Full wwPDB EM Validation Report ⓘ

Nov 21, 2022 – 08:58 AM EST

PDB ID	:	7U1S
EMDB ID	:	EMD-26304
Title	:	Cryo-EM structure of the pancreatic ATP-sensitive potassium channel bound to ATP and repaglinide with SUR1-out conformation
Authors	:	Shyng, S.L.; Sung, M.W.; Driggers, C.M.
Deposited on	:	2022-02-22
Resolution	:	3.80 Å(reported)
Based on initial models	:	6PZ9, 6BAA

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

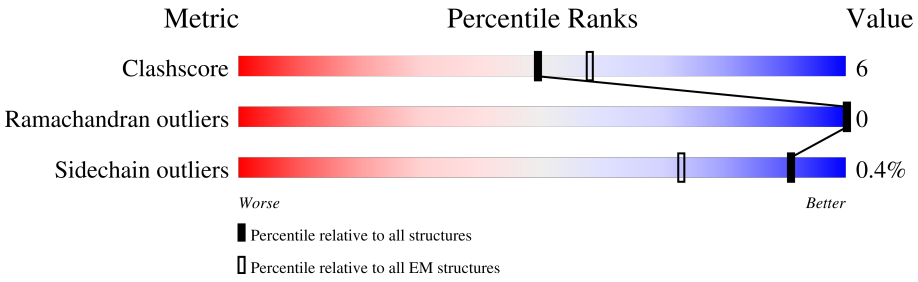
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance

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

The reported resolution of this entry is 3.80 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	390	7%, 74%, 17%, 8%
1	B	390	70%, 15%, 15%
1	C	390	72%, 13%, 15%
1	D	390	69%, 15%, 15%
2	E	1582	12%, 81%, 10%, 9%
3	F	2	100%, 100%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 21225 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 ATP-sensitive inward rectifier potassium channel 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	360	Total	C	N	O	S	0	0
			2641	1701	461	462	17		
1	B	331	Total	C	N	O	S	0	0
			2508	1621	437	433	17		
1	C	332	Total	C	N	O	S	0	0
			2497	1616	434	432	15		
1	D	330	Total	C	N	O	S	0	0
			2485	1612	431	426	16		

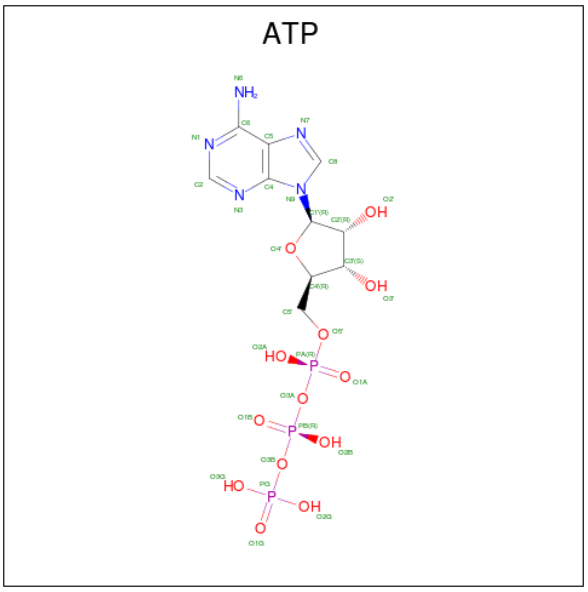
- Molecule 2 is a protein called ATP-binding cassette sub-family C member 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	1439	Total	C	N	O	S	0	0
			10181	6581	1762	1790	48		

- Molecule 3 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
3	F	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).

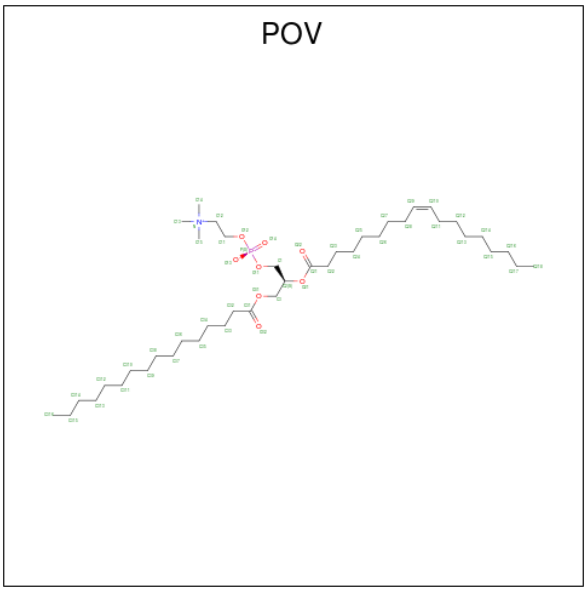


Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			62	20	10	26	6	
4	A	1	Total	C	N	O	P	0
			62	20	10	26	6	
4	C	1	Total	C	N	O	P	0
			62	20	10	26	6	
4	C	1	Total	C	N	O	P	0
			62	20	10	26	6	
4	E	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

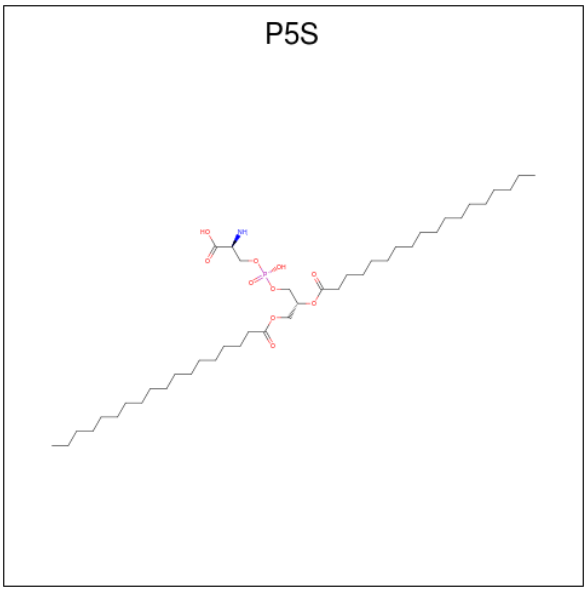
Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	K	0
			1	1	

- Molecule 6 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (three-letter code: POV) (formula: $C_{42}H_{82}NO_8P$).



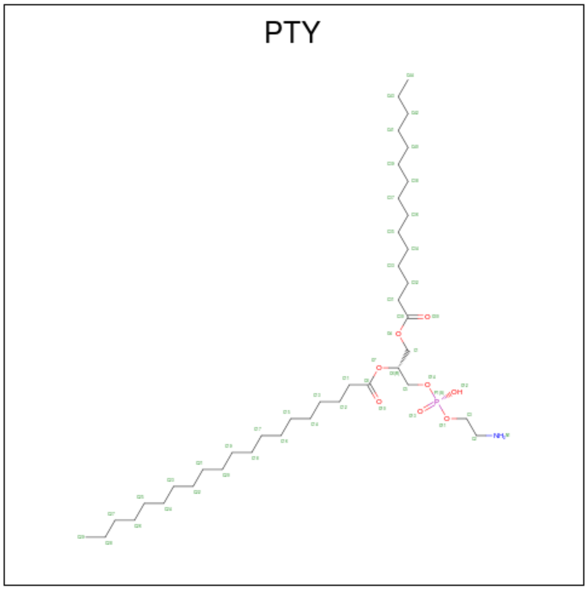
Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			36	26	1	8	1	
6	B	1	Total	C	N	O	P	0
			36	26	1	8	1	
6	C	1	Total	C	N	O	P	0
			36	26	1	8	1	
6	D	1	Total	C	N	O	P	0
			36	26	1	8	1	
6	E	1	Total	C	N	O	P	0
			36	26	1	8	1	

- Molecule 7 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-serine (three-letter code: P5S) (formula: $C_{42}H_{82}NO_{10}P$) (labeled as "Ligand of Interest" by depositor).



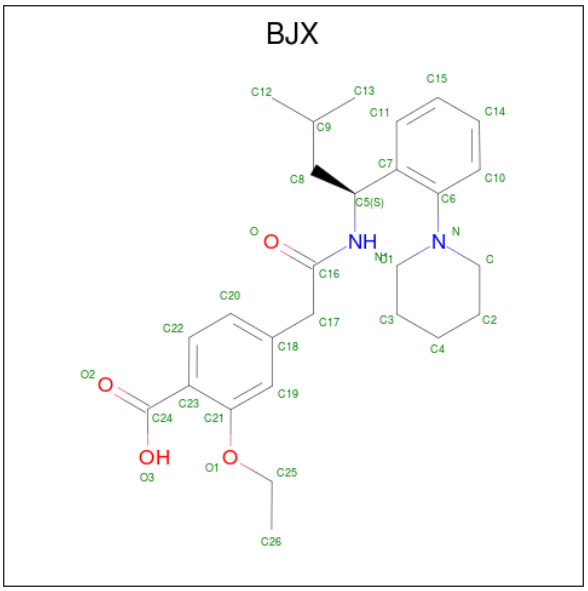
Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	N	O	P	0
			108	84	2	20	2	
7	A	1	Total	C	N	O	P	0
			108	84	2	20	2	
7	B	1	Total	C	N	O	P	0
			54	42	1	10	1	
7	C	1	Total	C	N	O	P	0
			54	42	1	10	1	
7	D	1	Total	C	N	O	P	0
			54	42	1	10	1	
7	E	1	Total	C	N	O	P	0
			54	42	1	10	1	

- Molecule 8 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: $C_{40}H_{80}NO_8P$).



