53
2:A:1605:SER:HB2	2:A:1608:LEU:HD13	1.90	0.53
2:A:34:GLU:OE2	2:A:34:GLU:N	2.42	0.53
2:A:1666:PHE:CE2	2:A:1739:TYR:CD2	2.97	0.53
2:A:1305:GLU:HA	2:A:1308:ARG:NH2	2.23	0.53
2:A:128:PHE:HE1	2:A:132:ILE:HD11	1.74	0.53
2:A:757:ASN:HD22	2:A:783:PHE:HD1	1.55	0.53
2:A:930:GLU:OE1	2:A:930:GLU:N	2.34	0.53
2:A:1363:GLN:O	2:A:1364:VAL:C	2.47	0.53
2:A:1426:LYS:HB2	2:A:1429:TYR:HB2	1.90	0.53
2:A:1518:ASP:N	2:A:1518:ASP:OD2	2.41	0.53
3:B:152:ARG:HB2	3:B:157:ILE:HD11	1.91	0.53
2:A:1184:THR:HG22	3:B:185:ILE:HG13	1.89	0.52
2:A:23:ILE:HG13	2:A:24:GLU:N	2.24	0.52
2:A:1528:ASN:O	2:A:1532:MET:HG3	2.10	0.52
2:A:1608:LEU:O	2:A:1612:ILE:HG12	2.09	0.52
2:A:742:MET:O	2:A:746:VAL:HG22	2.09	0.52
2:A:1573:TYR:HD2	2:A:1574:PHE:CE2	2.28	0.52
2:A:1651:LEU:HD13	2:A:1750:VAL:HG21	1.90	0.52
2:A:396:LEU:O	2:A:400:VAL:HG12	2.10	0.52
2:A:203:GLU:HG3	2:A:204:PHE:HD2	1.74	0.52
2:A:1480:LYS:HA	2:A:1483:ASN:HD22	1.75	0.52
2:A:1486:LYS:HD3	2:A:1639:MET:SD	2.50	0.52
2:A:210:VAL:HA	2:A:213:LEU:HD21	1.91	0.52
2:A:986:ASN:O	2:A:990:ILE:HG12	2.10	0.52
2:A:1581:PHE:CE1	7:A:2009:PCW:H182	2.45	0.52
2:A:1640:SER:O	2:A:1644:LEU:HD12	2.08	0.52
2:A:116:ARG:NH2	2:A:173:ALA:O	2.43	0.52
2:A:1487:LYS:HE2	2:A:1487:LYS:HA	1.92	0.52
2:A:737:ILE:CG1	2:A:797:ALA:HB2	2.39	0.51
2:A:806:VAL:O	2:A:810:ILE:HG23	2.10	0.51
2:A:1561:GLU:O	2:A:1565:LYS:HG2	2.11	0.51
3:B:24:VAL:HG23	3:B:39:LEU:HD13	1.92	0.51
2:A:932:MET:O	2:A:936:MET:HG3	2.10	0.51
2:A:969:SER:HA	2:A:973:SER:OG	2.09	0.51
2:A:1532:MET:SD	2:A:1620:ILE:HD11	2.50	0.51
1:C:46:ALA:HB3	1:C:114:LEU:HB3	1.91	0.51
2:A:1198:ILE:HG21	2:A:1303:ARG:HH21	1.75	0.51
2:A:1206:SER:O	2:A:1209:LEU:HB2	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1442:ILE:O	2:A:1446:PHE:HB3	2.11	0.51
2:A:154:ASN:HA	2:A:157:TYR:CD2	2.44	0.51
2:A:1697:SER:O	2:A:1697:SER:OG	2.23	0.51
2:A:395:ASN:HD22	2:A:1758:VAL:HB	1.76	0.51
2:A:1658:TYR:HD2	2:A:1739:TYR:HE1	1.56	0.51
2:A:156:LYS:O	2:A:160:THR:HG23	2.10	0.51
3:B:71:LEU:HD13	3:B:78:LEU:HD11	1.93	0.51
2:A:215:THR:O	2:A:218:VAL:N	2.44	0.51
3:B:92:TRP:CZ2	3:B:94:GLY:HA3	2.46	0.51
1:C:56:TYR:CZ	2:A:897:CYS:HB2	2.46	0.50
2:A:396:LEU:HD23	2:A:1762:ASN:HD21	1.76	0.50
2:A:807:GLY:O	2:A:810:ILE:HG12	2.10	0.50
2:A:1488:LEU:HA	2:A:1491:LYS:NZ	2.25	0.50
2:A:1685:GLY:O	2:A:1689:ILE:HG13	2.11	0.50
2:A:1587:ILE:O	2:A:1591:VAL:HG12	2.11	0.50
2:A:1595:LEU:O	2:A:1599:ILE:HG12	2.12	0.50
2:A:765:HIS:H	2:A:768:MET:CE	2.25	0.50
2:A:1586:VAL:O	2:A:1590:ILE:HG12	2.11	0.50
3:B:165:VAL:HG13	3:B:166:LEU:HD12	1.94	0.50
1:C:65:LEU:O	1:C:82:GLN:HG3	2.12	0.49
2:A:1485:MET:HA	2:A:1488:LEU:HD23	1.94	0.49
2:A:907:ARG:HD2	2:A:1413:TYR:CE1	2.47	0.49
2:A:1549:TRP:HA	2:A:1552:VAL:CG1	2.37	0.49
2:A:1608:LEU:H	2:A:1608:LEU:HD12	1.77	0.49
7:A:2009:PCW:H172	7:A:2009:PCW:H322	1.94	0.49
2:A:963:PHE:CD1	2:A:1446:PHE:HE1	2.30	0.49
1:C:80:PHE:CD1	1:C:81:LEU:HD23	2.38	0.49
2:A:993:THR:HA	2:A:996:LYS:HB2	1.94	0.49
2:A:1529:MET:O	2:A:1533:MET:HG3	2.13	0.49
2:A:217:ARG:O	2:A:218:VAL:C	2.48	0.49
2:A:289:ILE:HG21	2:A:302:TYR:CE1	2.48	0.49
2:A:346:THR:HG22	2:A:1536:LYS:HG3	1.95	0.49
2:A:395:ASN:OD1	2:A:1755:TYR:CE1	2.65	0.49
2:A:1492:LYS:O	2:A:1494:GLN:NE2	2.45	0.49
1:C:40:VAL:HG13	1:C:117:VAL:HG21	1.94	0.49
1:C:89:ASN:OD1	1:C:91:LYS:N	2.44	0.49
2:A:1491:LYS:HD3	2:A:1491:LYS:N	2.28	0.49
1:C:82:GLN:HG2	1:C:83:PHE:H	1.77	0.49
2:A:59:LEU:HB3	2:A:95:LYS:HG2	1.94	0.49
2:A:160:THR:O	2:A:164:THR:HG23	2.12	0.49
2:A:886:GLN:HA	2:A:886:GLN:OE1	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:112:THR:HG22	3:B:113:TYR:N	2.27	0.48
2:A:1315:ILE:O	2:A:1318:ILE:HG22	2.13	0.48
2:A:1528:ASN:HD21	2:A:1619:ARG:HH11	1.60	0.48
2:A:1407:GLY:N	2:A:1701:ASP:OD1	2.47	0.48
2:A:1195:GLU:O	2:A:1199:VAL:HG23	2.13	0.48
2:A:1628:LYS:HA	2:A:1631:ARG:HD2	1.95	0.48
2:A:742:MET:O	2:A:742:MET:HG3	2.14	0.48
2:A:1184:THR:HG21	3:B:182:TYR:CD1	2.49	0.48
2:A:1576:VAL:HB	2:A:1579:ASN:OD1	2.13	0.48
2:A:1647:ILE:HG21	2:A:1754:MET:HG2	1.95	0.48
2:A:170:LYS:O	2:A:174:ARG:N	2.33	0.48
2:A:158:THR:O	2:A:162:ILE:HG13	2.14	0.48
2:A:812:ASP:O	2:A:816:VAL:HG13	2.13	0.48
7:A:2009:PCW:H42	7:A:2009:PCW:H82	1.36	0.48
3:B:112:THR:HG22	3:B:113:TYR:H	1.79	0.48
2:A:327:GLY:C	2:A:328:TYR:HD1	2.17	0.48
2:A:1305:GLU:HA	2:A:1308:ARG:HH22	1.79	0.48
2:A:1616:ARG:HB2	2:A:1619:ARG:HH22	1.78	0.48
3:B:59:PHE:CE2	3:B:117:GLY:HA3	2.49	0.48
2:A:10:GLN:OE1	2:A:10:GLN:N	2.44	0.48
2:A:265:GLN:NE2	2:A:1613:ARG:HB3	2.29	0.48
2:A:857:LYS:HA	2:A:857:LYS:HD3	1.64	0.48
2:A:1318:ILE:N	2:A:1319:PRO:HD2	2.28	0.48
2:A:1504:ILE:O	2:A:1508:ILE:HG12	2.14	0.48
2:A:1735:VAL:HG23	6:A:2006:LPE:H21	1.95	0.48
2:A:1581:PHE:HE1	7:A:2009:PCW:H182	1.79	0.48
2:A:66:ILE:HD11	2:A:70:MET:HB2	1.95	0.47
2:A:1462:GLN:O	2:A:1465:LYS:HG2	2.14	0.47
1:C:65:LEU:O	1:C:82:GLN:HA	2.14	0.47
2:A:732:LYS:HA	2:A:735:LYS:NZ	2.28	0.47
2:A:842:VAL:HB	2:A:1334:ILE:HD11	1.95	0.47
2:A:910:MET:HG3	2:A:919:ILE:HD12	1.96	0.47
2:A:1197:PHE:O	2:A:1201:MET:HG2	2.14	0.47
2:A:1199:VAL:HG22	2:A:1303:ARG:HG2	1.96	0.47
2:A:1348:TYR:HD2	2:A:1382:TRP:CD1	2.31	0.47
2:A:1349:GLU:HB2	2:A:1358:ARG:HD3	1.95	0.47
2:A:86:LYS:HE3	2:A:86:LYS:HB3	1.66	0.47
2:A:231:LEU:H	2:A:231:LEU:HD12	1.77	0.47
2:A:1658:TYR:CD2	2:A:1739:TYR:HE1	2.33	0.47
2:A:992:VAL:HG22	2:A:996:LYS:HG2	1.95	0.47
2:A:908:TRP:CH2	2:A:922:ARG:HD3	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1295:LEU:HD22	2:A:1298:LEU:CD1	2.45	0.47
2:A:1321:ILE:HD12	2:A:1321:ILE:H	1.80	0.47
2:A:1532:MET:HE3	2:A:1616:ARG:HG3	1.95	0.47
2:A:301:LYS:HG2	2:A:302:TYR:CD2	2.50	0.47
2:A:155:VAL:O	2:A:156:LYS:C	2.53	0.47
2:A:1333:LEU:HB2	2:A:1396:TYR:OH	2.15	0.47
3:B:52:GLU:HA	3:B:99:LYS:O	2.15	0.47
2:A:16:THR:O	2:A:19:SER:OG	2.33	0.47
2:A:128:PHE:CE1	2:A:132:ILE:HD11	2.50	0.47
2:A:998:GLY:O	2:A:1002:VAL:HG23	2.15	0.47
2:A:1742:SER:O	2:A:1746:ILE:HG13	2.16	0.46
2:A:192:ASP:O	2:A:196:ILE:HG22	2.15	0.46
3:B:183:LYS:O	3:B:186:ALA:HB3	2.16	0.46
2:A:935:CYS:O	2:A:938:VAL:HG12	2.15	0.46
2:A:1385:LEU:HA	2:A:1385:LEU:HD12	1.74	0.46
3:B:126:LEU:HD23	3:B:128:PHE:CZ	2.49	0.46
2:A:1658:TYR:CD2	2:A:1739:TYR:CE1	2.99	0.46
7:A:2008:PCW:H19	7:A:2008:PCW:H162	1.63	0.46
7:A:2009:PCW:H122	7:A:2010:PCW:H2	1.98	0.46
2:A:1490:SER:HA	2:A:1492:LYS:NZ	2.31	0.46
3:B:39:LEU:HD22	3:B:41:ILE:HD11	1.96	0.46
1:C:126:ASN:HB2	1:C:141:LYS:NZ	2.31	0.46
3:B:185:ILE:O	3:B:188:ALA:HB3	2.15	0.46
1:C:38:LEU:N	1:C:143:HIS:O	2.41	0.46
2:A:79:ASP:O	2:A:83:ALA:N	2.49	0.46
2:A:278:ASN:OD1	2:A:329:THR:HG23	2.16	0.46
2:A:732:LYS:HA	2:A:735:LYS:HZ2	1.80	0.46
2:A:1348:TYR:HE1	2:A:1384:ASN:HD22	1.62	0.46
1:C:67:TRP:CH2	1:C:127:CYS:HB3	2.50	0.45
2:A:23:ILE:O	2:A:27:ILE:HG12	2.16	0.45
2:A:750:ILE:O	2:A:754:ILE:HG13	2.16	0.45
3:B:175:VAL:O	3:B:179:ILE:HG23	2.16	0.45
3:B:116:SER:HB3	3:B:146:VAL:HG12	1.97	0.45
3:B:28:THR:HB	3:B:143:HIS:O	2.17	0.45
2:A:154:ASN:HA	2:A:157:TYR:HD2	1.81	0.45
2:A:280:LEU:HD23	2:A:280:LEU:HA	1.73	0.45
1:C:42:ASN:HD21	1:C:119:PRO:HG3	1.82	0.45
2:A:964:LEU:HA	2:A:964:LEU:HD23	1.72	0.45
2:A:1395:GLY:O	2:A:1399:LEU:HG	2.17	0.45
2:A:1435:ILE:O	2:A:1439:VAL:HG23	2.17	0.45
1:C:81:LEU:HD13	1:C:89:ASN:HA	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:16:THR:HG23	2:A:19:SER:H	1.81	0.45
2:A:77:ASP:HA	2:A:89:ILE:HG23	1.99	0.45
2:A:172:LEU:HD23	2:A:173:ALA:N	2.32	0.45
2:A:1007:ARG:HH11	2:A:1011:LEU:HD12	1.82	0.45
2:A:1206:SER:HB3	2:A:1656:PHE:HE2	1.81	0.45
2:A:1666:PHE:HE2	2:A:1739:TYR:CE2	2.34	0.45
3:B:120:GLU:HB3	3:B:141:LYS:CA	2.32	0.45
2:A:164:THR:HG22	2:A:196:ILE:HD11	1.97	0.44
2:A:203:GLU:HG3	2:A:204:PHE:CD2	2.52	0.44
2:A:217:ARG:HG3	2:A:220:ARG:CZ	2.46	0.44
2:A:817:THR:O	2:A:821:VAL:HG23	2.17	0.44
2:A:905:LEU:HD13	2:A:909:HIS:CD2	2.53	0.44
2:A:1296:ARG:HG2	2:A:1299:ARG:NH2	2.33	0.44
2:A:27:ILE:HA	2:A:30:ARG:HD3	1.99	0.44
2:A:199:ALA:CA	2:A:217:ARG:HH22	2.24	0.44
2:A:356:ARG:NH2	2:A:362:TYR:O	2.50	0.44
3:B:57:TRP:HB2	3:B:71:LEU:HG	1.98	0.44
2:A:1326:LEU:HD23	2:A:1326:LEU:HA	1.76	0.44
3:B:26:SER:OG	3:B:142:ILE:CG2	2.66	0.44
1:C:35:PRO:O	1:C:142:ILE:HG12	2.17	0.44
1:C:59:ASN:OD1	1:C:61:LYS:HG2	2.17	0.44
1:C:143:HIS:HB3	1:C:145:GLN:HE21	1.82	0.44
2:A:22:LEU:O	2:A:25:GLN:HB3	2.18	0.44
2:A:851:THR:CG2	2:A:1327:VAL:HG21	2.48	0.44
2:A:1374:MET:HG3	2:A:1380:VAL:HG23	1.99	0.44
2:A:1394:LEU:HA	2:A:1394:LEU:HD23	1.72	0.44
1:C:32:VAL:HG11	1:C:140:GLY:HA3	2.00	0.44
1:C:34:VAL:HG12	1:C:49:PRO:O	2.17	0.44
2:A:19:SER:O	2:A:23:ILE:N	2.50	0.44
2:A:20:LEU:O	2:A:24:GLU:HG3	2.18	0.44
2:A:363:TRP:HZ3	2:A:367:TYR:CD1	2.36	0.44
2:A:1289:LEU:HD12	2:A:1289:LEU:HA	1.77	0.44
2:A:1558:PHE:HA	2:A:1561:GLU:HG3	2.00	0.44
2:A:1653:LEU:O	2:A:1657:ILE:HG13	2.17	0.44
7:A:2014:PCW:H41	7:A:2014:PCW:H82	1.79	0.44
2:A:136:ILE:HG21	2:A:224:THR:HG22	2.00	0.44
2:A:154:ASN:O	2:A:157:TYR:HB2	2.18	0.44
2:A:1325:LEU:O	2:A:1329:LEU:HB2	2.18	0.44
2:A:1502:ASN:N	2:A:1505:GLN:HE21	2.16	0.44
3:B:168:VAL:O	3:B:172:ILE:HG12	2.16	0.44
1:C:67:TRP:HB2	1:C:81:LEU:O	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:82:TYR:HD2	2:A:99:ARG:HD3	1.83	0.44
2:A:119:SER:OG	2:A:172:LEU:HD22	2.18	0.44
2:A:1228:TYR:CD2	3:B:159:SER:HB2	2.40	0.44
2:A:1232:ILE:HD11	3:B:163:MET:HA	1.99	0.44
2:A:1519:ILE:O	2:A:1523:VAL:HG23	2.18	0.44
2:A:1542:HIS:O	2:A:1546:VAL:HG23	2.17	0.44
2:A:737:ILE:CD1	2:A:797:ALA:HB2	2.47	0.44
2:A:951:VAL:O	2:A:952:MET:C	2.55	0.44
2:A:1229:ALA:O	2:A:1233:PHE:CD1	2.71	0.44
2:A:1666:PHE:CE2	2:A:1739:TYR:HD2	2.36	0.44
3:B:62:LYS:HE2	3:B:62:LYS:HB2	1.80	0.44
1:C:47:ARG:HG2	1:C:113:MET:SD	2.58	0.43
1:C:69:TYR:HE2	1:C:123:GLY:HA3	1.81	0.43
2:A:413:ILE:HG13	2:A:414:GLU:N	2.33	0.43
2:A:766:HIS:N	2:A:1390:ASP:O	2.50	0.43
2:A:1549:TRP:O	2:A:1553:VAL:HG12	2.18	0.43
2:A:729:TYR:CA	2:A:732:LYS:HE2	2.34	0.43
2:A:907:ARG:HD2	2:A:1413:TYR:CD1	2.53	0.43
2:A:908:TRP:HZ3	2:A:922:ARG:HB2	1.82	0.43
2:A:1324:VAL:CG2	2:A:1455:VAL:HG21	2.47	0.43
2:A:1532:MET:CE	2:A:1616:ARG:HG3	2.48	0.43
2:A:395:ASN:HD22	2:A:1758:VAL:CB	2.31	0.43
2:A:1211:PHE:O	2:A:1216:ILE:HD13	2.18	0.43
2:A:1400:LEU:HD21	2:A:1744:ILE:HD11	1.99	0.43
2:A:1485:MET:CE	2:A:1639:MET:HA	2.44	0.43
2:A:27:ILE:HD11	2:A:84:ASP:O	2.19	0.43
2:A:764:GLU:HA	2:A:768:MET:HE1	2.00	0.43
2:A:791:MET:HG3	2:A:816:VAL:HG21	2.00	0.43
2:A:918:LEU:HD23	2:A:918:LEU:HA	1.80	0.43
3:B:44:LYS:HB2	3:B:44:LYS:HE3	1.84	0.43
3:B:92:TRP:CE2	3:B:94:GLY:HA3	2.52	0.43
3:B:154:MET:O	3:B:158:VAL:HG12	2.19	0.43
1:C:48:LEU:HD23	1:C:142:ILE:HD12	2.00	0.43
2:A:813:SER:HA	2:A:816:VAL:HG22	2.00	0.43
2:A:999:ILE:HG13	2:A:1000:ASN:N	2.34	0.43
2:A:976:LEU:HD23	2:A:976:LEU:HA	1.83	0.43
2:A:1229:ALA:HB1	2:A:1233:PHE:CE1	2.52	0.43
2:A:1477:GLU:HA	2:A:1480:LYS:NZ	2.34	0.43
1:C:35:PRO:HD2	1:C:142:ILE:HD11	2.01	0.43
2:A:1359:PHE:HD2	2:A:1359:PHE:HA	1.59	0.43
7:A:2010:PCW:H63	7:A:2010:PCW:H42	1.56	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:53:THR:HG21	3:B:123:VAL:HG12	1.98	0.43
2:A:1324:VAL:HG21	2:A:1455:VAL:HG21	2.00	0.43
3:B:166:LEU:HA	3:B:169:VAL:HG22	2.00	0.43
1:C:141:LYS:HE3	1:C:141:LYS:HA	2.01	0.43
2:A:1580:ILE:O	2:A:1584:VAL:HG12	2.19	0.42
2:A:67:PRO:HA	2:A:68:PRO:HD3	1.95	0.42
2:A:1591:VAL:HG22	2:A:1595:LEU:HD12	2.02	0.42
3:B:106:ILE:HD12	3:B:106:ILE:HA	1.89	0.42
1:C:143:HIS:O	1:C:145:GLN:NE2	2.52	0.42
2:A:1198:ILE:O	2:A:1202:ILE:HG13	2.19	0.42
2:A:1211:PHE:HB2	2:A:1226:LEU:HD11	2.01	0.42
2:A:1528:ASN:ND2	2:A:1619:ARG:HH11	2.17	0.42
7:A:2005:PCW:H212	7:A:2005:PCW:H182	1.78	0.42
2:A:58:GLN:OE1	2:A:58:GLN:HA	2.18	0.42
2:A:286:LEU:HD21	2:A:333:ILE:HG12	2.01	0.42
2:A:17:LYS:HD2	2:A:20:LEU:HD12	2.00	0.42
2:A:304:TYR:HB2	2:A:328:TYR:HE2	1.84	0.42
2:A:1359:PHE:HZ	4:D:1:NAG:C7	2.32	0.42
6:A:2013:LPE:H3N3	6:A:2013:LPE:H312	1.61	0.42
2:A:98:PHE:CE2	2:A:124:VAL:HG12	2.54	0.42
2:A:191:LEU:O	2:A:195:VAL:HG23	2.18	0.42
2:A:296:GLU:O	2:A:300:ARG:HG3	2.19	0.42
2:A:421:LEU:O	2:A:425:GLN:HG2	2.20	0.42
2:A:1530:VAL:HA	2:A:1533:MET:SD	2.59	0.42
3:B:180:TYR:CZ	3:B:184:LYS:HD3	2.55	0.42
2:A:18:GLN:H	2:A:18:GLN:CD	2.23	0.42
2:A:1236:ILE:HD11	3:B:170:LEU:CD1	2.47	0.42
7:A:2008:PCW:H72	7:A:2008:PCW:H41	1.64	0.42
1:C:52:PHE:CE1	1:C:129:ILE:HG21	2.55	0.42
2:A:133:MET:O	2:A:137:LEU:HD23	2.19	0.42
2:A:174:ARG:HD2	2:A:174:ARG:HA	1.70	0.42
2:A:1244:LYS:HE2	2:A:1244:LYS:HB2	1.91	0.42
2:A:1536:LYS:HB3	2:A:1536:LYS:HE3	1.76	0.42
2:A:282:ASN:O	2:A:284:GLU:HG3	2.20	0.42
2:A:748:LEU:O	2:A:752:ILE:HG12	2.20	0.42
2:A:779:ARG:HA	2:A:779:ARG:HD2	1.83	0.42
2:A:1349:GLU:HG3	2:A:1351:ILE:HG23	2.02	0.42
2:A:1627:ALA:HB1	2:A:1630:ILE:HD12	2.02	0.42
7:A:2009:PCW:H121	7:A:2009:PCW:H152	1.39	0.42
1:C:56:TYR:HE2	2:A:895:CYS:HA	1.84	0.42
2:A:285:THR:HG23	2:A:287:GLU:N	2.35	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:285:THR:N	2:A:288:SER:OG	2.52	0.42
2:A:119:SER:O	2:A:122:ILE:HG22	2.18	0.41
2:A:276:PHE:HB2	2:A:331:VAL:CG2	2.50	0.41
2:A:306:LEU:HD12	2:A:306:LEU:HA	1.84	0.41
2:A:405:TYR:HE2	2:A:968:LEU:HG	1.85	0.41
2:A:1329:LEU:HD12	2:A:1329:LEU:HA	1.84	0.41
2:A:140:CYS:HA	2:A:143:MET:HE2	2.02	0.41
2:A:174:ARG:HG3	2:A:183:PHE:N	2.35	0.41
2:A:741:VAL:O	2:A:741:VAL:HG12	2.20	0.41
2:A:750:ILE:HD13	2:A:750:ILE:HA	1.88	0.41
2:A:985:ALA:HB1	2:A:990:ILE:HG23	2.02	0.41
2:A:1715:CYS:HB2	2:A:1730:CYS:HB3	1.21	0.41
2:A:98:PHE:CZ	2:A:124:VAL:HG12	2.56	0.41
2:A:182:THR:HG23	2:A:184:LEU:H	1.84	0.41
2:A:1524:LEU:CD2	2:A:1557:LEU:HD21	2.51	0.41
2:A:119:SER:HA	2:A:122:ILE:HG22	2.02	0.41
2:A:140:CYS:O	2:A:144:THR:HG23	2.20	0.41
2:A:1499:ARG:HE	2:A:1499:ARG:HB3	1.75	0.41
2:A:1573:TYR:HD2	2:A:1574:PHE:HE2	1.67	0.41
2:A:1497:ILE:HD12	2:A:1497:ILE:HA	1.95	0.41
2:A:282:ASN:O	2:A:282:ASN:OD1	2.39	0.41
2:A:407:GLU:OE2	2:A:407:GLU:HA	2.21	0.41
2:A:418:GLN:OE1	2:A:418:GLN:HA	2.21	0.41
2:A:963:PHE:CD1	2:A:1446:PHE:CE1	3.09	0.41
7:A:2009:PCW:H121	7:A:2009:PCW:H32	1.89	0.41
1:C:98:ARG:NH2	1:C:117:VAL:HA	2.35	0.41
2:A:117:ARG:O	2:A:120:ILE:HG13	2.20	0.41
2:A:202:THR:HA	2:A:205:VAL:HG12	2.02	0.41
3:B:185:ILE:HD13	3:B:185:ILE:HA	1.86	0.41
1:C:61:LYS:HA	1:C:85:MET:CE	2.51	0.41
2:A:136:ILE:HD11	2:A:223:LYS:NZ	2.36	0.41
2:A:210:VAL:O	2:A:213:LEU:HG	2.21	0.41
2:A:405:TYR:OH	2:A:965:ALA:HA	2.20	0.41
7:A:2010:PCW:H121	7:A:2010:PCW:H152	1.77	0.41
7:A:2014:PCW:H351	7:A:2014:PCW:H322	1.94	0.41
1:C:69:TYR:OH	1:C:71:GLU:HG3	2.21	0.41
2:A:396:LEU:HD23	2:A:1762:ASN:ND2	2.35	0.41
2:A:922:ARG:HG2	2:A:927:GLU:HB2	2.03	0.41
2:A:1179:TRP:NE1	2:A:1183:LYS:NZ	2.69	0.41
2:A:1245:TRP:O	2:A:1249:GLY:N	2.43	0.41
2:A:1384:ASN:OD1	2:A:1385:LEU:N	2.41	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1434:TYR:O	2:A:1438:VAL:HG23	2.21	0.41
2:A:1493:PRO:HA	2:A:1494:GLN:OE1	2.21	0.41
6:A:2007:LPE:H2N3	6:A:2007:LPE:H312	1.61	0.41
1:C:39:ASN:OD1	1:C:145:GLN:HB2	2.21	0.41
2:A:995:ILE:O	2:A:999:ILE:HG23	2.21	0.41
2:A:1287:LYS:HE3	2:A:1287:LYS:HB2	1.85	0.41
2:A:1424:GLN:OE1	2:A:1425:PRO:HD2	2.21	0.41
2:A:1575:THR:HG23	2:A:1576:VAL:HG23	2.03	0.41
2:A:1694:ILE:HG21	2:A:1703:LEU:HD12	2.02	0.40
6:A:2011:LPE:H1N2	6:A:2011:LPE:H312	1.60	0.40
2:A:73:GLU:OE2	2:A:117:ARG:NH2	2.49	0.40
2:A:76:GLU:H	2:A:76:GLU:CD	2.25	0.40
2:A:122:ILE:HD12	2:A:122:ILE:HA	1.88	0.40
2:A:125:HIS:O	2:A:128:PHE:HB3	2.21	0.40
2:A:189:ASN:O	2:A:193:PHE:CD1	2.73	0.40
6:A:2003:LPE:H21	7:A:2005:PCW:H141	2.02	0.40
1:C:82:GLN:CG	1:C:83:PHE:H	2.33	0.40
2:A:409:ASN:O	2:A:413:ILE:HG23	2.21	0.40
2:A:811:PHE:CZ	2:A:815:ILE:HD11	2.56	0.40
3:B:144:ILE:HA	3:B:144:ILE:HD13	1.76	0.40
2:A:121:LYS:N	2:A:121:LYS:HD3	2.36	0.40
2:A:267:PHE:O	2:A:268:MET:C	2.57	0.40
2:A:339:TYR:HB2	2:A:341:TYR:CD1	2.56	0.40
2:A:1611:VAL:O	2:A:1614:LEU:HG	2.21	0.40
2:A:1683:THR:HG22	2:A:1684:PHE:N	2.37	0.40
3:B:155:ALA:HA	3:B:158:VAL:HG12	2.04	0.40
2:A:774:ASN:O	2:A:778:ILE:HG12	2.21	0.40
2:A:1494:GLN:N	2:A:1494:GLN:CD	2.74	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	C	120/227 (53%)	112 (93%)	7 (6%)	1 (1%)	19 51
2	A	1274/2031 (63%)	1212 (95%)	61 (5%)	1 (0%)	51 82
3	B	171/230 (74%)	163 (95%)	8 (5%)	0	100 100
All	All	1565/2488 (63%)	1487 (95%)	76 (5%)	2 (0%)	54 82

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	97	ASP
2	A	149	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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	114/205 (56%)	113 (99%)	1 (1%)	78 90
2	A	1150/1811 (64%)	1127 (98%)	23 (2%)	55 77
3	B	157/202 (78%)	147 (94%)	10 (6%)	17 47
All	All	1421/2218 (64%)	1387 (98%)	34 (2%)	51 74

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

Mol	Chain	Res	Type
1	C	86	LYS
2	A	151	TRP
2	A	217	ARG
2	A	296	GLU
2	A	331	VAL
2	A	365	ASN
2	A	377	THR
2	A	817	THR
2	A	834	LEU
2	A	838	ARG
2	A	945	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	949	MET
2	A	1278	LEU
2	A	1283	LEU
2	A	1359	PHE
2	A	1369	GLU
2	A	1454	CYS
2	A	1456	ILE
2	A	1471	ASP
2	A	1499	ARG
2	A	1549	TRP
2	A	1628	LYS
2	A	1709	ASN
2	A	1714	ASP
3	B	41	ILE
3	B	43	CYS
3	B	64	THR
3	B	84	GLU
3	B	101	LEU
3	B	120	GLU
3	B	123	VAL
3	B	132	TYR
3	B	148	ASP
3	B	170	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	139	HIS
2	A	270	ASN
2	A	273	HIS
2	A	395	ASN
2	A	412	ASN
2	A	809	ASN
2	A	1483	ASN
2	A	1505	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

4 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	2,4	14,14,15	0.48	0	17,19,21	0.45	0
4	NAG	D	2	4	14,14,15	0.19	0	17,19,21	0.43	0
4	NAG	E	1	2,4	14,14,15	0.53	0	17,19,21	2.49	5 (29%)
4	NAG	E	2	4	14,14,15	0.43	0	17,19,21	0.93	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	NAG	E	1	2,4	-	5/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	1	NAG	O5-C1-C2	-6.85	100.47	111.29
4	E	1	NAG	C1-C2-N2	4.73	118.58	110.49
4	E	1	NAG	C2-N2-C7	3.75	128.24	122.90
4	E	1	NAG	C4-C3-C2	-2.61	107.20	111.02
4	E	1	NAG	O4-C4-C3	-2.44	104.70	110.35

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	1	NAG	C1-C2-N2-C7
4	E	1	NAG	C8-C7-N2-C2
4	E	1	NAG	O7-C7-N2-C2
4	D	2	NAG	O5-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6

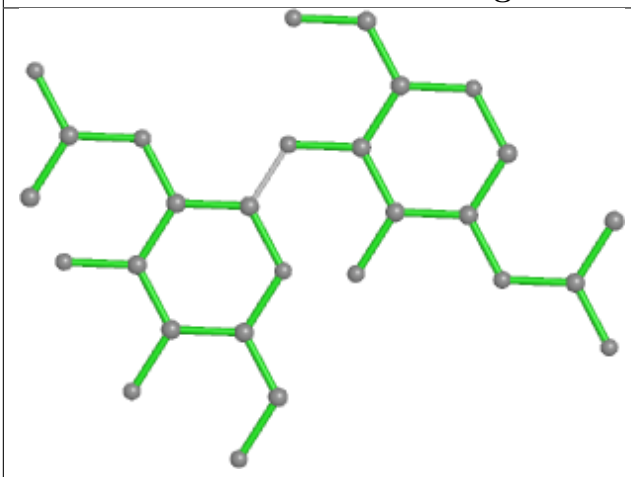
There are no ring outliers.