Mol	Chain	Residues	Atoms	AltConf
8	E	1	Total C N O P 192 132 6 48 6	0
8	E	1	Total C N O P 192 132 6 48 6	0
8	E	1	Total C N O P 192 132 6 48 6	0
8	E	1	Total C N O P 192 132 6 48 6	0
8	E	1	Total C N O P 192 132 6 48 6	0
8	E	1	Total C N O P 192 132 6 48 6	0

- Molecule 9 is Repaglinide (three-letter code: BJX) (formula: $C_{27}H_{36}N_2O_4$) (labeled as "Ligand of Interest" by depositor).



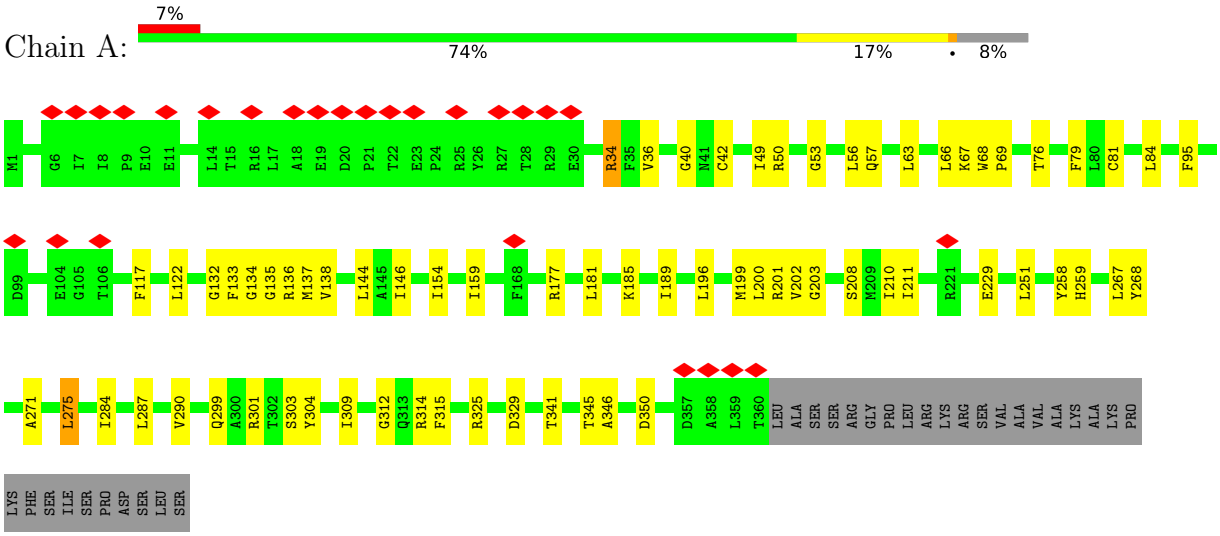
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
9	E	1	33	27	2	4	0

3 Residue-property plots (i)

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

• Molecule 1: ATP-sensitive inward rectifier potassium channel 11

Chain A:

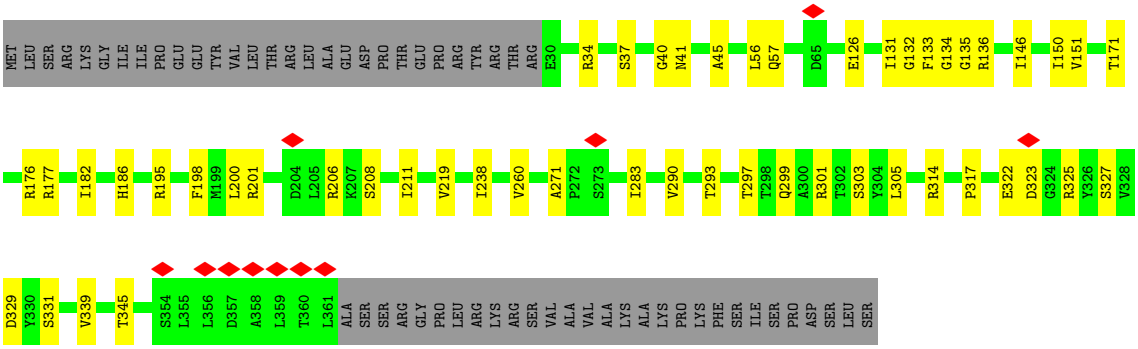


• Molecule 1: ATP-sensitive inward rectifier potassium channel 11

Chain B:

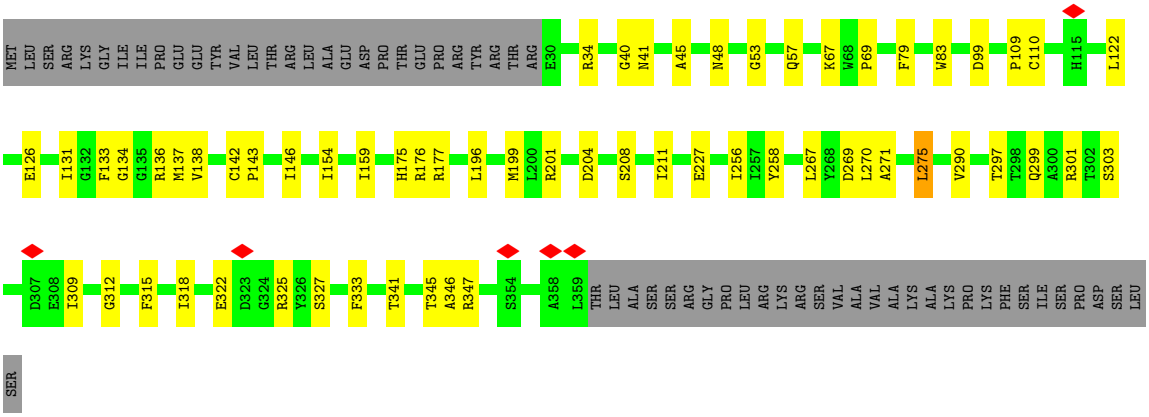
• Molecule 1: ATP-sensitive inward rectifier potassium channel 11

Chain C:



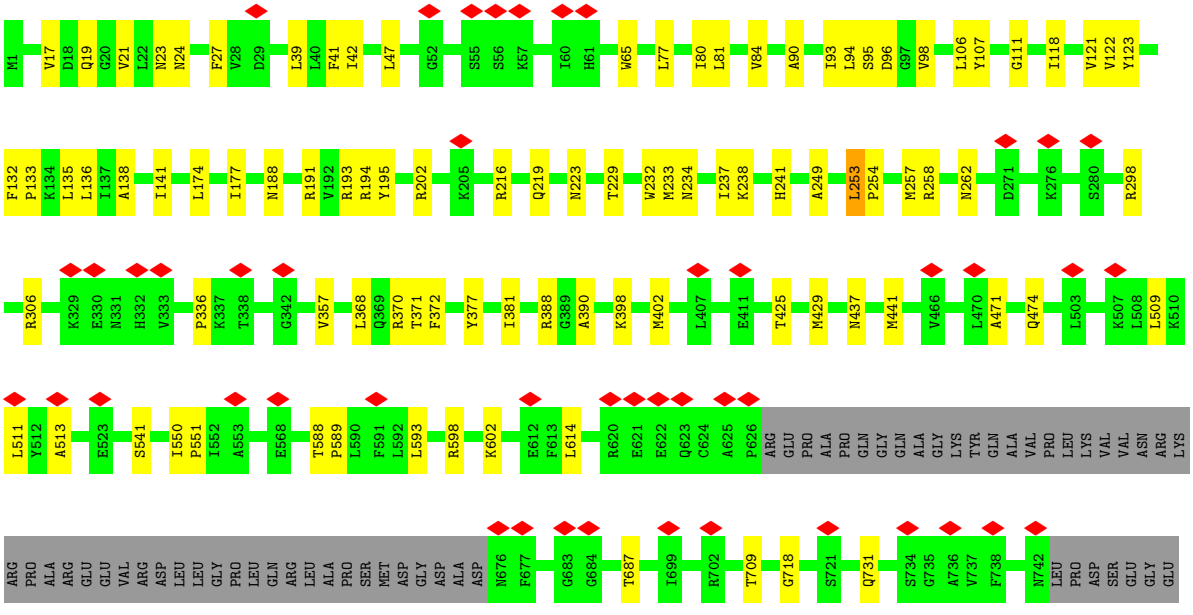
• Molecule 1: ATP-sensitive inward rectifier potassium channel 11

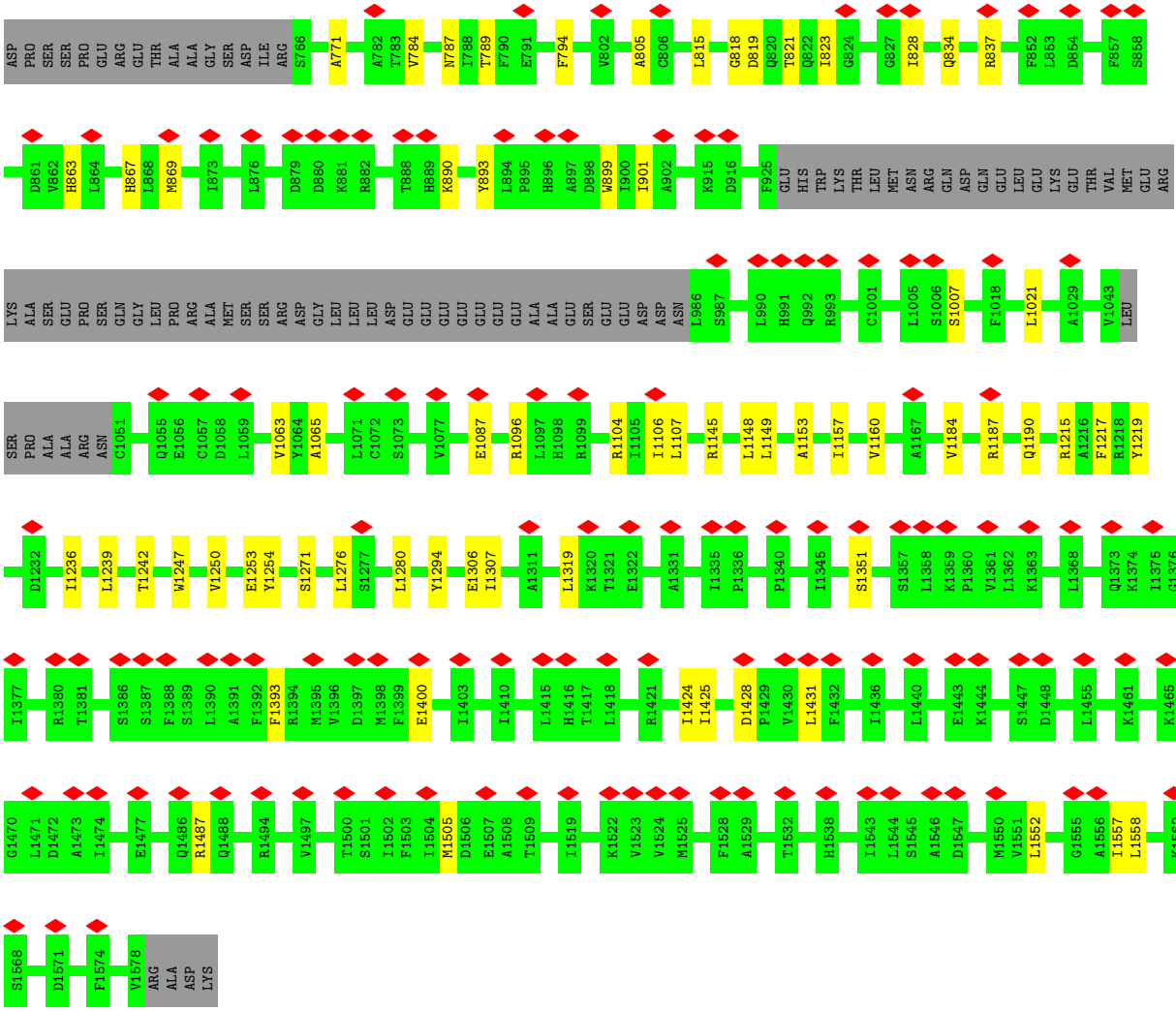
Chain D:



• Molecule 2: ATP-binding cassette sub-family C member 8

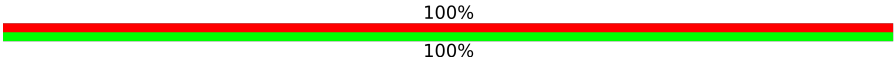
Chain E:





• Molecule 3: 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	28289	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	14.489	Depositor
Minimum map value	-8.835	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1.0	Depositor
Map size (Å)	178.69499, 113.905, 146.29999	wwPDB
Map dimensions	140, 109, 171	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.045, 1.045, 1.045	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PTY, K, POV, BJX, ATP, NAG, P5S

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.24	0/2700	0.48	0/3691
1	B	0.24	0/2565	0.47	0/3496
1	C	0.24	0/2554	0.47	0/3486
1	D	0.24	0/2542	0.47	0/3469
2	E	0.24	0/10395	0.43	0/14237
All	All	0.24	0/20756	0.45	0/28379

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	A	2641	0	2542	56	0
1	B	2508	0	2503	47	0
1	C	2497	0	2457	37	0
1	D	2485	0	2468	43	0
2	E	10181	0	9378	102	0
3	F	28	0	25	0	0
4	A	62	0	24	3	0
4	C	62	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	31	0	12	1	0
5	A	1	0	0	0	0
6	A	36	0	45	3	0
6	B	36	0	45	1	0
6	C	36	0	45	0	0
6	D	36	0	45	0	0
6	E	36	0	45	0	0
7	A	108	0	160	8	0
7	B	54	0	80	5	0
7	C	54	0	80	0	0
7	D	54	0	80	4	0
7	E	54	0	80	4	0
8	E	192	0	222	7	0
9	E	33	0	0	0	0
All	All	21225	0	20360	253	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 6.