1 monomer is involved in 1 short contact:

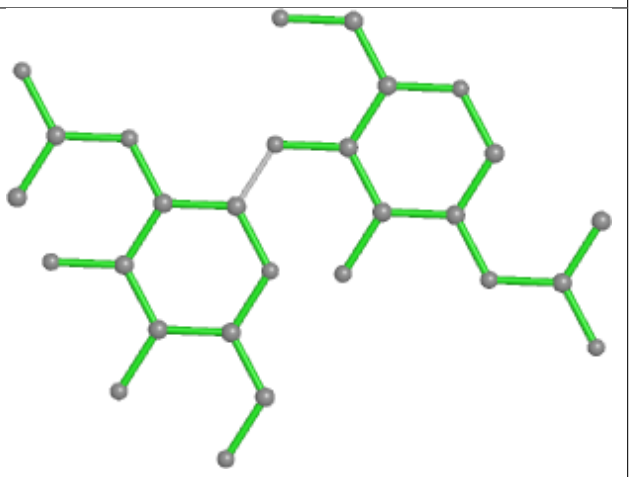
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	NAG	1	0

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

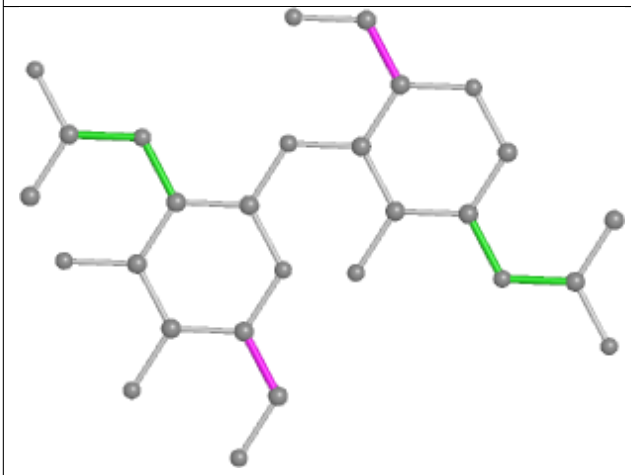
Oligosaccharide Chain D



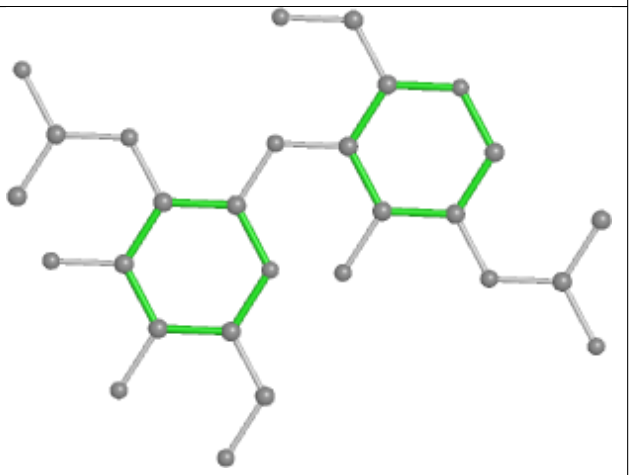
Bond lengths



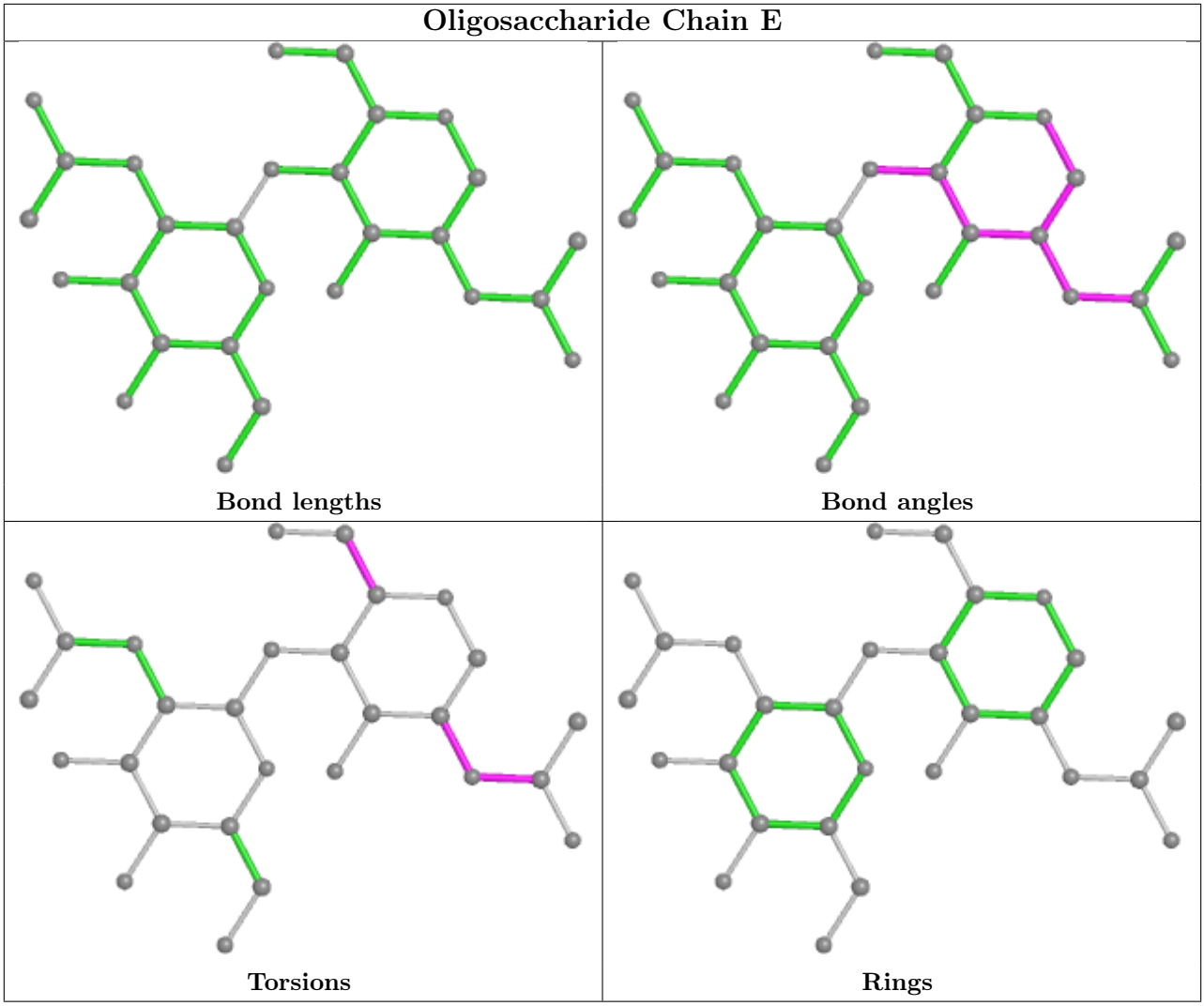
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

18 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	A	2001	2	14,14,15	0.35	0	17,19,21	0.56	0
6	LPE	A	2007	-	27,27,33	0.51	0	31,33,39	0.58	0
5	NAG	B	303	3	14,14,15	0.23	0	17,19,21	1.32	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	PCW	A	2005	-	52,52,53	0.94	2 (3%)	58,60,61	1.02	3 (5%)
6	LPE	A	2004	-	19,19,33	0.64	0	23,25,39	0.71	1 (4%)
5	NAG	B	301	3	14,14,15	0.51	0	17,19,21	1.14	2 (11%)
6	LPE	A	2012	-	24,24,33	0.61	0	28,30,39	0.80	1 (3%)
7	PCW	A	2009	-	43,43,53	0.98	3 (6%)	49,51,61	1.22	6 (12%)
7	PCW	A	2008	-	46,46,53	0.95	2 (4%)	52,54,61	1.26	5 (9%)
5	NAG	B	304	3	14,14,15	0.41	0	17,19,21	2.01	2 (11%)
7	PCW	A	2014	-	43,43,53	1.04	2 (4%)	49,51,61	1.15	4 (8%)
6	LPE	A	2013	-	16,16,33	0.66	0	20,22,39	0.68	1 (5%)
7	PCW	A	2010	-	43,43,53	1.01	2 (4%)	49,51,61	1.10	5 (10%)
6	LPE	A	2011	-	24,24,33	0.59	0	28,30,39	0.67	1 (3%)
5	NAG	A	2002	2	14,14,15	0.26	0	17,19,21	0.49	0
6	LPE	A	2003	-	24,24,33	0.33	0	25,27,39	0.73	0
6	LPE	A	2006	-	27,27,33	0.54	0	31,33,39	0.55	0
5	NAG	B	302	3	14,14,15	0.35	0	17,19,21	0.70	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	NAG	A	2001	2	-	2/6/23/26	0/1/1/1
6	LPE	A	2007	-	-	10/28/28/34	-
5	NAG	B	303	3	-	0/6/23/26	0/1/1/1
7	PCW	A	2005	-	-	18/56/56/57	-
6	LPE	A	2004	-	-	8/20/20/34	-
5	NAG	B	301	3	-	4/6/23/26	0/1/1/1
6	LPE	A	2012	-	-	12/25/25/34	-
7	PCW	A	2009	-	-	18/47/47/57	-
7	PCW	A	2008	-	-	12/50/50/57	-
5	NAG	B	304	3	-	0/6/23/26	0/1/1/1
7	PCW	A	2014	-	-	14/47/47/57	-
6	LPE	A	2013	-	-	8/17/17/34	-
7	PCW	A	2010	-	-	13/47/47/57	-
6	LPE	A	2011	-	-	10/25/25/34	-
5	NAG	A	2002	2	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	LPE	A	2003	-	-	11/25/25/34	-
6	LPE	A	2006	-	-	11/28/28/34	-
5	NAG	B	302	3	-	2/6/23/26	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	2014	PCW	O3-C11	4.33	1.46	1.33
7	A	2005	PCW	O3-C11	4.12	1.45	1.33
7	A	2014	PCW	O2-C31	4.09	1.45	1.34
7	A	2005	PCW	O2-C31	4.09	1.45	1.34
7	A	2010	PCW	O2-C31	4.08	1.45	1.34
7	A	2010	PCW	O3-C11	3.96	1.44	1.33
7	A	2008	PCW	O3-C11	3.89	1.44	1.33
7	A	2009	PCW	O3-C11	3.80	1.44	1.33
7	A	2008	PCW	O2-C31	3.59	1.44	1.34
7	A	2009	PCW	O2-C31	3.51	1.44	1.34
7	A	2009	PCW	O2-C2	-2.09	1.41	1.46

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	304	NAG	C1-O5-C5	7.23	121.99	112.19
7	A	2008	PCW	O2-C31-C32	4.94	122.15	111.50
7	A	2014	PCW	O2-C31-C32	4.47	121.13	111.50
7	A	2009	PCW	O2-C31-C32	4.30	120.77	111.50
5	B	303	NAG	O5-C1-C2	-4.04	104.91	111.29
7	A	2010	PCW	O2-C31-C32	3.95	120.01	111.50
7	A	2005	PCW	O2-C31-C32	3.36	118.75	111.50
7	A	2008	PCW	C4-C5-N	-3.04	105.64	115.78
7	A	2009	PCW	C2-O2-C31	-2.97	110.47	117.79
7	A	2008	PCW	C2-O2-C31	-2.95	110.52	117.79
5	B	301	NAG	C2-N2-C7	-2.85	118.84	122.90
6	A	2012	LPE	C31-C32-N	-2.82	106.37	115.78
7	A	2010	PCW	O3-C11-C12	2.79	120.66	111.91
5	B	304	NAG	O5-C1-C2	2.77	115.66	111.29
7	A	2010	PCW	C2-O2-C31	-2.70	111.14	117.79
7	A	2008	PCW	O2-C31-O31	-2.68	117.22	123.70
5	B	303	NAG	C1-O5-C5	2.65	115.78	112.19
5	B	301	NAG	O5-C1-C2	-2.62	107.15	111.29
7	A	2014	PCW	O3-C11-C12	2.53	119.84	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	2014	PCW	C4-C5-N	-2.50	107.43	115.78
7	A	2005	PCW	O3-C11-C12	2.46	119.62	111.91
7	A	2008	PCW	O3-C11-C12	2.36	119.31	111.91
6	A	2013	LPE	C31-C32-N	-2.27	108.20	115.78
7	A	2005	PCW	C4-C5-N	-2.26	108.23	115.78
7	A	2009	PCW	O2-C31-O31	-2.24	118.29	123.70
6	A	2011	LPE	C31-C32-N	-2.21	108.39	115.78
7	A	2014	PCW	C2-O2-C31	-2.19	112.40	117.79
7	A	2009	PCW	C4-C5-N	-2.17	108.54	115.78
7	A	2009	PCW	C3-C2-C1	-2.13	106.75	111.79
6	A	2004	LPE	C31-C32-N	-2.11	108.73	115.78
7	A	2010	PCW	O3-C11-O11	-2.09	118.32	123.59
7	A	2009	PCW	C14-C13-C12	-2.05	105.83	113.19
7	A	2010	PCW	C4-C5-N	-2.02	109.04	115.78

There are no chirality outliers.

All (155) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	2003	LPE	C3-O3-P-O32
6	A	2003	LPE	C3-O3-P-O33
6	A	2003	LPE	C31-O33-P-O31
6	A	2004	LPE	C31-O33-P-O3
6	A	2004	LPE	C31-O33-P-O31
6	A	2007	LPE	C3-O3-P-O31
6	A	2007	LPE	C3-O3-P-O32
6	A	2011	LPE	C31-O33-P-O32
6	A	2011	LPE	O33-C31-C32-N
6	A	2012	LPE	C3-O3-P-O32
6	A	2012	LPE	O33-C31-C32-N
6	A	2013	LPE	C31-O33-P-O31
7	A	2005	PCW	C4-O4P-P-O1P
7	A	2005	PCW	C4-O4P-P-O2P
7	A	2008	PCW	C1-O3P-P-O1P
7	A	2008	PCW	C1-O3P-P-O2P
7	A	2008	PCW	C4-O4P-P-O3P
7	A	2009	PCW	C1-O3P-P-O1P
7	A	2009	PCW	C1-O3P-P-O2P
7	A	2009	PCW	C1-O3P-P-O4P
7	A	2009	PCW	C4-O4P-P-O1P
7	A	2009	PCW	C4-O4P-P-O2P
7	A	2009	PCW	C4-O4P-P-O3P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	A	2010	PCW	C32-C31-O2-C2
7	A	2010	PCW	C1-O3P-P-O1P
7	A	2010	PCW	C1-O3P-P-O2P
7	A	2010	PCW	C4-O4P-P-O1P
7	A	2014	PCW	C32-C31-O2-C2
7	A	2014	PCW	O31-C31-O2-C2
7	A	2014	PCW	C1-O3P-P-O2P
7	A	2014	PCW	C4-O4P-P-O1P
7	A	2014	PCW	C4-O4P-P-O2P
7	A	2014	PCW	C4-O4P-P-O3P
7	A	2009	PCW	O11-C11-O3-C3
7	A	2014	PCW	O11-C11-O3-C3
7	A	2009	PCW	C12-C11-O3-C3
7	A	2014	PCW	C12-C11-O3-C3
7	A	2009	PCW	O31-C31-O2-C2
7	A	2010	PCW	O31-C31-O2-C2
7	A	2009	PCW	C32-C31-O2-C2
6	A	2003	LPE	O2H-C2-C3-O3
7	A	2008	PCW	C32-C31-O2-C2
5	A	2002	NAG	O5-C5-C6-O6
6	A	2011	LPE	C31-C32-N-C1N
6	A	2012	LPE	C31-C32-N-C2N
6	A	2012	LPE	C31-C32-N-C3N
7	A	2005	PCW	C4-C5-N-C6
5	A	2002	NAG	C4-C5-C6-O6
7	A	2009	PCW	C31-C32-C33-C34
7	A	2005	PCW	C11-C12-C13-C14
5	B	301	NAG	O5-C5-C6-O6
7	A	2008	PCW	O31-C31-O2-C2
7	A	2005	PCW	C4-C5-N-C7
7	A	2005	PCW	C32-C31-O2-C2
6	A	2004	LPE	C3-O3-P-O33
6	A	2006	LPE	C3-O3-P-O33
6	A	2007	LPE	C3-O3-P-O33
6	A	2012	LPE	C3-O3-P-O33
6	A	2012	LPE	C31-O33-P-O3
7	A	2005	PCW	C4-O4P-P-O3P
7	A	2008	PCW	C1-O3P-P-O4P
7	A	2010	PCW	C1-O3P-P-O4P
5	B	302	NAG	C8-C7-N2-C2
7	A	2005	PCW	O31-C31-O2-C2
6	A	2013	LPE	C31-C32-N-C3N