All (253) 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:E:238:LYS:HE3	8:E:1607:PTY:HC51	1.64	0.80
1:D:322:GLU:HG3	1:D:327:SER:HB2	1.69	0.75
1:A:299:GLN:HG3	1:B:211:ILE:HG23	1.68	0.74
1:D:312:GLY:HA3	1:D:341:THR:HG21	1.72	0.71
1:C:299:GLN:HG3	1:D:211:ILE:HG23	1.75	0.69
1:A:146:ILE:HG12	1:B:122:LEU:HD21	1.75	0.69
1:D:201:ARG:HH21	1:D:315:PHE:HB3	1.57	0.69
1:A:177:ARG:NH1	1:A:208:SER:OG	2.25	0.68
2:E:1217:PHE:HB2	2:E:1219:TYR:HB2	1.76	0.67
2:E:234:ASN:OD1	2:E:1247:TRP:NE1	2.26	0.67
1:A:201:ARG:HH21	1:A:315:PHE:HB3	1.59	0.66
1:A:122:LEU:HD21	1:D:146:ILE:HG12	1.78	0.65
1:B:214:THR:HG23	1:B:247:ASN:HB3	1.78	0.64
1:C:322:GLU:HG3	1:C:327:SER:HB2	1.79	0.64
2:E:216:ARG:NH1	2:E:249:ALA:O	2.28	0.64
2:E:1431:LEU:HD11	2:E:1487:ARG:HB2	1.79	0.64
1:A:56:LEU:HD21	2:E:135:LEU:HD22	1.81	0.63
1:B:173:GLN:NE2	1:C:293:THR:O	2.31	0.62
1:D:177:ARG:NH1	1:D:208:SER:OG	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:271:ALA:HB2	1:C:345:THR:HG22	1.81	0.62
1:C:146:ILE:HG12	1:D:122:LEU:HD21	1.82	0.62
1:A:329:ASP:OD1	1:D:48:ASN:ND2	2.33	0.61
2:E:253:LEU:HD12	2:E:257:MET:HB3	1.82	0.61
2:E:805:ALA:HB1	2:E:869:MET:HA	1.82	0.61
2:E:81:LEU:HA	2:E:84:VAL:HG22	1.81	0.60
1:A:271:ALA:HB2	1:A:345:THR:HG22	1.81	0.60
1:A:325:ARG:HD2	1:D:45:ALA:HB2	1.83	0.60
1:A:49:ILE:HG12	1:B:330:TYR:HD2	1.67	0.60
1:C:34:ARG:NH2	1:C:303:SER:OG	2.34	0.60
1:D:34:ARG:NH2	1:D:303:SER:OG	2.34	0.60
2:E:371:THR:HG21	7:E:1609:P5S:H48	1.83	0.60
2:E:398:LYS:NZ	2:E:614:LEU:O	2.36	0.59
1:C:126:GLU:OE2	1:C:136:ARG:NH1	2.35	0.59
2:E:834:GLN:HA	2:E:837:ARG:HD2	1.84	0.59
2:E:1007:SER:O	2:E:1096:ARG:NH2	2.36	0.59
1:B:36:VAL:HA	1:B:42:CYS:HA	1.85	0.58
1:C:177:ARG:NH1	1:C:208:SER:OG	2.37	0.58
2:E:17:VAL:HB	2:E:21:VAL:HG12	1.84	0.58
2:E:402:MET:O	2:E:1215:ARG:NH1	2.36	0.58
1:C:57:GLN:HE22	7:D:402:P5S:H1A	1.69	0.57
2:E:19:GLN:O	2:E:23:ASN:ND2	2.33	0.57
1:D:40:GLY:HA2	1:D:301:ARG:HB2	1.87	0.57
2:E:863:HIS:O	2:E:867:HIS:ND1	2.31	0.56
2:E:1104:ARG:NH1	2:E:1319:LEU:O	2.38	0.56
1:D:176:ARG:HH21	7:D:402:P5S:HB	1.70	0.56
1:D:176:ARG:NH2	7:D:402:P5S:O13	2.38	0.56
2:E:372:PHE:HZ	7:E:1609:P5S:H28	1.70	0.56
1:C:37:SER:HB3	1:C:41:ASN:HB3	1.88	0.56
4:A:405:ATP:H1'	1:B:182:ILE:HD12	1.87	0.55
1:B:176:ARG:HH21	7:B:402:P5S:HA	1.71	0.55
2:E:371:THR:HG1	2:E:1254:TYR:HH	1.54	0.55
1:B:299:GLN:HG3	1:C:211:ILE:HG23	1.89	0.55
1:A:67:LYS:HB3	1:A:69:PRO:HD2	1.87	0.54
1:A:211:ILE:HG23	1:D:299:GLN:HG3	1.90	0.54
1:B:58:ASP:HB2	1:C:206:ARG:HH22	1.72	0.54
2:E:229:THR:HA	2:E:1250:VAL:HG11	1.90	0.54
2:E:441:MET:HB3	2:E:593:LEU:HD12	1.89	0.54
7:A:406:P5S:H52A	7:B:402:P5S:H28A	1.88	0.54
1:A:81:CYS:HB3	2:E:41:PHE:HB3	1.90	0.54
1:B:287:LEU:HB3	1:B:300:ALA:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:329:ASP:OD1	1:C:331:SER:OG	2.25	0.53
8:E:1603:PTY:H122	8:E:1605:PTY:H112	1.89	0.53
7:A:406:P5S:H27	7:B:402:P5S:H46A	1.92	0.52
2:E:98:VAL:HG11	2:E:336:PRO:HG3	1.90	0.52
2:E:1351:SER:O	2:E:1400:GLU:N	2.37	0.52
2:E:784:VAL:HG22	2:E:823:ILE:HB	1.89	0.52
1:A:36:VAL:HA	1:A:42:CYS:HA	1.92	0.52
1:B:200:LEU:HD11	1:B:285:VAL:HG21	1.92	0.52
1:C:200:LEU:HD23	1:C:201:ARG:H	1.74	0.52
1:A:211:ILE:HB	1:A:290:VAL:HG23	1.92	0.52
2:E:1190:GLN:HG2	2:E:1307:ILE:HD13	1.91	0.51
7:E:1609:P5S:H20A	7:E:1609:P5S:O47	2.10	0.51
1:B:34:ARG:NH2	1:B:303:SER:O	2.44	0.51
1:B:138:VAL:O	1:C:136:ARG:NH2	2.44	0.51
1:D:211:ILE:HB	1:D:290:VAL:HG13	1.93	0.51
1:D:126:GLU:OE2	1:D:136:ARG:NH1	2.44	0.50
2:E:122:VAL:HG22	8:E:1603:PTY:H112	1.93	0.50
7:A:406:P5S:H3A	2:E:132:PHE:HZ	1.77	0.50
1:D:269:ASP:OD1	1:D:347:ARG:NE	2.39	0.50
1:A:40:GLY:HA2	1:A:301:ARG:HB2	1.94	0.50
6:A:403:POV:H25A	1:D:143:PRO:HB3	1.94	0.50
1:A:138:VAL:O	1:B:136:ARG:NH2	2.41	0.50
2:E:388:ARG:HG2	2:E:425:THR:HG22	1.94	0.49
1:A:68:TRP:HB2	7:A:404:P5S:H3	1.94	0.49
2:E:370:ARG:HD3	2:E:1253:GLU:HB3	1.93	0.49
2:E:1021:LEU:HD23	2:E:1148:LEU:HD21	1.95	0.49
2:E:84:VAL:HG11	2:E:174:LEU:HD22	1.95	0.49
2:E:253:LEU:HB3	2:E:1236:ILE:HD13	1.95	0.49
1:A:117:PHE:N	6:A:403:POV:O14	2.46	0.49
1:C:314:ARG:HE	1:C:339:VAL:HG11	1.78	0.48
7:A:406:P5S:H26A	7:B:402:P5S:H49A	1.94	0.48
1:C:195:ARG:HH21	1:C:260:VAL:HG11	1.78	0.48
1:C:290:VAL:HA	1:C:297:THR:HA	1.95	0.48
1:D:199:MET:HG2	1:D:258:TYR:HB3	1.96	0.48
2:E:298:ARG:HH12	7:E:1609:P5S:H3A	1.77	0.48
1:C:56:LEU:HD13	1:C:57:GLN:N	2.27	0.48
2:E:388:ARG:NE	2:E:429:MET:SD	2.86	0.48
1:A:137:MET:SD	1:B:135:GLY:HA3	2.53	0.48
2:E:257:MET:HG2	2:E:1239:LEU:HD11	1.95	0.48
2:E:687:THR:N	2:E:731:GLN:O	2.46	0.48
2:E:890:LYS:HZ2	2:E:893:TYR:H	1.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:GLY:HA3	1:A:341:THR:HG21	1.96	0.48
1:D:41:ASN:H	1:D:301:ARG:HH21	1.61	0.48
1:B:107:ASN:OD1	1:B:108:VAL:N	2.47	0.47
1:C:150:ILE:HG23	1:D:83:TRP:HZ3	1.79	0.47
2:E:94:LEU:HD12	2:E:357:VAL:HG21	1.96	0.47
1:A:202:VAL:HG21	1:A:287:LEU:HD22	1.96	0.47
2:E:718:GLY:N	4:E:1610:ATP:O2A	2.47	0.47
1:A:63:LEU:HA	1:A:66:LEU:HD12	1.96	0.47
1:B:177:ARG:NH1	1:B:208:SER:OG	2.47	0.47
1:B:126:GLU:OE2	1:B:136:ARG:NH1	2.47	0.47
1:B:288:GLU:HG2	1:B:299:GLN:HG2	1.96	0.47
1:C:45:ALA:HB2	1:D:325:ARG:HD2	1.96	0.47
1:D:201:ARG:NH1	1:D:333:PHE:O	2.47	0.47
1:D:318:ILE:HD12	1:D:333:PHE:HA	1.96	0.47
1:B:30:GLU:N	1:C:323:ASP:O	2.48	0.47
2:E:511:LEU:HB3	2:E:1424:ILE:HD13	1.97	0.47
1:B:67:LYS:HB3	1:B:69:PRO:HD2	1.97	0.47
2:E:789:THR:HG21	2:E:794:PHE:HD1	1.80	0.47
1:A:275:LEU:HD21	1:A:309:ILE:HB	1.97	0.46
1:B:134:GLY:HA3	1:C:133:PHE:O	2.15	0.46
1:B:293:THR:OG1	1:B:294:THR:N	2.48	0.46
2:E:550:ILE:HG13	2:E:551:PRO:HD3	1.98	0.46
1:A:134:GLY:HA3	1:B:133:PHE:O	2.15	0.46
1:B:117:PHE:HB3	6:B:401:POV:H1A	1.97	0.46
1:B:202:VAL:HG21	1:B:287:LEU:HD22	1.98	0.46
1:A:136:ARG:NH2	1:D:138:VAL:O	2.49	0.46
1:B:112:THR:OG1	1:B:137:MET:N	2.44	0.46
1:B:216:HIS:HB2	1:B:286:ILE:HB	1.97	0.46
1:D:196:LEU:HD23	1:D:346:ALA:HB2	1.98	0.46
2:E:65:TRP:HE1	8:E:1605:PTY:HC22	1.81	0.46
2:E:39:LEU:HA	2:E:42:ILE:HG22	1.98	0.46
1:A:117:PHE:HB3	6:A:403:POV:H1A	1.98	0.46
1:A:132:GLY:HA3	1:B:131:ILE:O	2.16	0.46
1:B:137:MET:SD	1:C:135:GLY:HA3	2.56	0.46
1:C:40:GLY:HA2	1:C:301:ARG:HB2	1.98	0.45
1:D:275:LEU:HD21	1:D:309:ILE:HB	1.99	0.45
1:D:290:VAL:HA	1:D:297:THR:HA	1.97	0.45
2:E:107:TYR:O	2:E:111:GLY:N	2.41	0.45
2:E:1145:ARG:HG3	2:E:1145:ARG:HH11	1.82	0.45
1:C:151:VAL:HG22	7:D:402:P5S:H35	1.99	0.45
1:C:200:LEU:HD23	1:C:201:ARG:N	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:241:HIS:HA	2:E:1184:VAL:HG11	1.98	0.45
1:A:268:TYR:OH	1:A:350:ASP:OD2	2.35	0.45
1:B:290:VAL:HA	1:B:297:THR:HA	1.99	0.45
1:A:95:PHE:HE2	2:E:27:PHE:HA	1.82	0.45
1:B:60:PHE:CE2	1:C:171:THR:HG22	2.52	0.45
2:E:541:SER:HB3	2:E:1087:GLU:HG3	1.99	0.45
2:E:1552:LEU:HA	2:E:1557:ILE:HA	1.99	0.45
2:E:377:TYR:O	2:E:381:ILE:HG12	2.16	0.45
1:A:36:VAL:HG22	1:A:284:ILE:HD12	1.99	0.45
2:E:93:ILE:HD12	8:E:1606:PTY:H321	1.99	0.45
1:A:189:ILE:HG22	1:A:196:LEU:HD11	1.99	0.44
1:B:220:VAL:HG22	1:B:235:GLN:HG2	1.99	0.44
2:E:133:PRO:HB2	2:E:195:TYR:CZ	2.52	0.44
2:E:90:ALA:HA	8:E:1606:PTY:H131	1.99	0.44
1:A:79:PHE:HE1	1:A:159:ILE:HG22	1.82	0.44
2:E:77:LEU:O	2:E:80:ILE:HG13	2.18	0.44
2:E:133:PRO:HG3	2:E:193:ARG:HE	1.82	0.44
1:A:76:THR:HG23	1:D:154:ILE:HD13	1.99	0.44
1:A:181:LEU:HD21	1:A:210:ILE:HD12	1.99	0.44
2:E:96:ASP:HB3	2:E:106:LEU:HD12	1.98	0.44
1:A:84:LEU:HD22	2:E:41:PHE:CE2	2.53	0.44
2:E:1160:VAL:HG22	2:E:1280:LEU:HB3	1.99	0.44
2:E:1393:PHE:CZ	2:E:1424:ILE:HD12	2.52	0.44
1:D:79:PHE:HE1	1:D:159:ILE:HG22	1.83	0.44
2:E:471:ALA:O	2:E:474:GLN:HG2	2.17	0.44
2:E:815:LEU:HB2	2:E:818:GLY:HA2	2.00	0.44
2:E:1149:LEU:HD23	2:E:1294:TYR:CZ	2.53	0.44
1:A:144:LEU:HD21	8:E:1601:PTY:H142	2.00	0.44
2:E:1063:VAL:HG22	2:E:1065:ALA:H	1.83	0.44
1:B:132:GLY:HA3	1:C:131:ILE:O	2.18	0.43
2:E:188:ASN:OD1	2:E:191:ARG:NH2	2.50	0.43
2:E:306:ARG:NH1	2:E:437:ASN:OD1	2.50	0.43
1:A:135:GLY:HA3	1:D:137:MET:SD	2.57	0.43
2:E:138:ALA:O	2:E:141:ILE:HG13	2.17	0.43
1:A:50:ARG:H	4:A:405:ATP:HN62	1.67	0.43
1:D:67:LYS:HB3	1:D:69:PRO:HD2	2.00	0.43
2:E:821:THR:HB	2:E:828:ILE:HG13	2.00	0.43
1:D:110:CYS:SG	1:D:142:CYS:N	2.86	0.43
1:D:201:ARG:HE	1:D:256:ILE:HD11	1.83	0.43
2:E:133:PRO:O	2:E:136:LEU:HG	2.18	0.43
7:A:404:P5S:H33	7:A:404:P5S:H30	1.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ILE:HG12	1:B:330:TYR:CD2	2.50	0.43
1:A:199:MET:HG2	1:A:258:TYR:HB3	2.01	0.43
2:E:219:GLN:HG2	2:E:232:TRP:HE1	1.83	0.43
1:A:200:LEU:HD23	1:A:201:ARG:N	2.34	0.42
1:B:232:PRO:HD3	1:C:317:PRO:HB3	2.02	0.42
2:E:381:ILE:HG21	2:E:1242:THR:HG21	2.02	0.42
1:D:177:ARG:NH2	1:D:204:ASP:OD2	2.52	0.42
2:E:254:PRO:O	2:E:258:ARG:HG3	2.19	0.42
2:E:709:THR:HG22	2:E:901:ILE:HG22	2.02	0.42
2:E:1187:ARG:HD3	2:E:1306:GLU:HG2	1.99	0.42
1:A:229:GLU:HG3	1:B:192:ARG:HE	1.84	0.42
1:B:68:TRP:CD1	7:B:402:P5S:H3	2.55	0.42
1:C:322:GLU:N	1:C:325:ARG:O	2.40	0.42
2:E:24:ASN:O	2:E:27:PHE:N	2.53	0.42
2:E:223:ASN:N	2:E:223:ASN:OD1	2.50	0.42
1:B:198:PHE:CE2	1:B:283:ILE:HG21	2.55	0.42
2:E:1106:ILE:HG22	2:E:1107:LEU:HD23	2.01	0.42
2:E:1428:ASP:O	2:E:1487:ARG:NH1	2.46	0.42
7:A:406:P5S:H33	7:A:406:P5S:H30A	1.89	0.42
2:E:95:SER:O	2:E:98:VAL:HG12	2.19	0.42
2:E:771:ALA:HA	2:E:1217:PHE:CE1	2.54	0.42
2:E:819:ASP:N	2:E:819:ASP:OD1	2.51	0.42
1:B:58:ASP:HB3	1:B:61:THR:HB	2.01	0.42
1:C:219:VAL:HG23	1:C:238:ILE:HG13	2.02	0.42
2:E:1271:SER:HA	2:E:1276:LEU:H	1.85	0.42
1:B:36:VAL:HG23	1:B:303:SER:HB3	2.01	0.42
1:C:134:GLY:HA3	1:D:133:PHE:O	2.19	0.42
2:E:1153:ALA:O	2:E:1157:ILE:HG12	2.19	0.42
1:A:34:ARG:NH2	1:A:303:SER:O	2.53	0.42
1:A:201:ARG:NH2	1:A:315:PHE:HB3	2.30	0.42
1:A:84:LEU:HD22	2:E:41:PHE:HE2	1.85	0.41
2:E:262:ASN:HB3	2:E:390:ALA:HB2	2.01	0.41
2:E:233:MET:O	2:E:237:ILE:HG12	2.19	0.41
2:E:588:THR:HB	2:E:589:PRO:HD3	2.01	0.41
1:C:182:ILE:HD13	1:C:182:ILE:HA	1.94	0.41
1:A:185:LYS:HB2	4:A:401:ATP:H5'2	2.02	0.41
1:D:271:ALA:HB2	1:D:345:THR:HG22	2.01	0.41
2:E:174:LEU:O	2:E:177:ILE:HG13	2.21	0.41
2:E:509:LEU:O	2:E:513:ALA:N	2.53	0.41
2:E:550:ILE:N	2:E:551:PRO:HD2	2.34	0.41
7:A:406:P5S:H23	7:A:406:P5S:H26	1.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:ASP:HB2	1:B:109:PRO:HB3	2.01	0.41
1:C:132:GLY:HA3	1:D:131:ILE:O	2.19	0.41
1:A:181:LEU:HD13	1:A:287:LEU:HD23	2.02	0.41
1:B:112:THR:HG1	1:B:137:MET:H	1.66	0.41
2:E:368:LEU:HD13	2:E:368:LEU:HA	1.97	0.41
1:A:314:ARG:NH2	1:D:227:GLU:O	2.53	0.41
1:C:198:PHE:CE2	1:C:283:ILE:HG21	2.56	0.41
1:D:99:ASP:HB2	1:D:109:PRO:HB3	2.02	0.41
2:E:598:ARG:HG2	2:E:602:LYS:HE3	2.02	0.41
1:B:199:MET:HG2	1:B:258:TYR:HB3	2.02	0.41
1:B:220:VAL:HG12	1:B:233:LEU:HD22	2.03	0.41
1:D:267:LEU:HD22	1:D:270:LEU:HD11	2.03	0.41
2:E:47:LEU:HD21	2:E:123:TYR:HA	2.02	0.41
2:E:194:ARG:HD2	2:E:202:ARG:NH1	2.36	0.41
2:E:1106:ILE:HD13	2:E:1106:ILE:HA	1.95	0.41
1:A:154:ILE:HG23	1:B:75:PHE:HE2	1.86	0.41
1:A:133:PHE:O	1:D:134:GLY:HA3	2.22	0.40
1:A:203:GLY:HA2	1:A:251:LEU:HD21	2.03	0.40
1:C:34:ARG:NH1	1:C:305:LEU:HD23	2.36	0.40
1:A:53:GLY:O	1:A:57:GLN:HG3	2.20	0.40
1:A:259:HIS:HD2	1:A:267:LEU:HD12	1.85	0.40
1:A:268:TYR:O	1:A:346:ALA:HB3	2.21	0.40
2:E:194:ARG:HD2	2:E:202:ARG:HH12	1.86	0.40
1:A:200:LEU:HD11	1:A:304:TYR:CE2	2.56	0.40
2:E:1425:ILE:HG12	2:E:1505:MET:HA	2.03	0.40
2:E:1552:LEU:HA	2:E:1558:LEU:H	1.86	0.40
1:D:53:GLY:O	1:D:57:GLN:N	2.46	0.40
2:E:118:ILE:O	2:E:121:VAL:HG12	2.21	0.40
2:E:709:THR:HA	2:E:899:TRP:O	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	358/390 (92%)	348 (97%)	10 (3%)	0	100	100
1	B	329/390 (84%)	314 (95%)	15 (5%)	0	100	100
1	C	330/390 (85%)	309 (94%)	21 (6%)	0	100	100
1	D	328/390 (84%)	308 (94%)	20 (6%)	0	100	100
2	E	1429/1582 (90%)	1340 (94%)	89 (6%)	0	100	100
All	All	2774/3142 (88%)	2619 (94%)	155 (6%)	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	A	263/341 (77%)	261 (99%)	2 (1%)	81	89
1	B	265/341 (78%)	265 (100%)	0	100	100
1	C	257/341 (75%)	255 (99%)	2 (1%)	81	89
1	D	258/341 (76%)	256 (99%)	2 (1%)	81	89
2	E	909/1373 (66%)	907 (100%)	2 (0%)	93	97
All	All	1952/2737 (71%)	1944 (100%)	8 (0%)	91	95