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	A	2011	LPE	O1-C11-C12-C13
5	A	2001	NAG	O5-C5-C6-O6
6	A	2004	LPE	C31-C32-N-C1N
6	A	2011	LPE	C31-C32-N-C2N
6	A	2012	LPE	C31-C32-N-C1N
6	A	2013	LPE	C31-C32-N-C1N
6	A	2003	LPE	O33-C31-C32-N
6	A	2006	LPE	C14-C15-C16-C17
6	A	2012	LPE	C13-C14-C15-C16
7	A	2005	PCW	C13-C14-C15-C16
6	A	2004	LPE	C31-C32-N-C3N
6	A	2011	LPE	C31-C32-N-C3N
6	A	2013	LPE	C31-C32-N-C2N
7	A	2005	PCW	C4-C5-N-C8
5	B	302	NAG	O7-C7-N2-C2
6	A	2011	LPE	C31-O33-P-O3
7	A	2010	PCW	C1-C2-C3-O3
5	B	301	NAG	C8-C7-N2-C2
7	A	2005	PCW	C34-C35-C36-C37
7	A	2014	PCW	C21-C22-C23-C24
6	A	2007	LPE	O2H-C2-C3-O3
6	A	2003	LPE	C1-C2-C3-O3
6	A	2006	LPE	C13-C14-C15-C16
7	A	2005	PCW	C12-C13-C14-C15
7	A	2008	PCW	C23-C24-C25-C26
5	B	301	NAG	C4-C5-C6-O6
6	A	2003	LPE	C2-C1-O1-C11
6	A	2003	LPE	C31-O33-P-O3
7	A	2010	PCW	O2-C2-C3-O3
7	A	2009	PCW	C19-C20-C21-C22
5	B	301	NAG	O7-C7-N2-C2
6	A	2004	LPE	C31-C32-N-C2N
7	A	2010	PCW	C12-C13-C14-C15
6	A	2003	LPE	C3-O3-P-O31
6	A	2004	LPE	C3-O3-P-O31
6	A	2006	LPE	C3-O3-P-O32
6	A	2006	LPE	C31-C32-N-C1N
6	A	2006	LPE	C31-C32-N-C2N
6	A	2011	LPE	C31-O33-P-O31
6	A	2012	LPE	C31-O33-P-O31
6	A	2013	LPE	C31-O33-P-O32
7	A	2008	PCW	C4-O4P-P-O1P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	A	2009	PCW	C4-C5-N-C7
7	A	2009	PCW	C4-C5-N-C8
6	A	2012	LPE	C32-C31-O33-P
6	A	2011	LPE	C12-C11-O1-C1
6	A	2007	LPE	C31-C32-N-C2N
6	A	2004	LPE	O33-C31-C32-N
6	A	2006	LPE	O33-C31-C32-N
6	A	2013	LPE	O33-C31-C32-N
7	A	2005	PCW	O4P-C4-C5-N
7	A	2008	PCW	O4P-C4-C5-N
7	A	2009	PCW	O4P-C4-C5-N
7	A	2010	PCW	O4P-C4-C5-N
7	A	2014	PCW	O4P-C4-C5-N
6	A	2012	LPE	C12-C11-O1-C1
7	A	2005	PCW	C43-C44-C45-C46
6	A	2007	LPE	C31-C32-N-C3N
6	A	2006	LPE	C31-O33-P-O3
6	A	2007	LPE	C31-O33-P-O3
6	A	2013	LPE	C31-O33-P-O3
7	A	2014	PCW	C1-O3P-P-O4P
6	A	2003	LPE	C12-C11-O1-C1
5	A	2001	NAG	C3-C2-N2-C7
7	A	2005	PCW	C19-C20-C21-C22
7	A	2005	PCW	C15-C16-C17-C18
6	A	2006	LPE	C2-C1-O1-C11
7	A	2009	PCW	C4-C5-N-C6
6	A	2006	LPE	C31-C32-N-C3N
6	A	2007	LPE	C31-C32-N-C1N
6	A	2003	LPE	C15-C16-C17-C18
6	A	2011	LPE	C12-C13-C14-C15
7	A	2010	PCW	C4-C5-N-C6
7	A	2014	PCW	C32-C33-C34-C35
7	A	2008	PCW	C17-C18-C19-C20
7	A	2005	PCW	O11-C11-O3-C3
7	A	2014	PCW	C19-C20-C21-C22
7	A	2005	PCW	C12-C11-O3-C3
7	A	2008	PCW	C37-C38-C39-C40
6	A	2007	LPE	C19-C20-C21-C22
6	A	2007	LPE	C17-C18-C19-C20
6	A	2006	LPE	C31-O33-P-O31
7	A	2010	PCW	C4-O4P-P-O2P
7	A	2009	PCW	C12-C13-C14-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	A	2013	LPE	C32-C31-O33-P
7	A	2008	PCW	C5-C4-O4P-P
7	A	2009	PCW	C5-C4-O4P-P
7	A	2014	PCW	C5-C4-O4P-P
6	A	2012	LPE	C2-C1-O1-C11
7	A	2010	PCW	C4-C5-N-C7

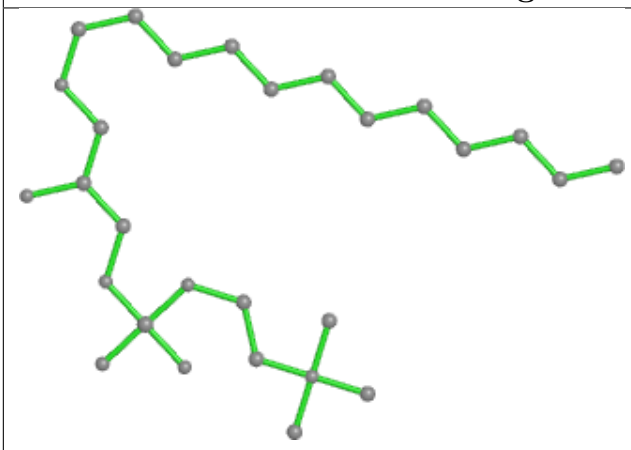
There are no ring outliers.

10 monomers are involved in 23 short contacts:

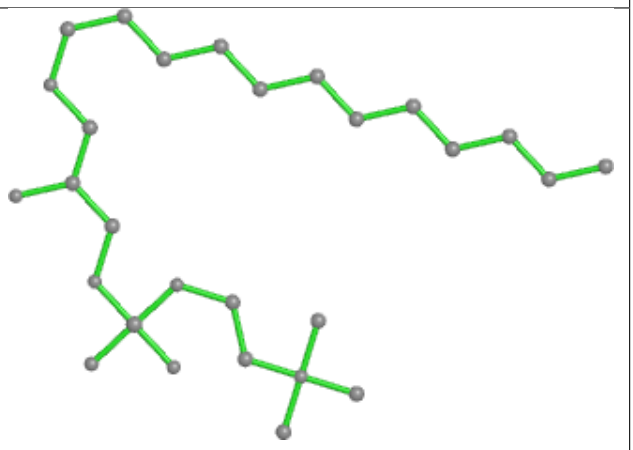
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2007	LPE	1	0
7	A	2005	PCW	2	0
7	A	2009	PCW	8	0
7	A	2008	PCW	3	0
7	A	2014	PCW	3	0
6	A	2013	LPE	1	0
7	A	2010	PCW	4	0
6	A	2011	LPE	1	0
6	A	2003	LPE	2	0
6	A	2006	LPE	1	0

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

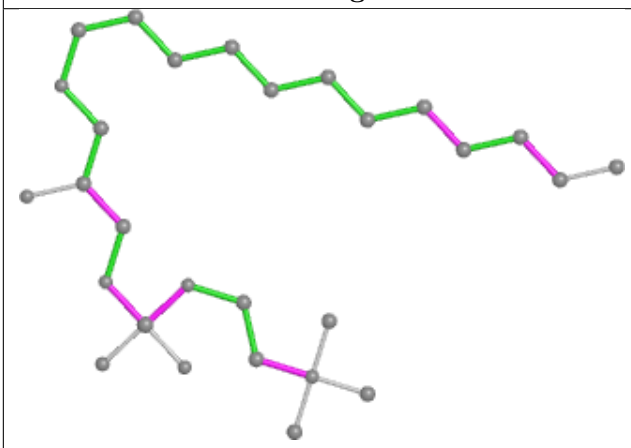
Ligand LPE A 2007



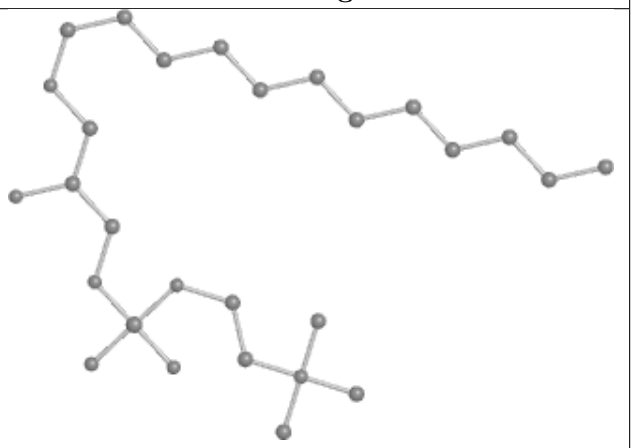
Bond lengths



Bond angles

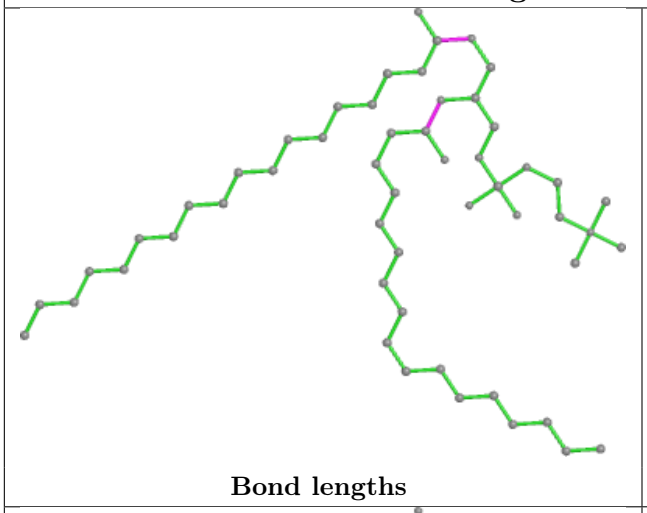


Torsions

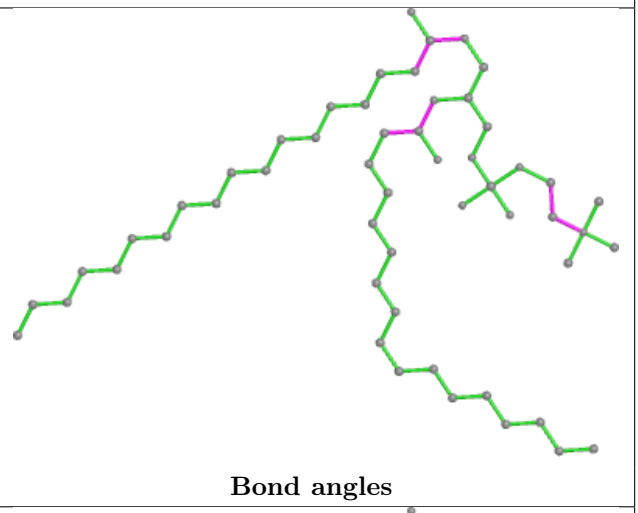


Rings

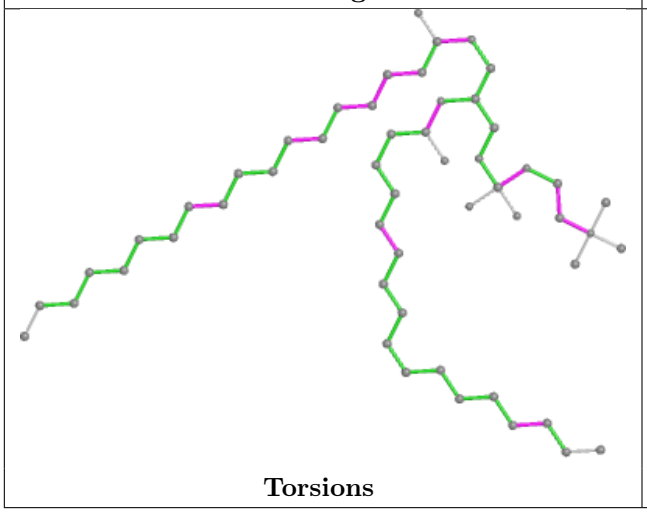
Ligand PCW A 2005



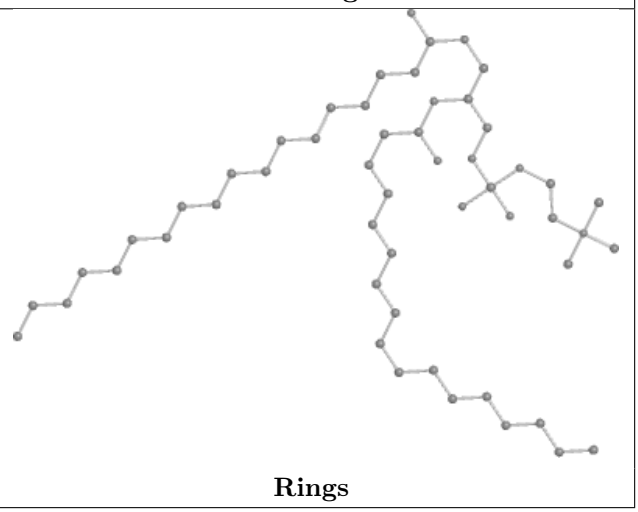
Bond lengths



Bond angles

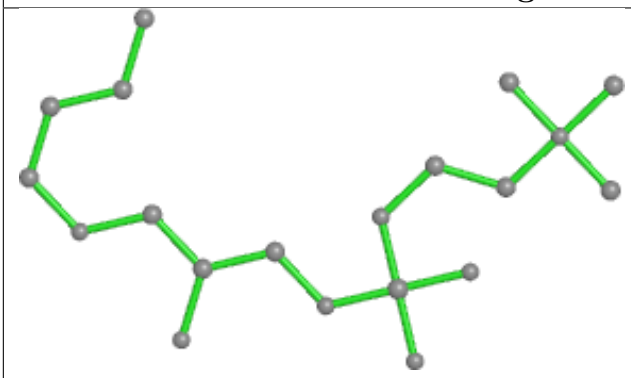


Torsions

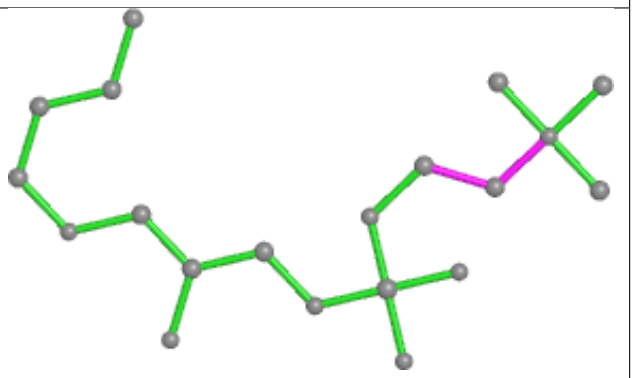


Rings

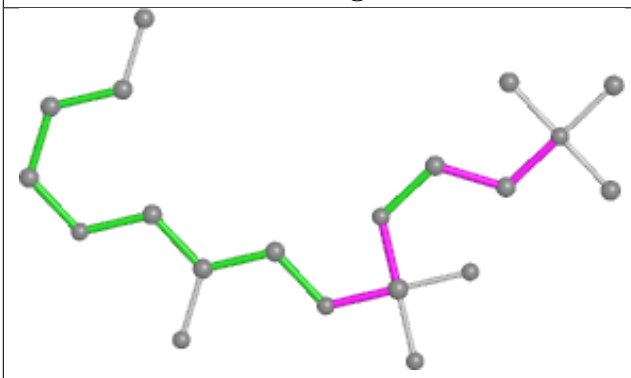
Ligand LPE A 2004



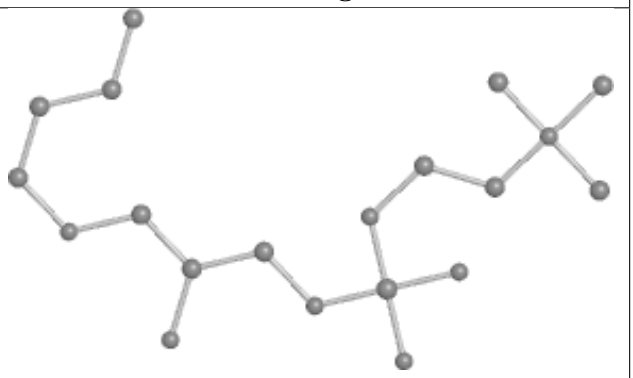
Bond lengths



Bond angles

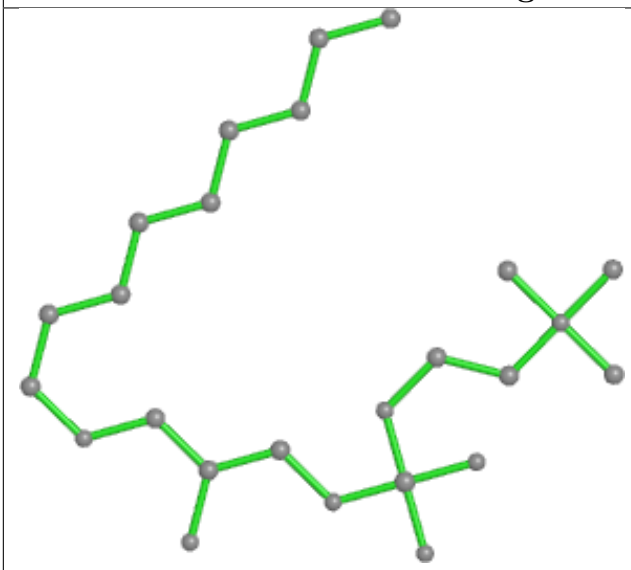


Torsions

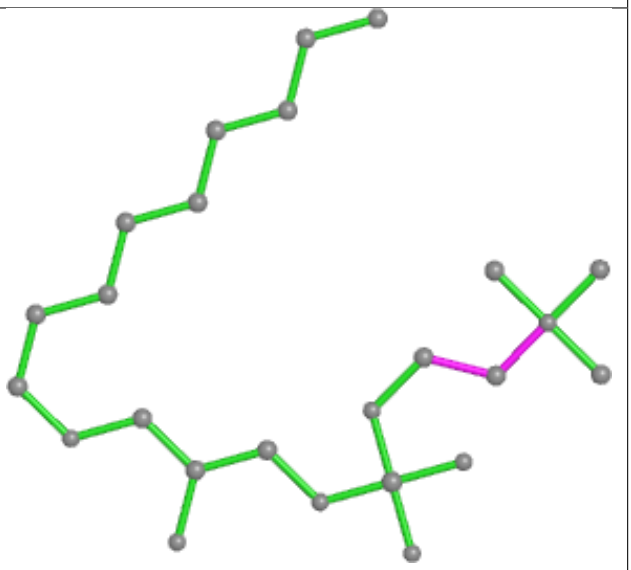


Rings

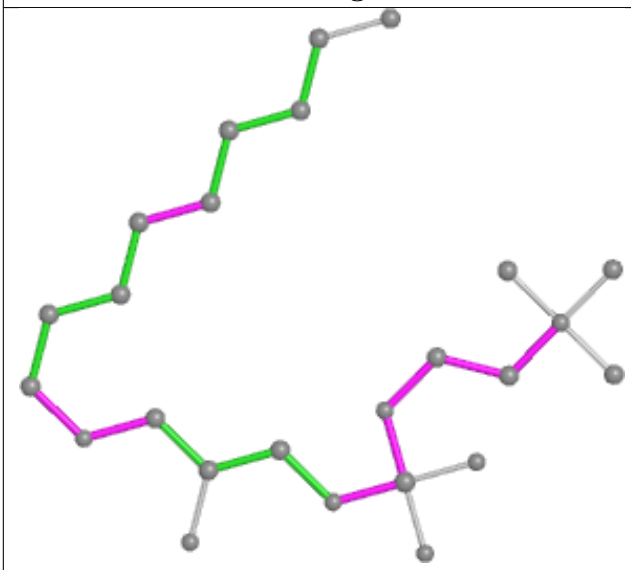
Ligand LPE A 2012



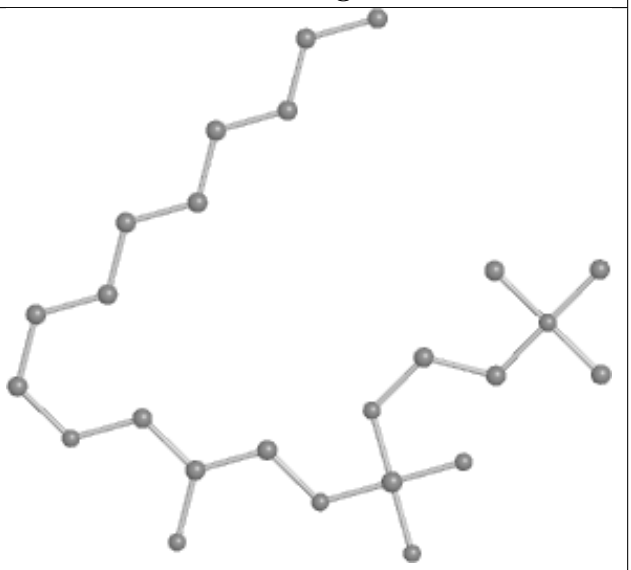
Bond lengths



Bond angles

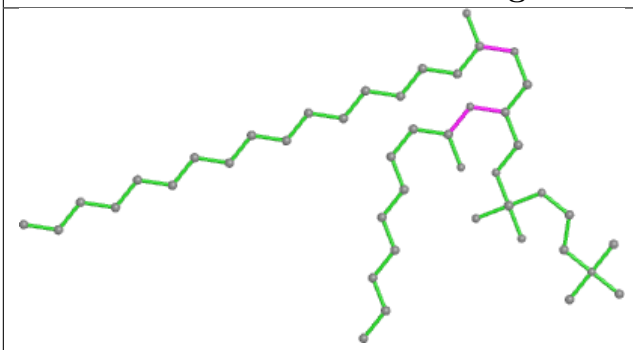


Torsions

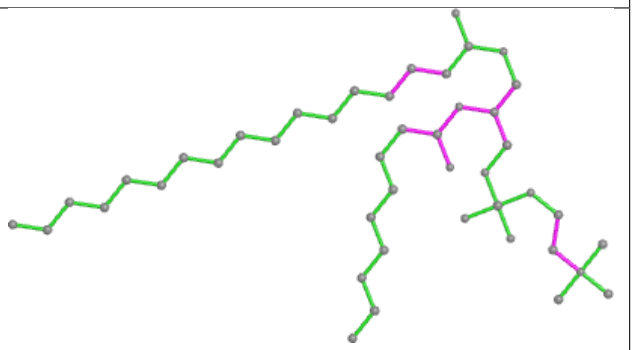


Rings

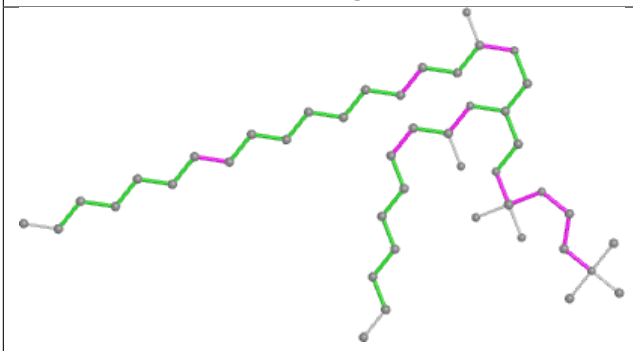
Ligand PCW A 2009



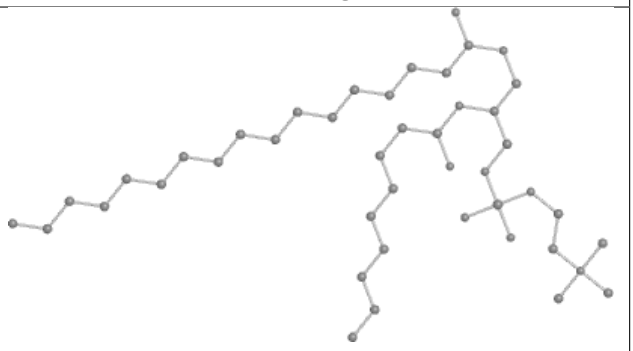
Bond lengths



Bond angles

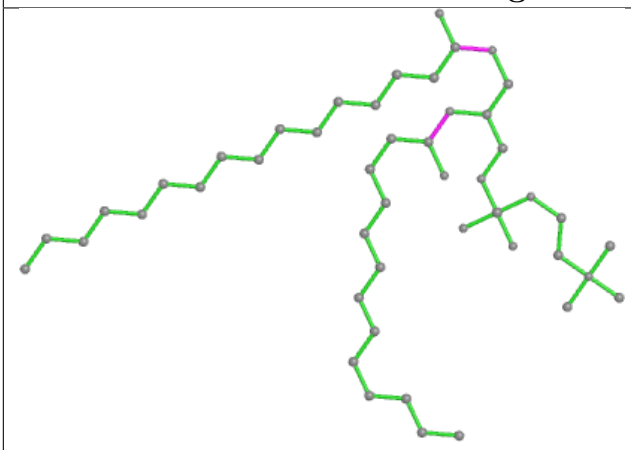


Torsions

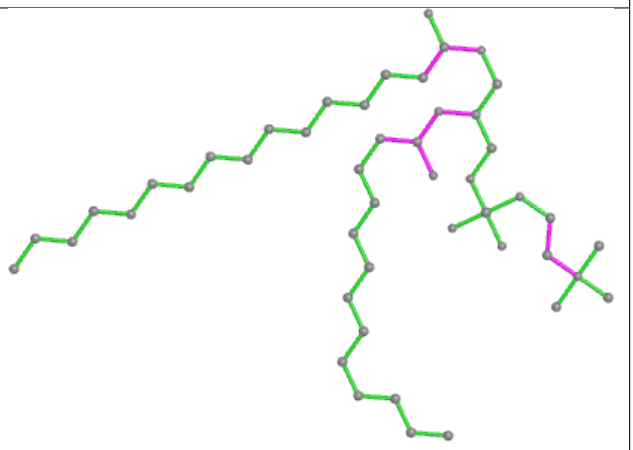


Rings

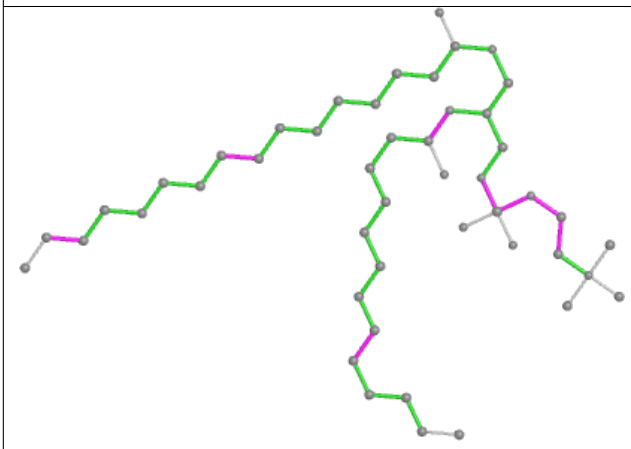
Ligand PCW A 2008



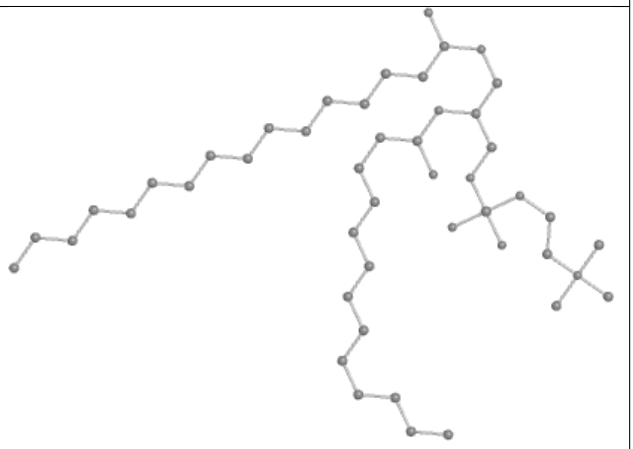
Bond lengths



Bond angles

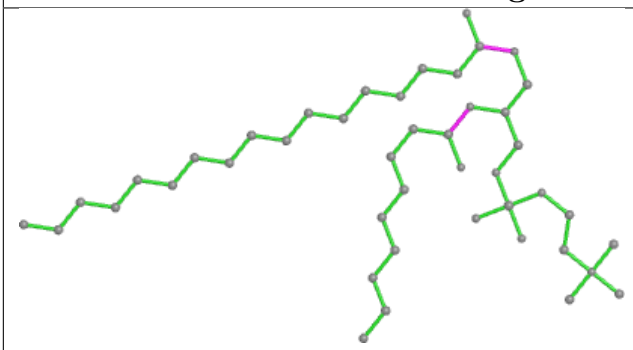


Torsions

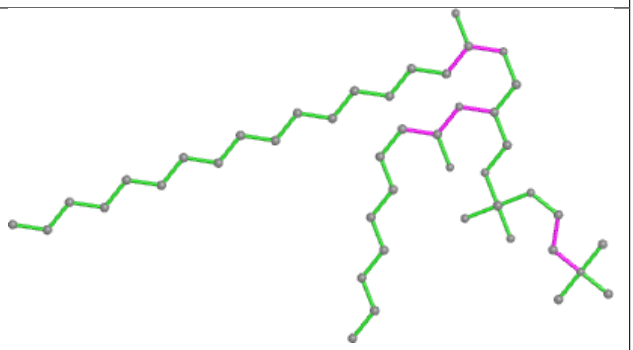


Rings

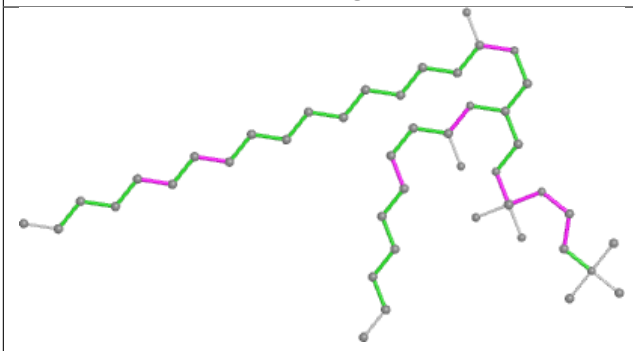
Ligand PCW A 2014



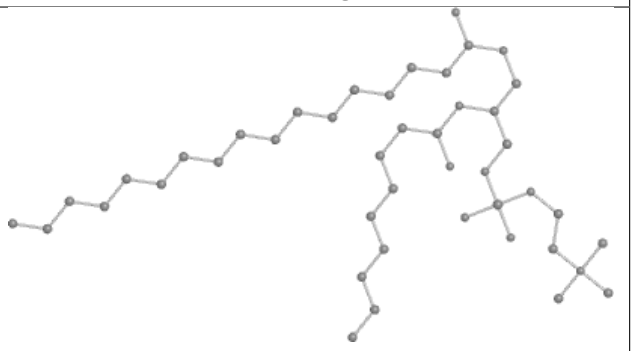
Bond lengths



Bond angles

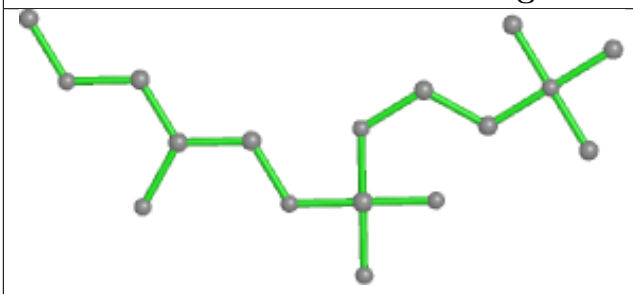


Torsions