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ARG
1	A	275	LEU
1	C	176	ARG
1	C	186	HIS
1	D	175	HIS
1	D	275	LEU
2	E	253	LEU
2	E	787	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such

sidechains are listed below:

Mol	Chain	Res	Type
1	C	57	GLN
2	E	1245	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

2 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	$\#\|Z\| > 2$
3	NAG	F	1	2,3	14,14,15	0.56	0	17,19,21	0.57	0
3	NAG	F	2	3	14,14,15	0.29	0	17,19,21	0.42	0

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

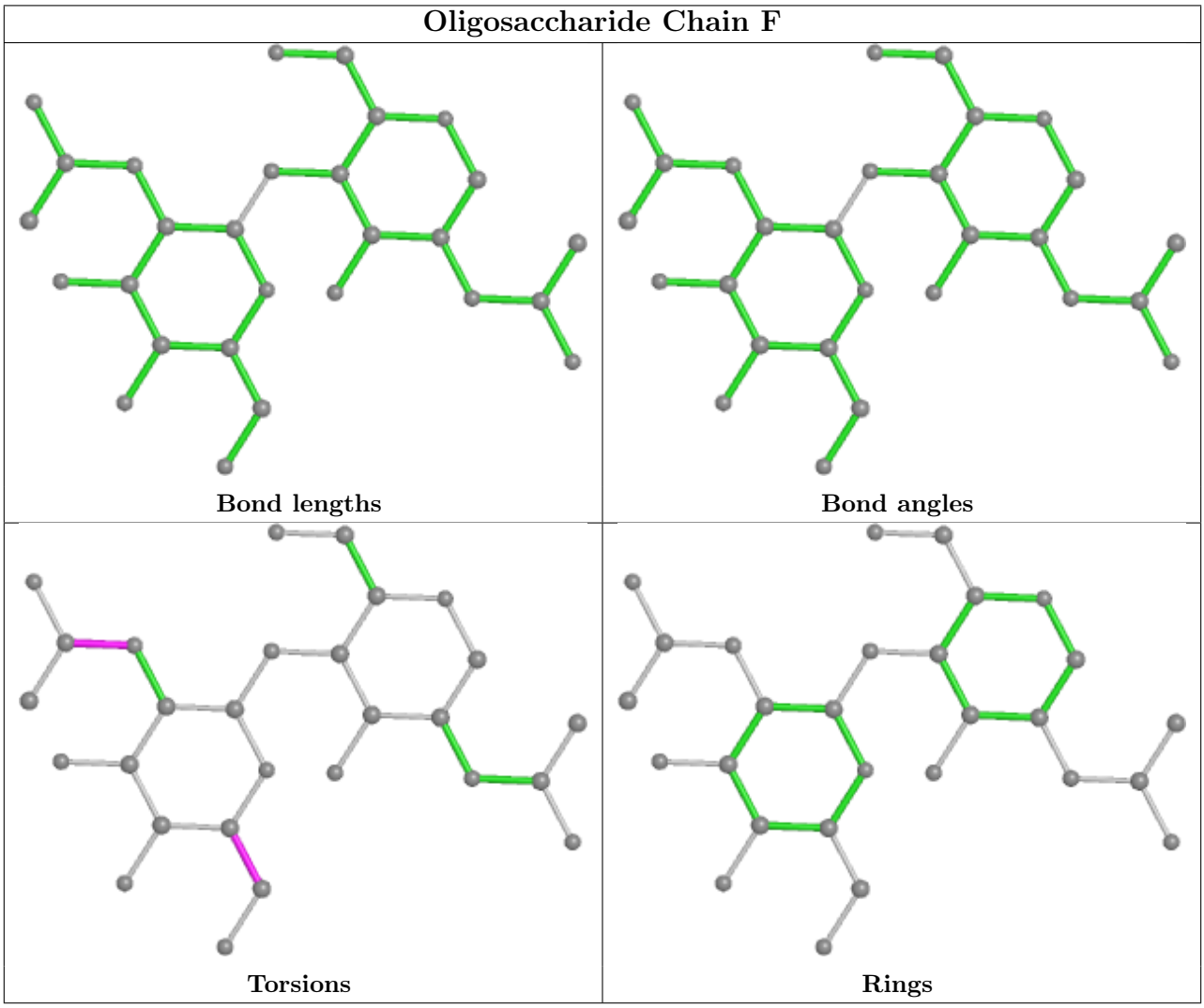
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	2	NAG	C8-C7-N2-C2
3	F	2	NAG	O7-C7-N2-C2
3	F	2	NAG	O5-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.



5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 1 is monoatomic - leaving 23 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	$\#\|Z\| > 2$
6	POV	E	1604	-	35,35,51	0.60	0	41,43,59	0.54	0
4	ATP	A	401	-	26,33,33	0.59	0	31,52,52	0.75	2 (6%)
7	P5S	E	1609	-	52,53,53	0.52	0	56,60,60	0.86	1 (1%)
8	PTY	E	1603	-	31,31,49	0.56	0	34,36,54	0.50	0
7	P5S	A	404	-	52,53,53	0.52	0	56,60,60	0.92	1 (1%)
4	ATP	E	1610	-	26,33,33	0.60	0	31,52,52	0.73	2 (6%)
6	POV	D	401	-	35,35,51	0.59	0	41,43,59	0.49	0
7	P5S	B	402	-	52,53,53	0.53	0	56,60,60	0.93	1 (1%)
7	P5S	A	406	-	52,53,53	0.52	0	56,60,60	0.90	1 (1%)
6	POV	B	401	-	35,35,51	0.59	0	41,43,59	0.53	0
4	ATP	A	405	-	26,33,33	0.60	0	31,52,52	0.73	2 (6%)
8	PTY	E	1607	-	31,31,49	0.57	0	34,36,54	0.55	0
8	PTY	E	1606	-	31,31,49	0.58	0	34,36,54	0.39	0
6	POV	A	403	-	35,35,51	0.60	0	41,43,59	0.53	0
7	P5S	C	403	-	52,53,53	0.53	0	56,60,60	0.79	1 (1%)
4	ATP	C	404	-	26,33,33	0.60	0	31,52,52	0.73	2 (6%)
7	P5S	D	402	-	52,53,53	0.53	0	56,60,60	0.79	1 (1%)
4	ATP	C	401	-	26,33,33	0.60	0	31,52,52	0.74	2 (6%)
8	PTY	E	1608	-	31,31,49	0.56	0	34,36,54	0.43	0
6	POV	C	402	-	35,35,51	0.59	0	41,43,59	0.50	0
8	PTY	E	1601	-	31,31,49	0.56	0	34,36,54	0.43	0
9	BJX	E	1602	-	35,35,35	2.94	15 (42%)	47,47,47	1.62	8 (17%)
8	PTY	E	1605	-	31,31,49	0.55	0	34,36,54	0.55	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	POV	E	1604	-	-	15/39/39/55	-
4	ATP	A	401	-	-	6/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	P5S	E	1609	-	-	28/59/59/59	-
8	PTY	E	1603	-	-	19/35/35/53	-
7	P5S	A	404	-	-	27/59/59/59	-
4	ATP	E	1610	-	-	4/18/38/38	0/3/3/3
6	POV	D	401	-	-	12/39/39/55	-
7	P5S	B	402	-	-	30/59/59/59	-
7	P5S	A	406	-	-	26/59/59/59	-
6	POV	B	401	-	-	15/39/39/55	-
4	ATP	A	405	-	-	6/18/38/38	0/3/3/3
8	PTY	E	1607	-	-	16/35/35/53	-
8	PTY	E	1606	-	-	14/35/35/53	-
6	POV	A	403	-	-	10/39/39/55	-
7	P5S	C	403	-	-	19/59/59/59	-
4	ATP	C	404	-	-	6/18/38/38	0/3/3/3
7	P5S	D	402	-	-	21/59/59/59	-
4	ATP	C	401	-	-	6/18/38/38	0/3/3/3
8	PTY	E	1608	-	-	15/35/35/53	-
6	POV	C	402	-	-	6/39/39/55	-
8	PTY	E	1601	-	-	14/35/35/53	-
9	BJX	E	1602	-	-	19/27/35/35	0/3/3/3
8	PTY	E	1605	-	-	19/35/35/53	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	E	1602	BJX	C8-C5	8.32	1.61	1.53
9	E	1602	BJX	C7-C5	6.54	1.62	1.52
9	E	1602	BJX	C6-C7	5.78	1.46	1.40
9	E	1602	BJX	C16-N1	5.60	1.46	1.34
9	E	1602	BJX	C6-N	4.80	1.51	1.41
9	E	1602	BJX	C5-N1	3.48	1.51	1.46
9	E	1602	BJX	C1-N	3.22	1.51	1.46
9	E	1602	BJX	C23-C24	3.04	1.56	1.49
9	E	1602	BJX	C17-C18	3.01	1.56	1.51
9	E	1602	BJX	O1-C21	2.66	1.42	1.37
9	E	1602	BJX	C-N	2.51	1.50	1.46
9	E	1602	BJX	C19-C18	2.22	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	E	1602	BJX	C19-C21	2.20	1.42	1.38
9	E	1602	BJX	C11-C7	2.15	1.42	1.39
9	E	1602	BJX	O2-C24	2.12	1.29	1.22