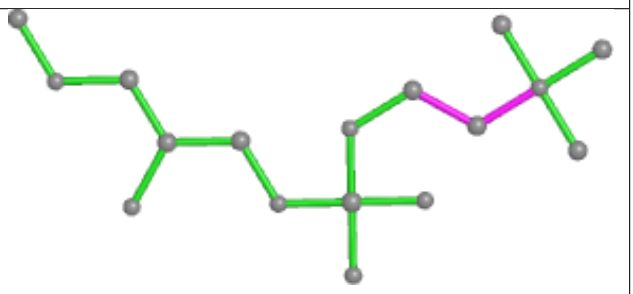


Rings

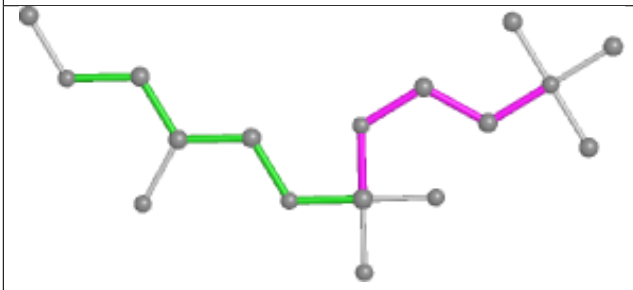
Ligand LPE A 2013



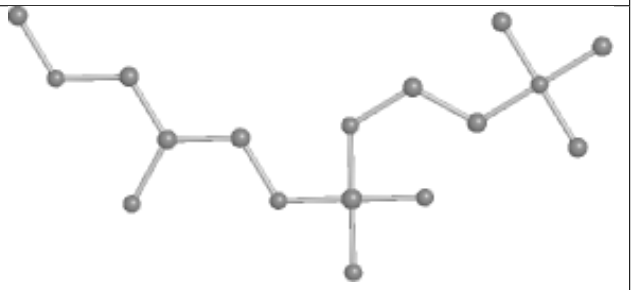
Bond lengths



Bond angles

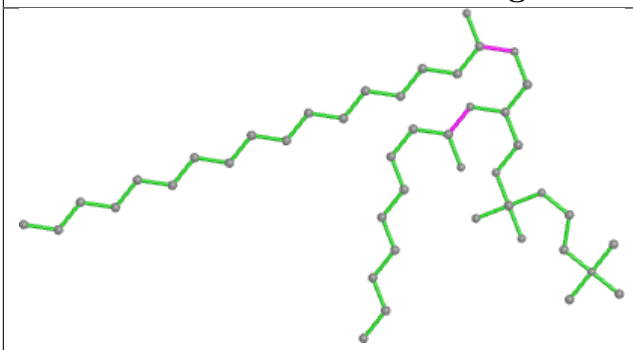


Torsions

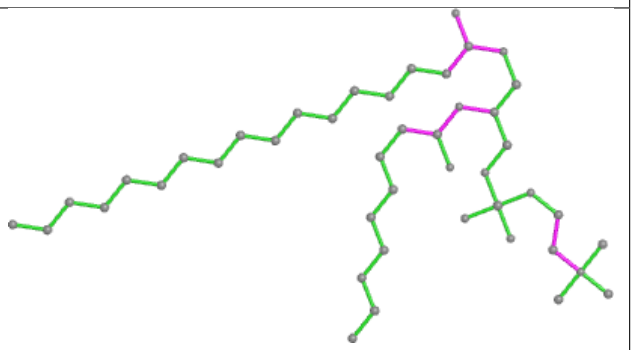


Rings

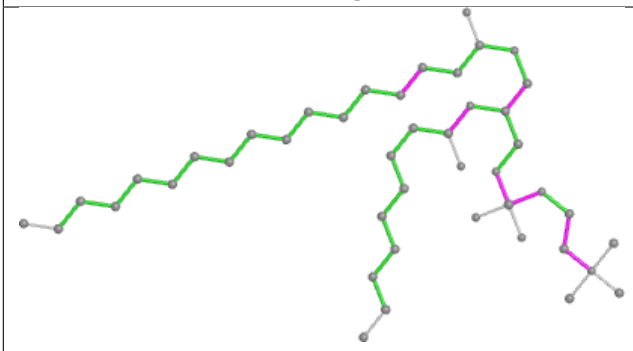
Ligand PCW A 2010



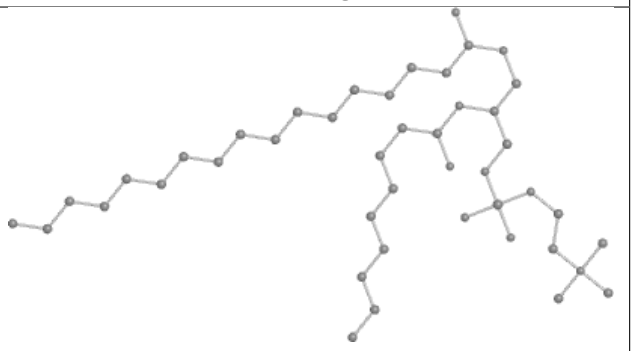
Bond lengths



Bond angles

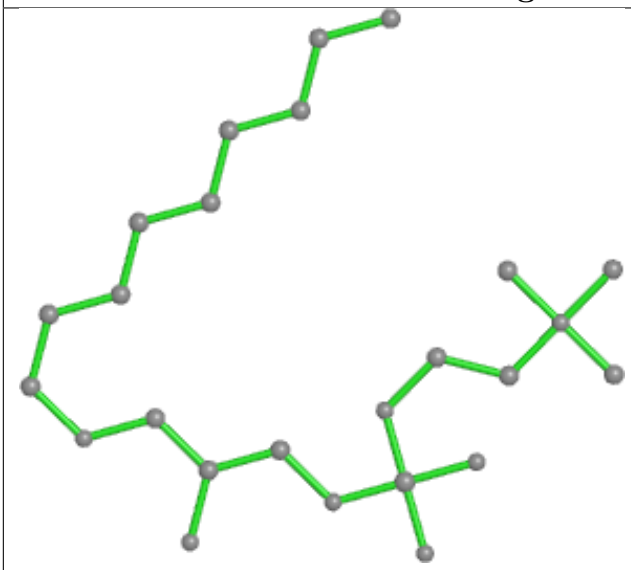


Torsions

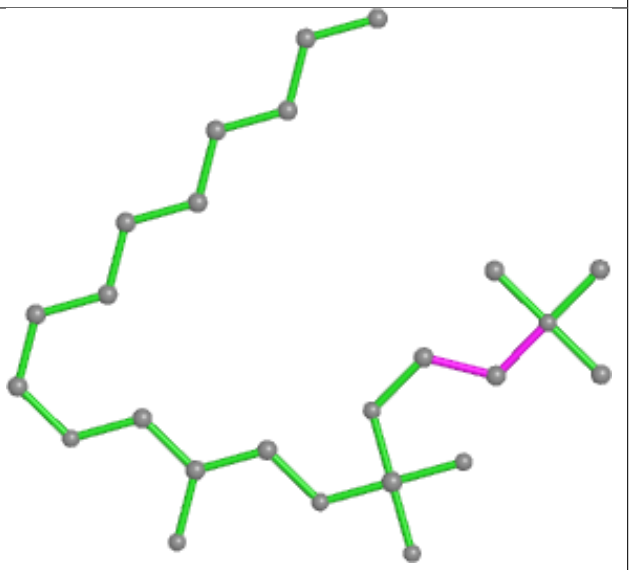


Rings

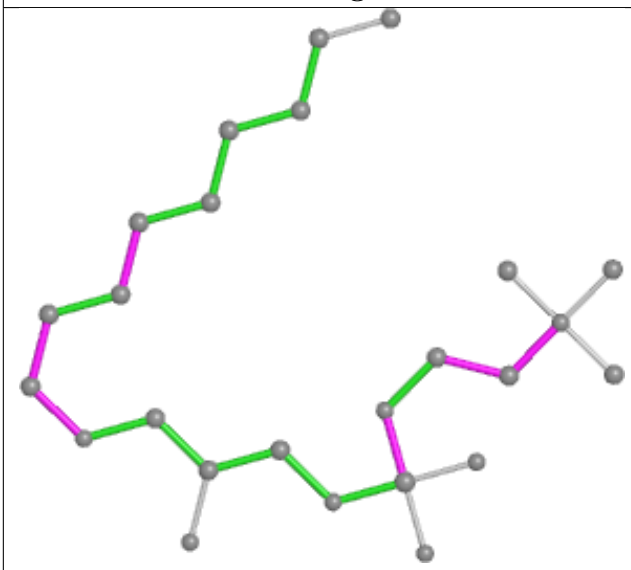
Ligand LPE A 2011



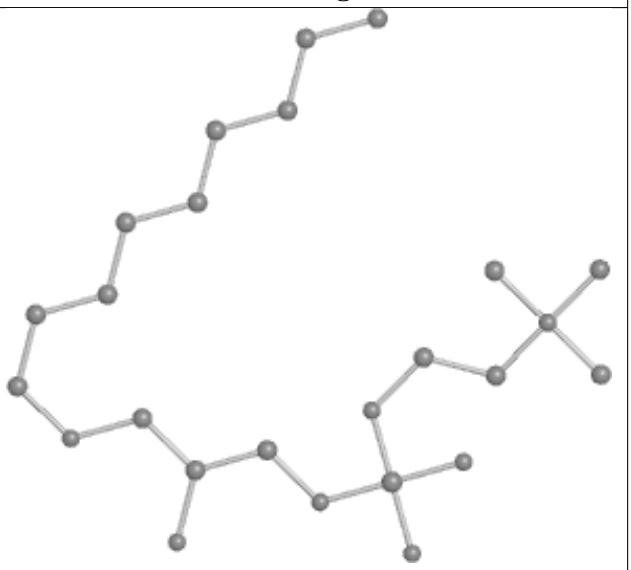
Bond lengths



Bond angles

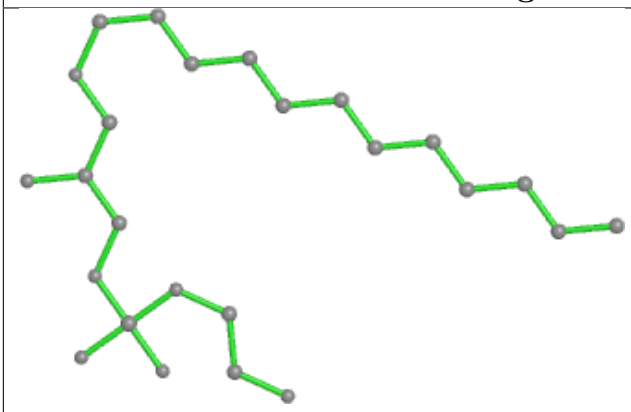


Torsions

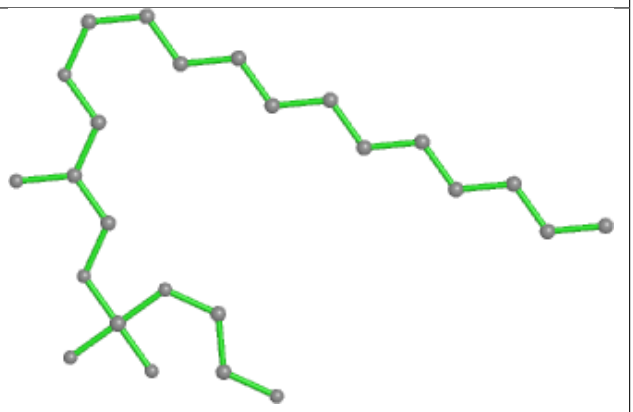


Rings

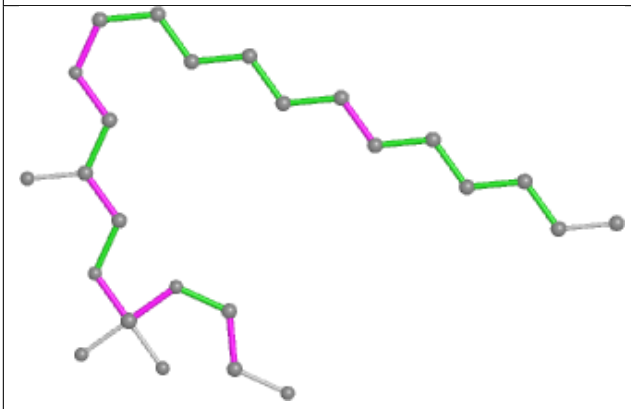
Ligand LPE A 2003



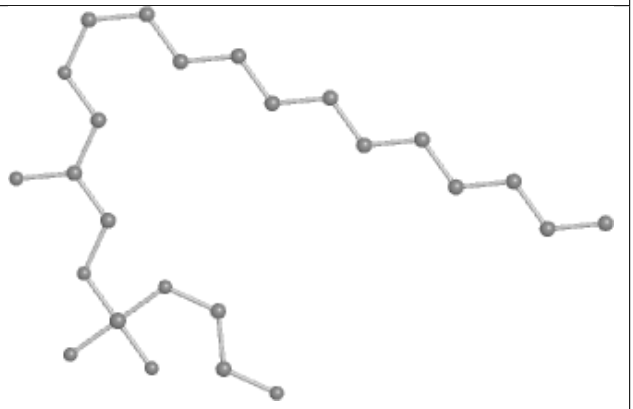
Bond lengths



Bond angles

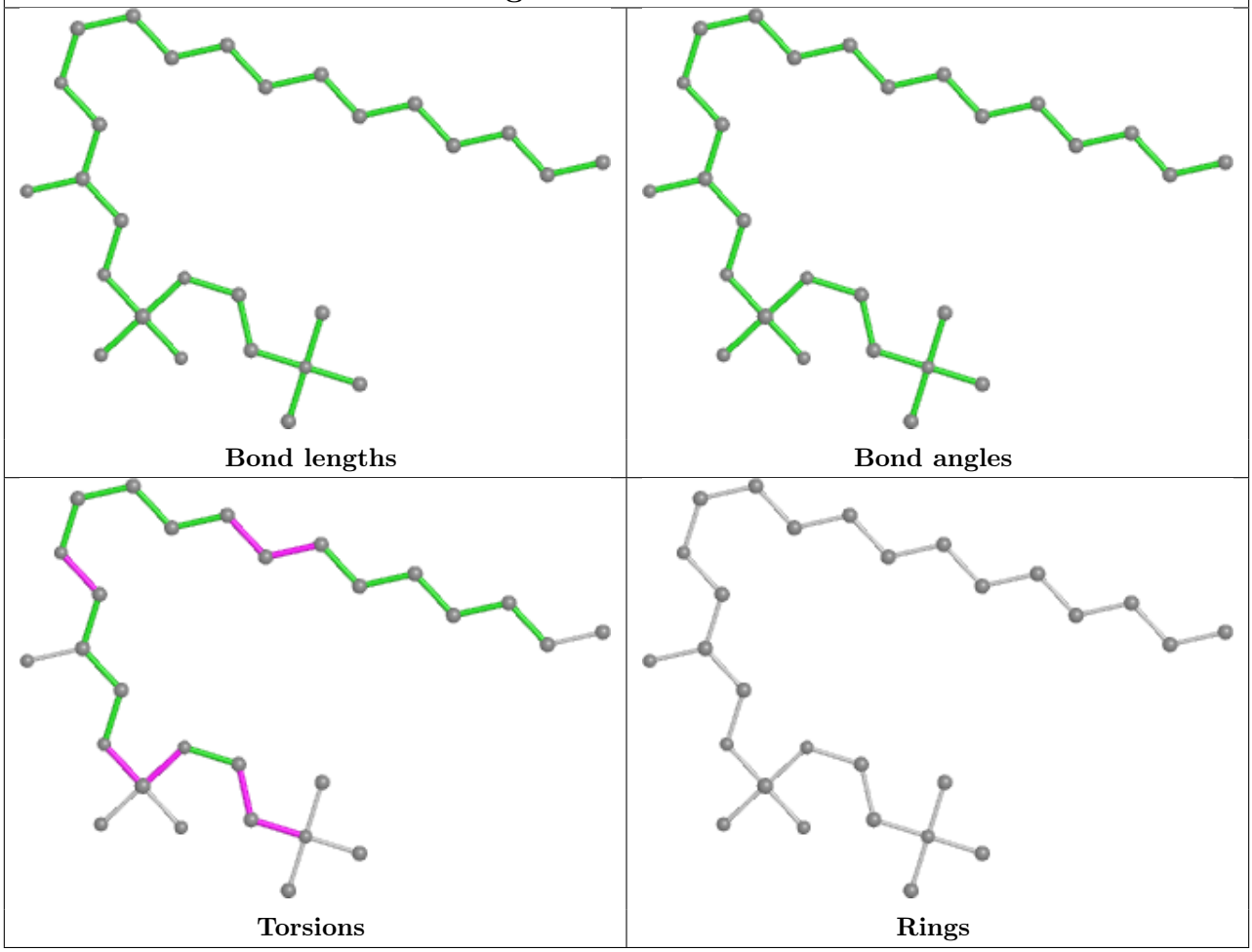


Torsions



Rings

Ligand LPE A 2006



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.

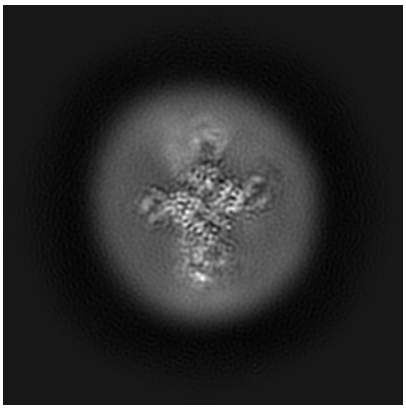
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-38484. These allow visual inspection of the internal detail of the map and identification of artifacts.

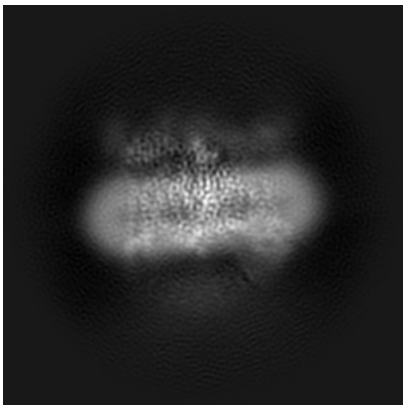
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

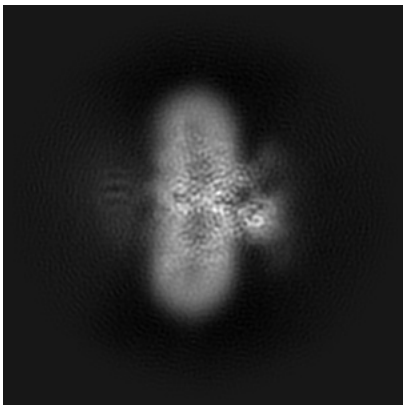
6.1.1 Primary map



X

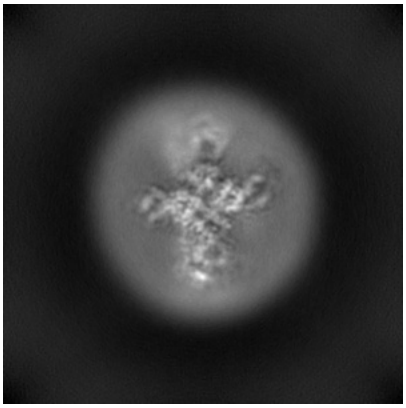


Y

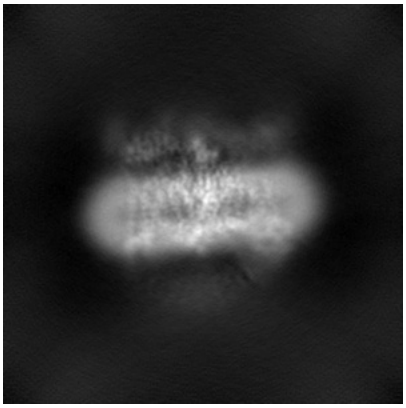


Z

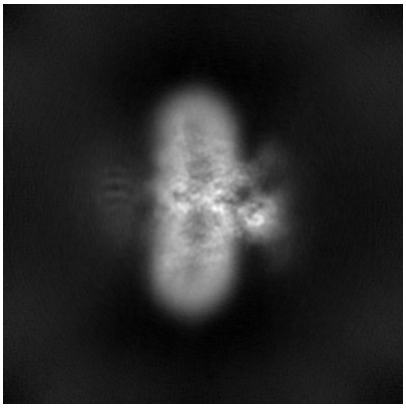
6.1.2 Raw map



X



Y

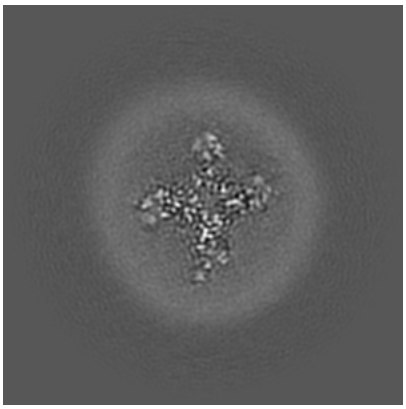


Z

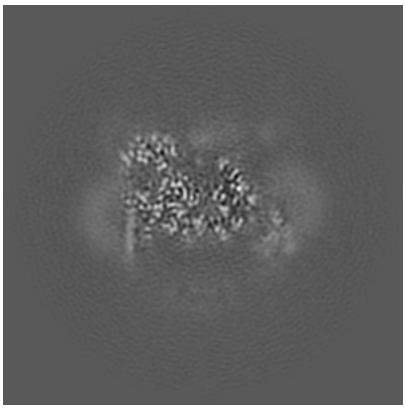
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

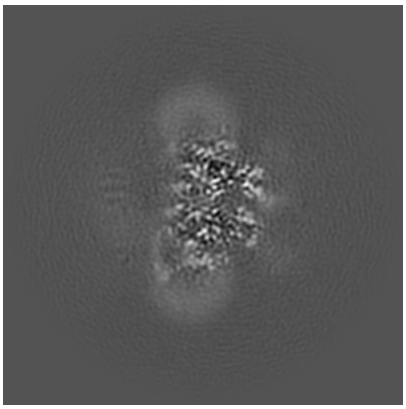
6.2.1 Primary map



X Index: 128

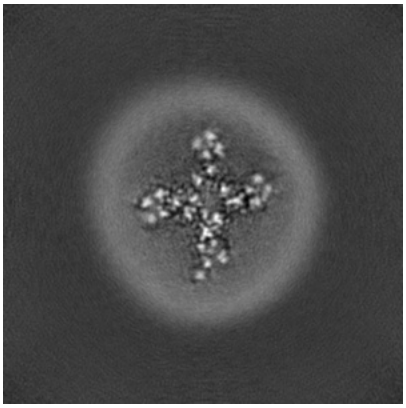


Y Index: 128

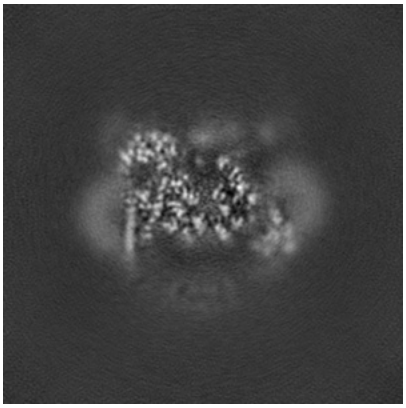


Z Index: 128

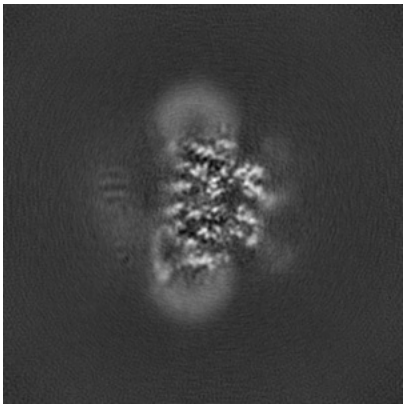
6.2.2 Raw map



X Index: 128



Y Index: 128

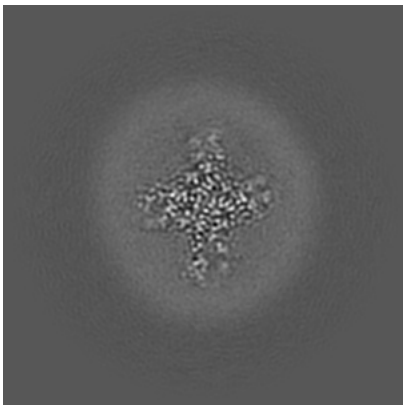


Z Index: 128

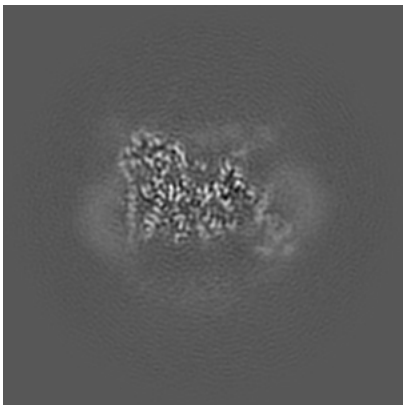
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

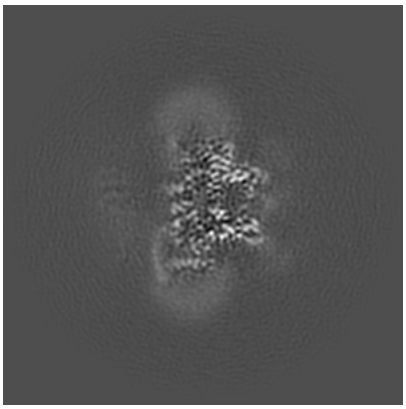
6.3.1 Primary map



X Index: 134

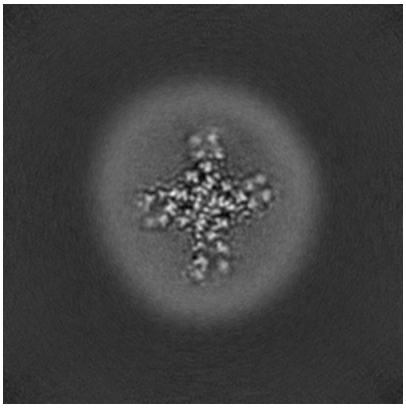


Y Index: 125

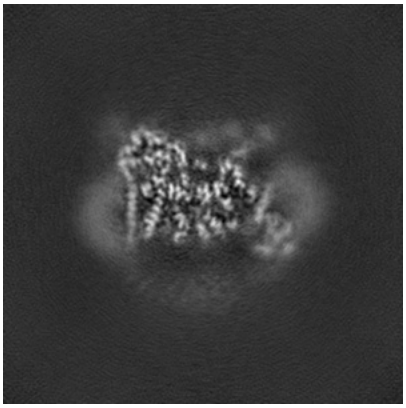


Z Index: 126

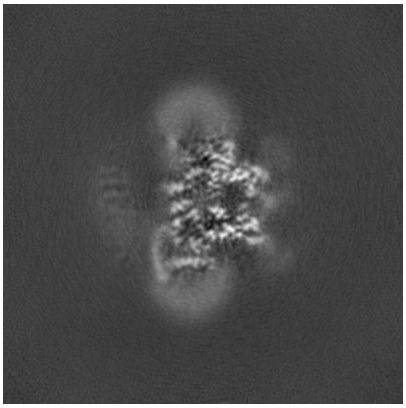
6.3.2 Raw map



X Index: 134



Y Index: 125

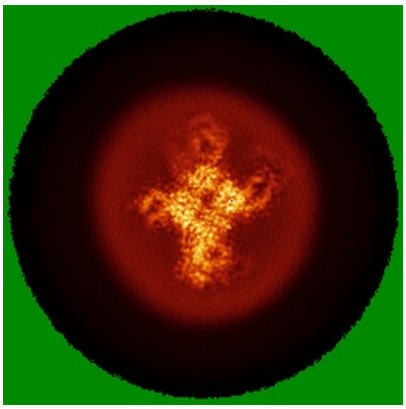


Z Index: 126

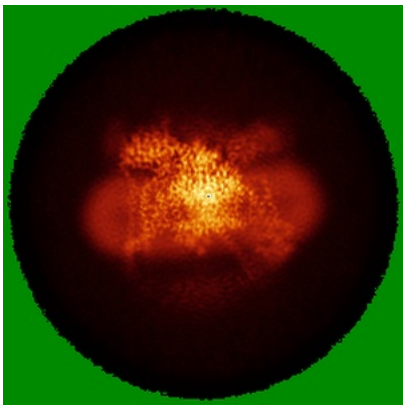
The images above show the largest variance slices of the map in three orthogonal directions.

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

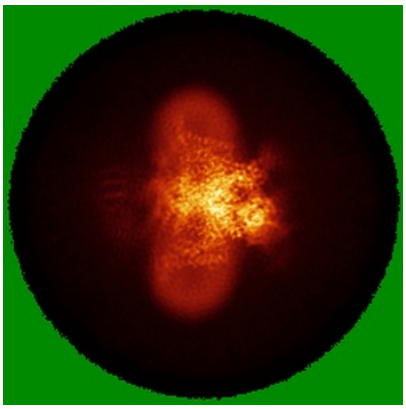
6.4.1 Primary map



X

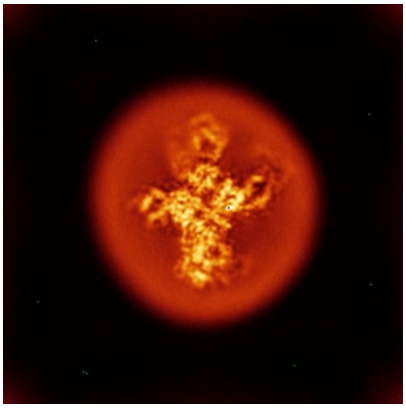


Y

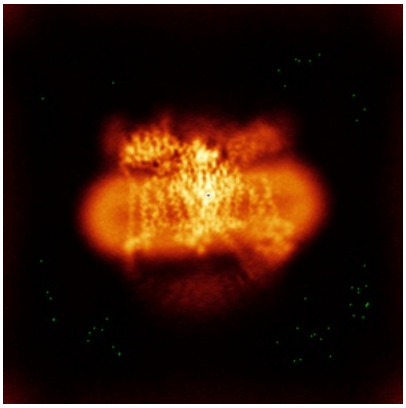


Z

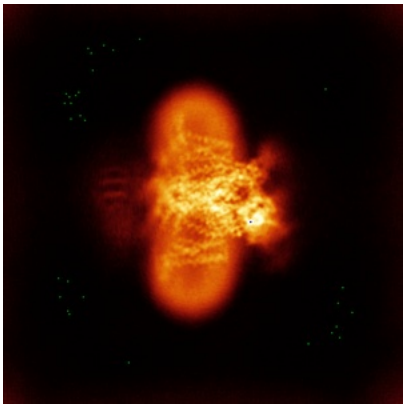
6.4.2 Raw map



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 0.25. 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.

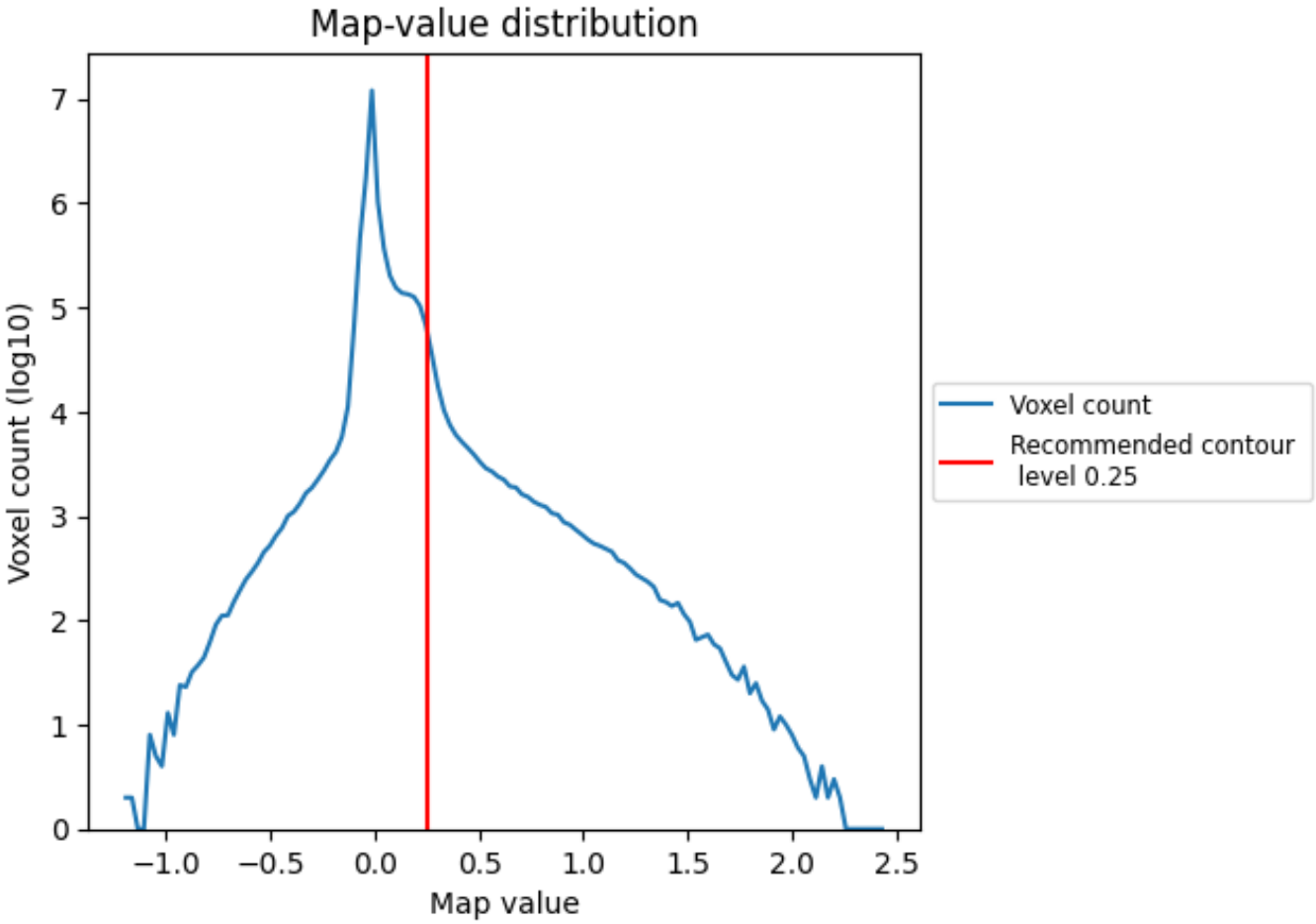
6.6 Mask visualisation (i)

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

7 Map analysis

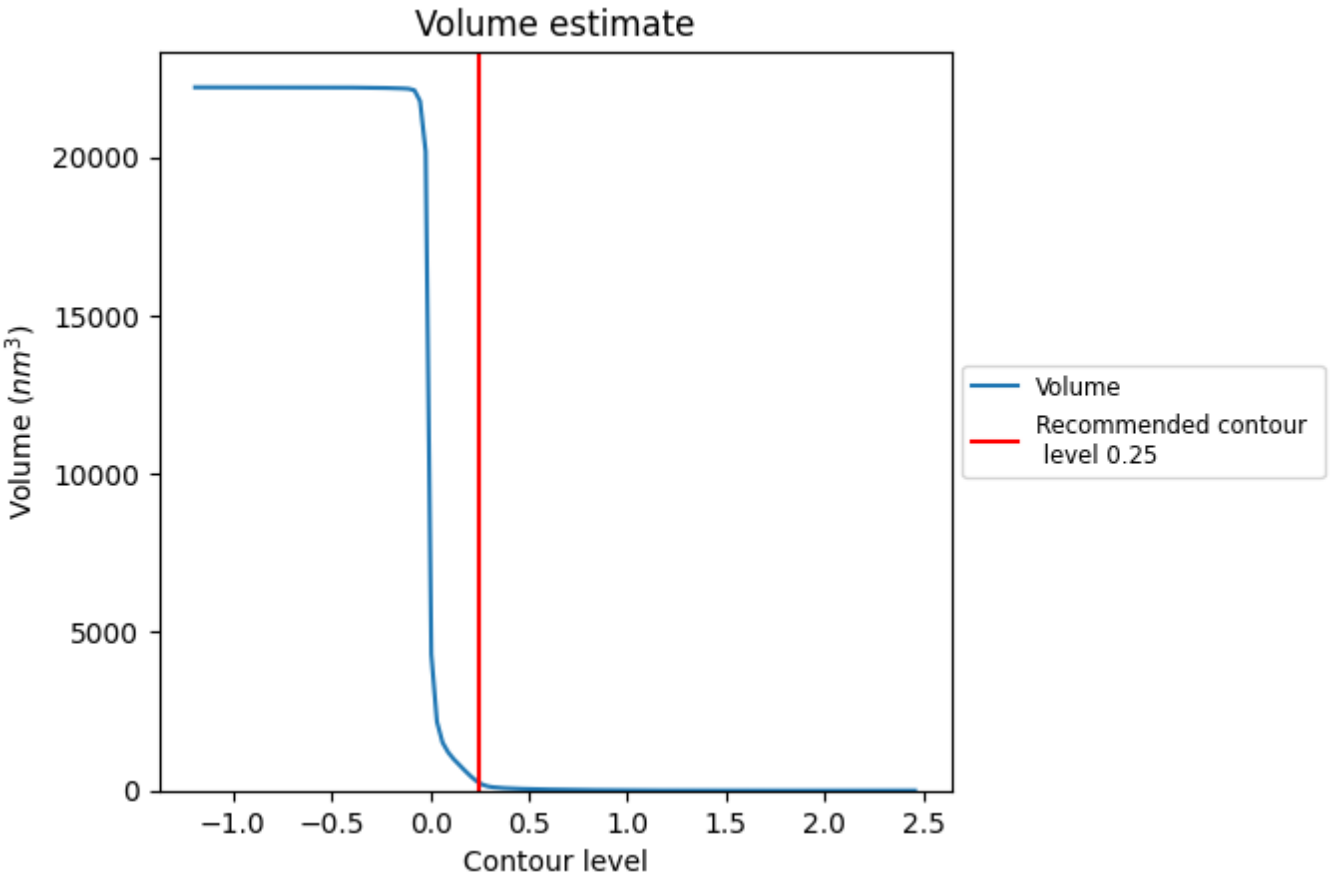
This section contains the results of statistical analysis of the map.