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	404	P5S	OG-CB-CA	5.41	112.78	108.06
7	B	402	P5S	OG-CB-CA	5.32	112.69	108.06
7	A	406	P5S	OG-CB-CA	5.11	112.52	108.06
9	E	1602	BJX	C17-C16-N1	4.86	123.71	115.88
7	C	403	P5S	OG-CB-CA	4.27	111.78	108.06
7	D	402	P5S	OG-CB-CA	4.17	111.69	108.06
7	E	1609	P5S	OG-CB-CA	4.01	111.55	108.06
9	E	1602	BJX	C7-C6-N	3.45	124.72	119.32
9	E	1602	BJX	C10-C6-N	-3.29	117.05	122.30
9	E	1602	BJX	O-C16-N1	-3.12	117.69	122.95
9	E	1602	BJX	C-N-C1	-2.84	105.24	111.52
4	E	1610	ATP	C5-C6-N6	2.30	123.85	120.35
4	C	401	ATP	C5-C6-N6	2.30	123.84	120.35
4	A	401	ATP	C5-C6-N6	2.29	123.84	120.35
4	C	404	ATP	C5-C6-N6	2.29	123.83	120.35
4	A	405	ATP	C5-C6-N6	2.29	123.83	120.35
9	E	1602	BJX	C5-N1-C16	2.25	126.91	123.33
9	E	1602	BJX	C14-C10-C6	2.11	122.68	118.26
4	C	401	ATP	PB-O3B-PG	2.06	139.90	132.83
9	E	1602	BJX	C1-N-C6	-2.06	111.39	116.27
4	C	404	ATP	PB-O3B-PG	2.05	139.88	132.83
4	A	405	ATP	PB-O3B-PG	2.05	139.86	132.83
4	E	1610	ATP	PB-O3B-PG	2.04	139.84	132.83
4	A	401	ATP	PB-O3B-PG	2.04	139.82	132.83

There are no chirality outliers.

All (353) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	401	ATP	C5'-O5'-PA-O1A
4	A	401	ATP	C5'-O5'-PA-O2A
4	A	405	ATP	C5'-O5'-PA-O3A
4	A	405	ATP	O4'-C4'-C5'-O5'
4	A	405	ATP	C3'-C4'-C5'-O5'
4	C	401	ATP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
4	C	401	ATP	O4'-C4'-C5'-O5'
4	C	401	ATP	C3'-C4'-C5'-O5'
4	C	404	ATP	PB-O3B-PG-O3G
4	C	404	ATP	C5'-O5'-PA-O1A
4	C	404	ATP	C5'-O5'-PA-O2A
4	C	404	ATP	C5'-O5'-PA-O3A
4	E	1610	ATP	PB-O3B-PG-O3G
4	E	1610	ATP	C5'-O5'-PA-O3A
6	A	403	POV	O12-C11-C12-N
6	B	401	POV	C1-O11-P-O14
6	B	401	POV	O21-C2-C3-O31
6	C	402	POV	C11-O12-P-O11
6	D	401	POV	C11-O12-P-O14
6	E	1604	POV	C11-O12-P-O14
7	A	404	P5S	O-C-CA-N
7	A	404	P5S	O19-C1-C2-O37
7	A	404	P5S	N-CA-CB-OG
7	A	404	P5S	C3-O16-P12-O13
7	A	406	P5S	O-C-CA-N
7	A	406	P5S	O-C-CA-CB
7	A	406	P5S	OXT-C-CA-CB
7	A	406	P5S	C-CA-CB-OG
7	A	406	P5S	N-CA-CB-OG
7	B	402	P5S	C-CA-CB-OG
7	B	402	P5S	N-CA-CB-OG
7	B	402	P5S	CB-OG-P12-O15
7	C	403	P5S	C3-O16-P12-O15
7	D	402	P5S	C-CA-CB-OG
7	E	1609	P5S	O-C-CA-CB
7	E	1609	P5S	OXT-C-CA-CB
7	E	1609	P5S	C-CA-CB-OG
7	E	1609	P5S	N-CA-CB-OG
7	E	1609	P5S	C3-O16-P12-OG
7	E	1609	P5S	C3-O16-P12-O13
7	E	1609	P5S	C3-O16-P12-O15
8	E	1603	PTY	C11-C8-O7-C6
8	E	1603	PTY	C3-O11-P1-O12
8	E	1603	PTY	C3-O11-P1-O13
8	E	1603	PTY	C3-O11-P1-O14
8	E	1605	PTY	N1-C2-C3-O11
8	E	1605	PTY	C5-O14-P1-O11
8	E	1605	PTY	C5-O14-P1-O12

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Mol	Chain	Res	Type	Atoms
8	E	1605	PTY	C5-O14-P1-O13
8	E	1606	PTY	N1-C2-C3-O11
8	E	1607	PTY	C3-O11-P1-O14
8	E	1607	PTY	C5-O14-P1-O12
8	E	1608	PTY	C3-O11-P1-O13
9	E	1602	BJX	C7-C5-C8-C9
9	E	1602	BJX	C8-C5-N1-C16
7	D	402	P5S	O18-C17-O19-C1
7	D	402	P5S	C20-C17-O19-C1
7	B	402	P5S	O18-C17-O19-C1
7	C	403	P5S	O18-C17-O19-C1
9	E	1602	BJX	C21-C23-C24-O2
9	E	1602	BJX	C21-C23-C24-O3
8	E	1603	PTY	O10-C8-O7-C6
8	E	1608	PTY	O10-C8-O7-C6
7	B	402	P5S	C20-C17-O19-C1
8	E	1608	PTY	C11-C8-O7-C6
7	A	404	P5S	C20-C17-O19-C1
7	A	406	P5S	C20-C17-O19-C1
7	C	403	P5S	C20-C17-O19-C1
7	E	1609	P5S	C20-C17-O19-C1
7	E	1609	P5S	O18-C17-O19-C1
7	B	402	P5S	C39-C38-O37-C2
7	A	404	P5S	O18-C17-O19-C1
7	A	406	P5S	C23-C24-C25-C26
7	B	402	P5S	O47-C38-O37-C2
7	A	406	P5S	O18-C17-O19-C1
9	E	1602	BJX	C5-C8-C9-C13
7	E	1609	P5S	C49-C50-C51-C52
7	E	1609	P5S	OXT-C-CA-N
7	A	404	P5S	C43-C44-C45-C46
6	E	1604	POV	C32-C31-O31-C3
8	E	1605	PTY	C31-C30-O4-C1
8	E	1608	PTY	C31-C30-O4-C1
7	C	403	P5S	C26-C27-C28-C29
6	D	401	POV	O21-C2-C3-O31
6	E	1604	POV	O32-C31-O31-C3
8	E	1605	PTY	O30-C30-O4-C1
8	E	1608	PTY	O30-C30-O4-C1
9	E	1602	BJX	C5-C8-C9-C12
7	A	406	P5S	OXT-C-CA-N
6	E	1604	POV	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
7	A	404	P5S	C30-C31-C32-C33
8	E	1606	PTY	C8-C11-C12-C13
8	E	1607	PTY	C11-C8-O7-C6
6	B	401	POV	C1-O11-P-O12
7	A	404	P5S	CB-OG-P12-O16
7	B	402	P5S	CB-OG-P12-O16
7	C	403	P5S	C3-O16-P12-OG
7	D	402	P5S	C3-O16-P12-OG
8	E	1603	PTY	C5-O14-P1-O11
8	E	1607	PTY	C5-O14-P1-O11
8	E	1607	PTY	C31-C30-O4-C1
7	A	404	P5S	C38-C39-C40-C41
8	E	1607	PTY	O10-C8-O7-C6
7	A	406	P5S	C39-C38-O37-C2
7	A	404	P5S	C26-C27-C28-C29
7	C	403	P5S	C44-C45-C46-C48
7	D	402	P5S	C42-C43-C44-C45
8	E	1605	PTY	C16-C17-C18-C19
8	E	1606	PTY	C11-C12-C13-C14
7	A	406	P5S	O47-C38-O37-C2
7	B	402	P5S	C27-C28-C29-C30
6	A	403	POV	C23-C24-C25-C26
9	E	1602	BJX	N1-C5-C8-C9
7	D	402	P5S	C22-C23-C24-C25
7	A	404	P5S	OXT-C-CA-N
8	E	1605	PTY	C12-C13-C14-C15
7	A	404	P5S	C40-C41-C42-C43
7	B	402	P5S	C29-C30-C31-C32
8	E	1601	PTY	C11-C8-O7-C6
7	A	406	P5S	C24-C25-C26-C27
7	B	402	P5S	C24-C25-C26-C27
7	B	402	P5S	C31-C32-C33-C34
7	B	402	P5S	C39-C40-C41-C42
7	C	403	P5S	C22-C23-C24-C25
8	E	1601	PTY	C15-C16-C17-C18
6	A	403	POV	C24-C25-C26-C27
8	E	1607	PTY	N1-C2-C3-O11
6	B	401	POV	C22-C23-C24-C25
8	E	1603	PTY	C13-C14-C15-C16
7	A	404	P5S	C31-C32-C33-C34
7	B	402	P5S	C43-C44-C45-C46
8	E	1601	PTY	O10-C8-O7-C6