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.

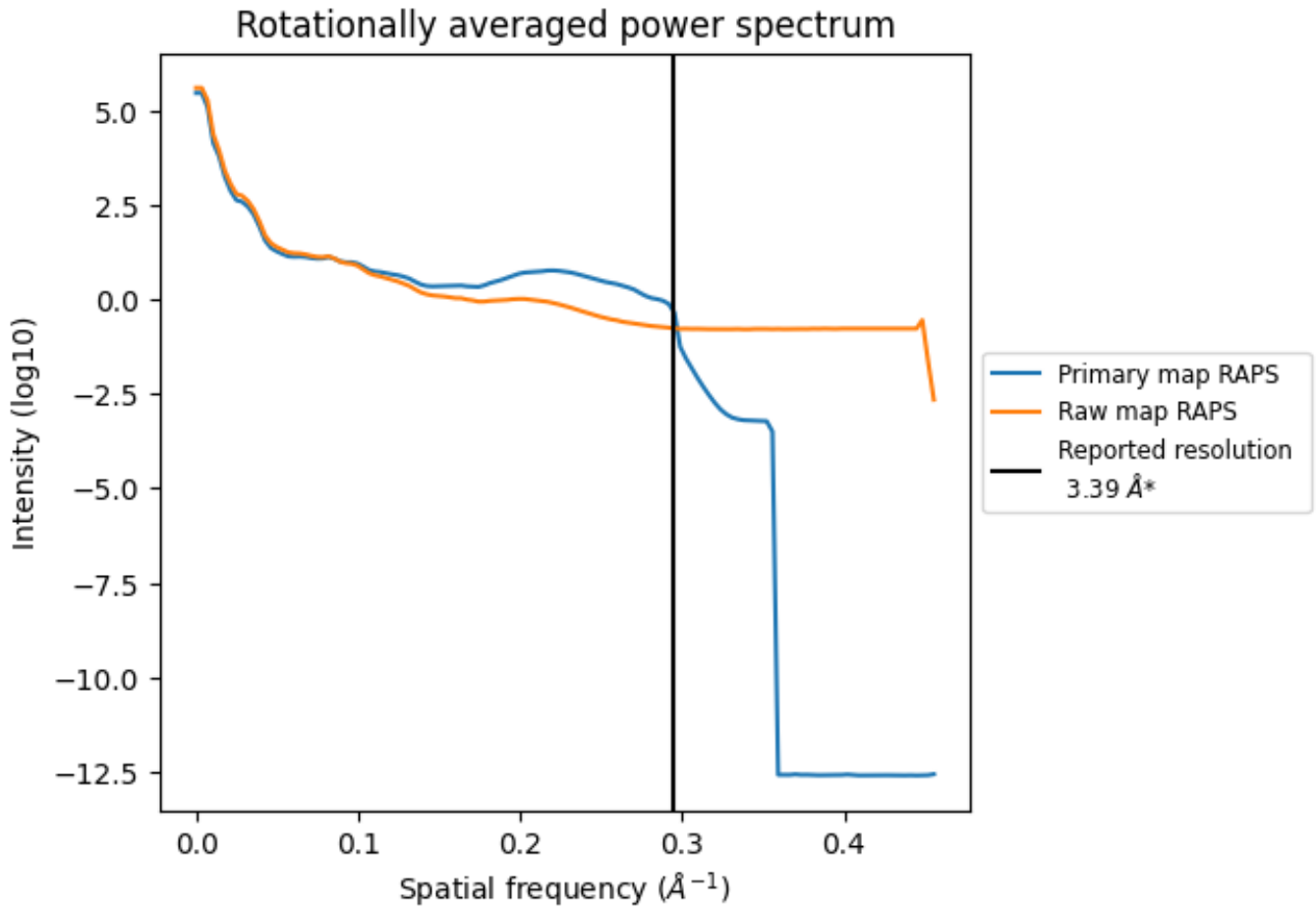
7.2 Volume estimate (i)



The volume at the recommended contour level is 242 nm^3; this corresponds to an approximate mass of 219 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)

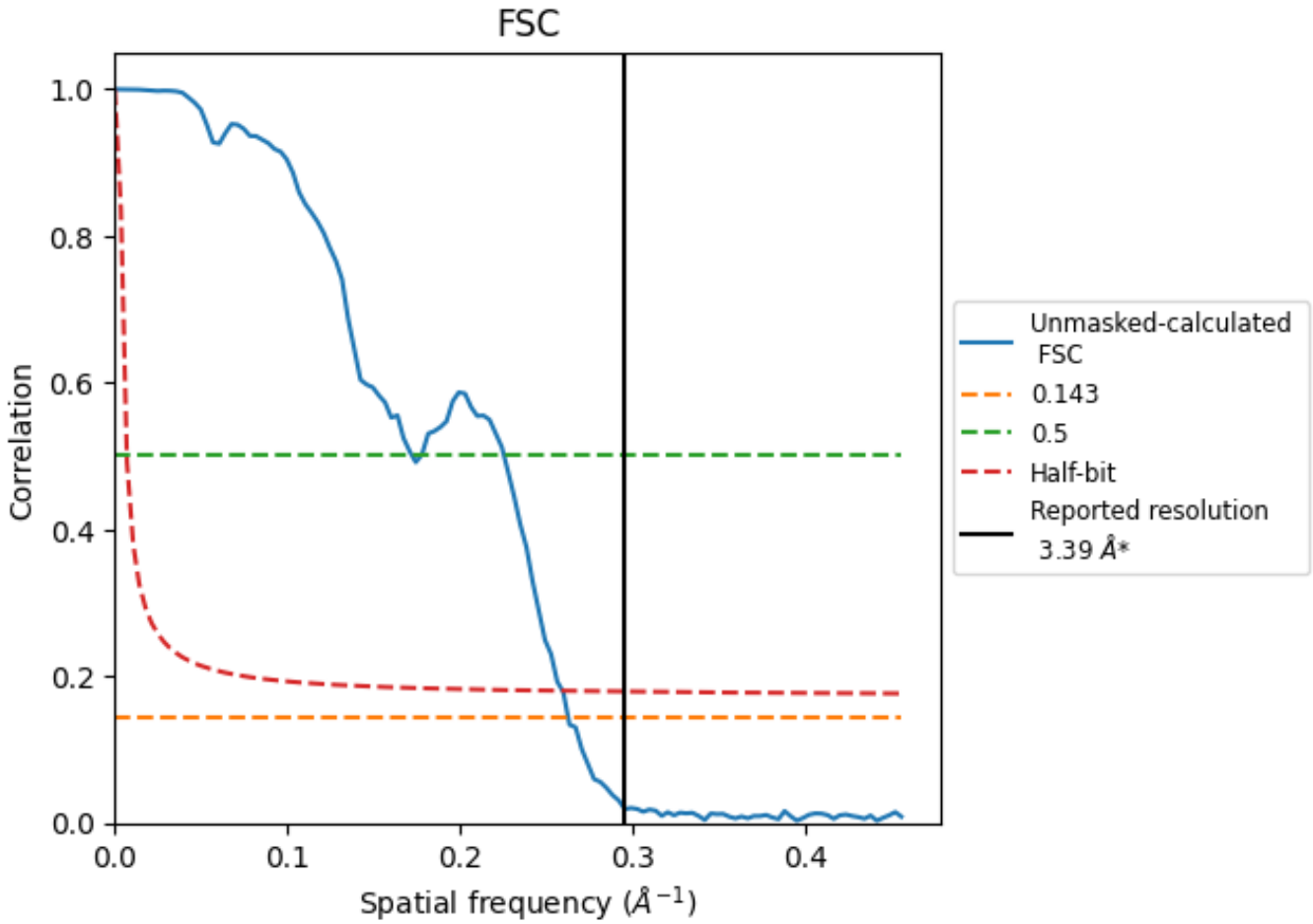


*Reported resolution corresponds to spatial frequency of 0.295 $Å^{-1}$

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 0.295 Å^{-1}

8.2 Resolution estimates (i)

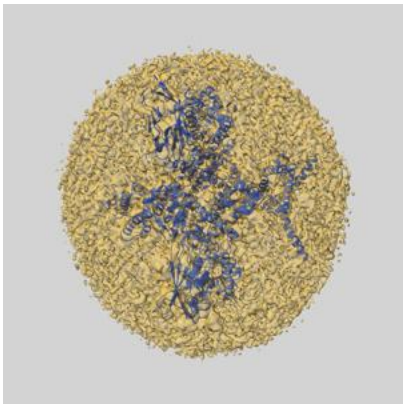
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.39	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.81	5.80	3.86

*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 3.81 differs from the reported value 3.39 by more than 10 %

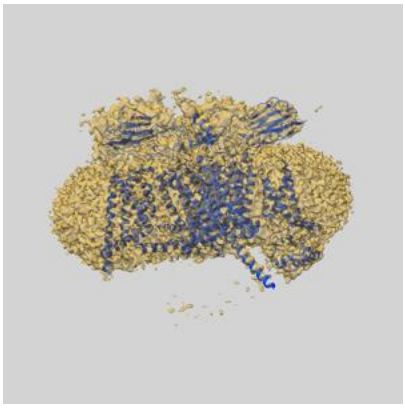
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-38484 and PDB model 8XMO. Per-residue inclusion information can be found in section 3 on page 9.

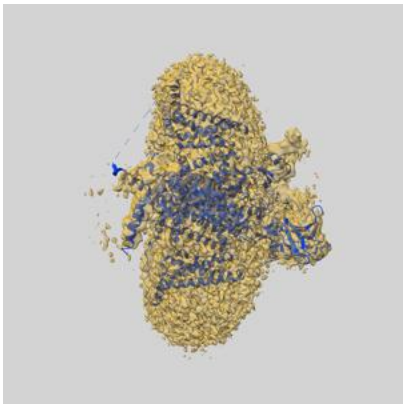
9.1 Map-model overlay



X



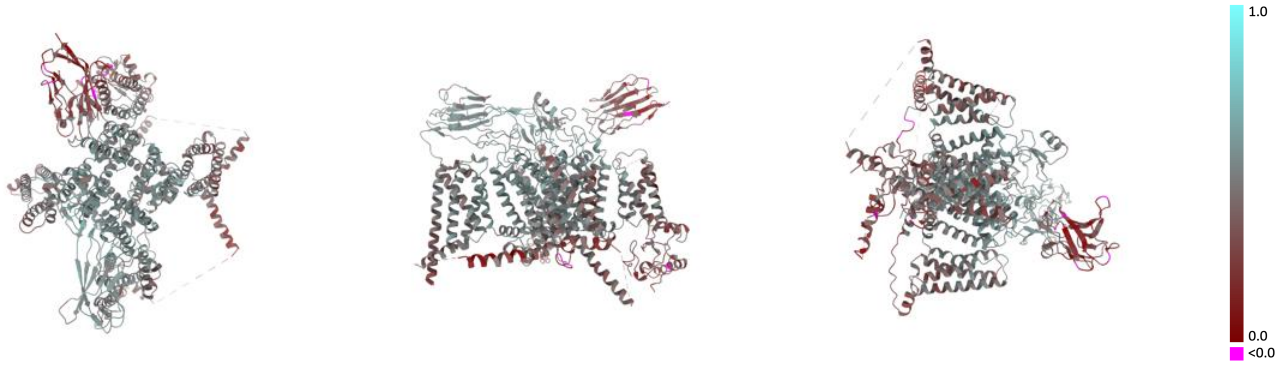
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.25 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.

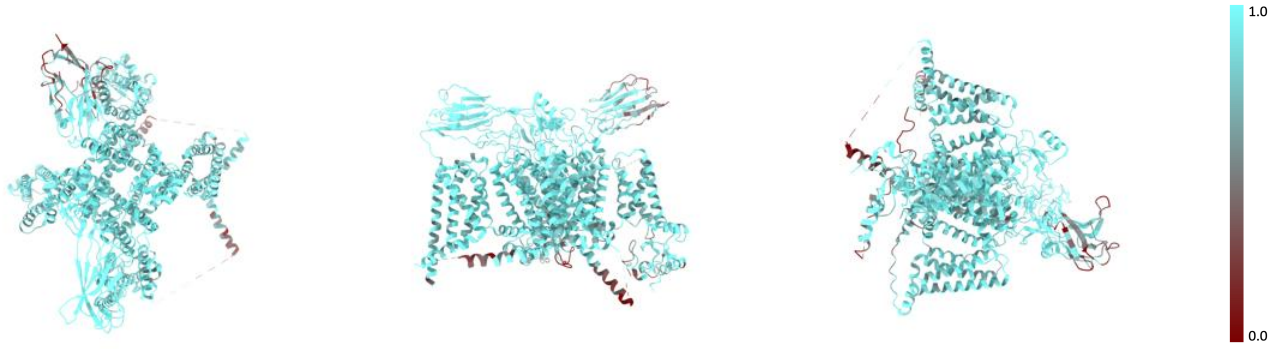
9.2 Q-score mapped to coordinate model (i)



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.

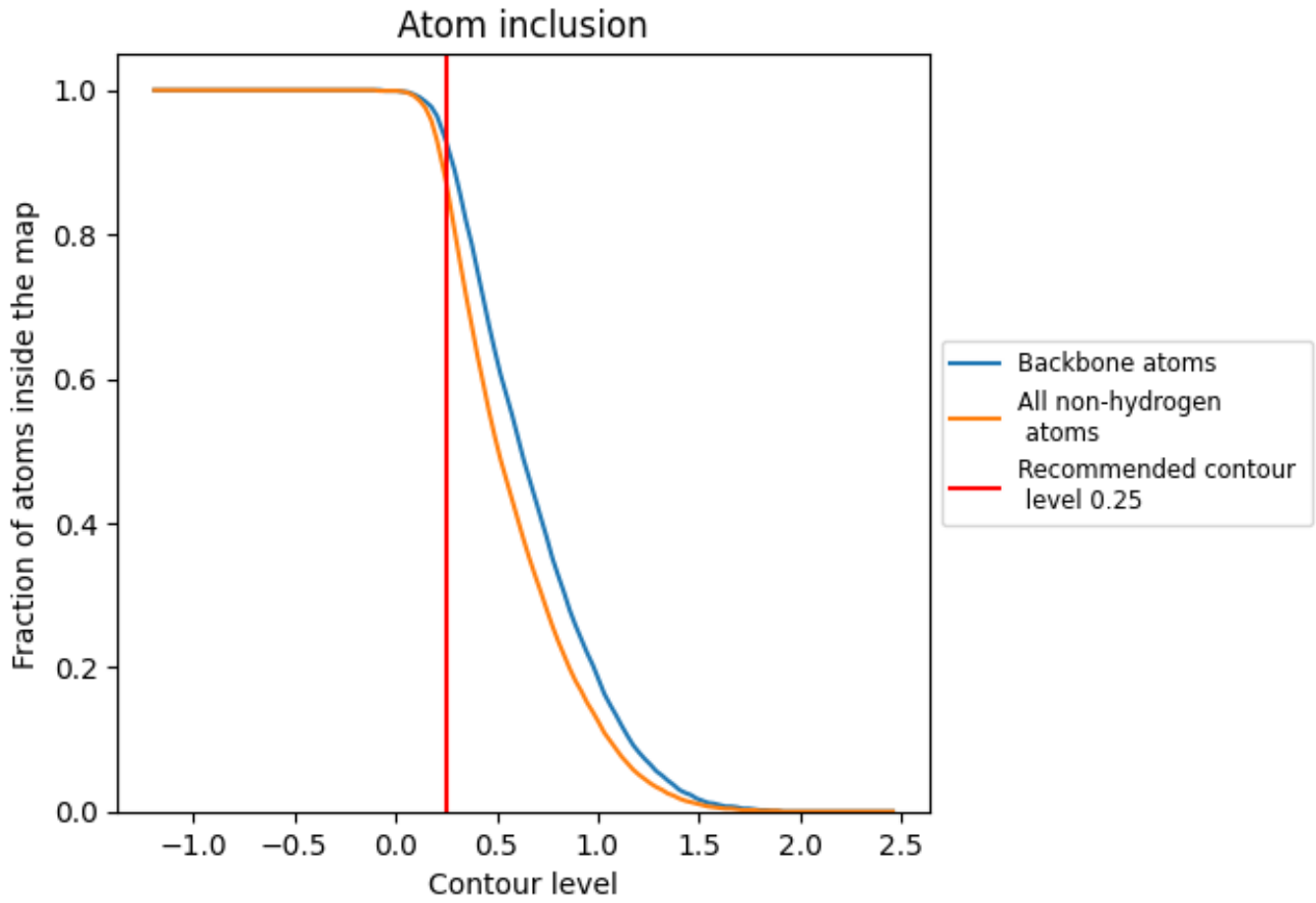
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.25).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 87% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8730	0.4550
A	0.8790	0.4650
B	0.9420	0.4950
C	0.6920	0.2830
D	0.8930	0.5020
E	0.9640	0.4640