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Mol	Chain	Res	Type	Atoms
6	E	1604	POV	C31-C32-C33-C34
7	B	402	P5S	C38-C39-C40-C41
8	E	1601	PTY	C8-C11-C12-C13
6	D	401	POV	C23-C24-C25-C26
7	E	1609	P5S	C39-C40-C41-C42
7	E	1609	P5S	C23-C24-C25-C26
8	E	1607	PTY	O30-C30-O4-C1
9	E	1602	BJX	C26-C25-O1-C21
6	A	403	POV	C32-C31-O31-C3
8	E	1605	PTY	C11-C8-O7-C6
7	E	1609	P5S	C40-C41-C42-C43
7	A	406	P5S	C22-C23-C24-C25
7	A	404	P5S	C27-C28-C29-C30
7	D	402	P5S	C20-C21-C22-C23
8	E	1603	PTY	C30-C31-C32-C33
8	E	1603	PTY	C14-C15-C16-C17
7	A	404	P5S	C-CA-CB-OG
6	B	401	POV	C22-C21-O21-C2
7	C	403	P5S	C39-C38-O37-C2
7	D	402	P5S	C39-C38-O37-C2
8	E	1606	PTY	C11-C8-O7-C6
7	B	402	P5S	O37-C2-C3-O16
8	E	1603	PTY	C11-C12-C13-C14
8	E	1603	PTY	C15-C16-C17-C18
7	B	402	P5S	O-C-CA-CB
7	D	402	P5S	OXT-C-CA-CB
7	B	402	P5S	C40-C41-C42-C43
7	C	403	P5S	C43-C44-C45-C46
7	E	1609	P5S	C53-C54-C55-C56
6	A	403	POV	O32-C31-O31-C3
7	C	403	P5S	O47-C38-O37-C2
7	D	402	P5S	O47-C38-O37-C2
8	E	1606	PTY	O10-C8-O7-C6
8	E	1601	PTY	C16-C17-C18-C19
7	A	404	P5S	C3-O16-P12-OG
7	B	402	P5S	C1-C2-C3-O16
8	E	1605	PTY	O14-C5-C6-C1
8	E	1605	PTY	C30-C31-C32-C33
6	B	401	POV	C33-C34-C35-C36
9	E	1602	BJX	C19-C21-O1-C25
8	E	1605	PTY	O10-C8-O7-C6
7	A	406	P5S	C48-C49-C50-C51

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Mol	Chain	Res	Type	Atoms
6	D	401	POV	C1-C2-C3-O31
8	E	1605	PTY	O4-C1-C6-C5
8	E	1607	PTY	O4-C1-C6-C5
7	B	402	P5S	C17-C20-C21-C22
7	D	402	P5S	C21-C22-C23-C24
8	E	1608	PTY	C13-C14-C15-C16
7	A	406	P5S	C30-C31-C32-C33
7	B	402	P5S	C21-C22-C23-C24
9	E	1602	BJX	C23-C21-O1-C25
9	E	1602	BJX	O-C16-C17-C18
8	E	1601	PTY	O14-C5-C6-O7
7	E	1609	P5S	C42-C43-C44-C45
8	E	1605	PTY	C17-C18-C19-C20
6	B	401	POV	O22-C21-O21-C2
6	E	1604	POV	C33-C34-C35-C36
4	A	401	ATP	PB-O3A-PA-O1A
8	E	1603	PTY	C31-C30-O4-C1
6	D	401	POV	C32-C33-C34-C35
8	E	1607	PTY	O14-C5-C6-C1
7	D	402	P5S	C46-C48-C49-C50
8	E	1605	PTY	C8-C11-C12-C13
6	E	1604	POV	C2-C1-O11-P
7	B	402	P5S	C23-C24-C25-C26
7	A	404	P5S	C29-C30-C31-C32
7	A	404	P5S	O19-C1-C2-C3
8	E	1601	PTY	O4-C1-C6-C5
8	E	1608	PTY	C12-C13-C14-C15
7	A	406	P5S	C45-C46-C48-C49
8	E	1606	PTY	C16-C17-C18-C19
8	E	1608	PTY	C8-C11-C12-C13
7	D	402	P5S	C23-C24-C25-C26
7	E	1609	P5S	O-C-CA-N
6	D	401	POV	C25-C26-C27-C28
8	E	1605	PTY	C11-C12-C13-C14
8	E	1603	PTY	C6-C5-O14-P1
7	C	403	P5S	C21-C22-C23-C24
9	E	1602	BJX	C8-C5-C7-C11
9	E	1602	BJX	C10-C6-N-C
7	E	1609	P5S	C44-C45-C46-C48
6	D	401	POV	O11-C1-C2-C3
7	C	403	P5S	C1-C2-C3-O16
7	E	1609	P5S	C1-C2-C3-O16

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Mol	Chain	Res	Type	Atoms
8	E	1601	PTY	O14-C5-C6-C1
7	E	1609	P5S	C41-C42-C43-C44
7	B	402	P5S	C41-C42-C43-C44
7	A	404	P5S	C41-C42-C43-C44
8	E	1605	PTY	C1-C6-O7-C8
7	A	404	P5S	C28-C29-C30-C31
7	A	406	P5S	O19-C1-C2-C3
7	E	1609	P5S	O19-C1-C2-C3
8	E	1608	PTY	O4-C1-C6-C5
7	A	406	P5S	C41-C42-C43-C44
7	C	403	P5S	O37-C2-C3-O16
7	E	1609	P5S	O37-C2-C3-O16
8	E	1607	PTY	O14-C5-C6-O7
8	E	1607	PTY	C14-C15-C16-C17
8	E	1603	PTY	O30-C30-O4-C1
8	E	1601	PTY	O4-C1-C6-O7
8	E	1606	PTY	O4-C1-C6-O7
8	E	1608	PTY	O4-C1-C6-O7
7	C	403	P5S	CA-CB-OG-P12
7	D	402	P5S	CA-CB-OG-P12
6	E	1604	POV	C34-C35-C36-C37
7	D	402	P5S	O-C-CA-CB
7	D	402	P5S	N-CA-CB-OG
6	A	403	POV	C11-O12-P-O11
8	E	1608	PTY	C3-O11-P1-O14
8	E	1606	PTY	C6-C5-O14-P1
8	E	1603	PTY	C31-C32-C33-C34
4	A	405	ATP	C5'-O5'-PA-O1A
4	A	405	ATP	C5'-O5'-PA-O2A
4	C	401	ATP	C5'-O5'-PA-O1A
4	C	401	ATP	C5'-O5'-PA-O2A
4	E	1610	ATP	C5'-O5'-PA-O1A
6	A	403	POV	C11-O12-P-O13
6	B	401	POV	C1-O11-P-O13
6	C	402	POV	C11-O12-P-O13
7	A	404	P5S	CB-OG-P12-O13
7	A	404	P5S	C3-O16-P12-O15
7	D	402	P5S	C3-O16-P12-O13
8	E	1603	PTY	C5-O14-P1-O13
8	E	1607	PTY	C3-O11-P1-O12
8	E	1606	PTY	C13-C14-C15-C16
6	C	402	POV	O11-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
9	E	1602	BJX	C22-C23-C24-O2
6	B	401	POV	C12-C11-O12-P
8	E	1606	PTY	C32-C33-C34-C35
6	D	401	POV	C22-C23-C24-C25
6	B	401	POV	O11-C1-C2-O21
6	C	402	POV	O11-C1-C2-O21
6	D	401	POV	O11-C1-C2-O21
7	D	402	P5S	O37-C2-C3-O16
9	E	1602	BJX	N1-C16-C17-C18
7	C	403	P5S	C32-C33-C34-C35
6	B	401	POV	C1-C2-C3-O31
6	B	401	POV	O12-C11-C12-N
6	E	1604	POV	O12-C11-C12-N
8	E	1606	PTY	O4-C1-C6-C5
7	E	1609	P5S	O19-C1-C2-O37
9	E	1602	BJX	C22-C23-C24-O3
8	E	1608	PTY	C17-C18-C19-C20
6	A	403	POV	C32-C33-C34-C35
8	E	1603	PTY	C32-C33-C34-C35
6	E	1604	POV	O22-C21-O21-C2
8	E	1605	PTY	C31-C32-C33-C34
8	E	1605	PTY	O14-C5-C6-O7
7	E	1609	P5S	C43-C44-C45-C46
8	E	1607	PTY	O4-C30-C31-C32
6	E	1604	POV	C22-C21-O21-C2
8	E	1607	PTY	O4-C1-C6-O7
6	B	401	POV	C11-O12-P-O11
6	D	401	POV	C1-O11-P-O12
6	D	401	POV	C11-O12-P-O11
6	E	1604	POV	C11-O12-P-O11
7	A	406	P5S	CB-OG-P12-O16
7	A	406	P5S	C3-O16-P12-OG
7	C	403	P5S	CB-OG-P12-O16
8	E	1601	PTY	C3-O11-P1-O14
8	E	1608	PTY	C5-O14-P1-O11
6	E	1604	POV	C1-C2-C3-O31
4	A	405	ATP	PA-O3A-PB-O2B
4	C	401	ATP	PA-O3A-PB-O2B
4	C	404	ATP	PB-O3A-PA-O2A
4	E	1610	ATP	PA-O3A-PB-O1B
8	E	1607	PTY	C15-C16-C17-C18
7	B	402	P5S	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
7	E	1609	P5S	C31-C32-C33-C34
6	B	401	POV	O11-C1-C2-C3
8	E	1606	PTY	O14-C5-C6-C1
8	E	1603	PTY	N1-C2-C3-O11
6	A	403	POV	O22-C21-O21-C2
8	E	1608	PTY	C6-C5-O14-P1
7	B	402	P5S	OXT-C-CA-CB
7	E	1609	P5S	C26-C27-C28-C29
7	E	1609	P5S	C48-C49-C50-C51
7	A	404	P5S	C48-C49-C50-C51
8	E	1606	PTY	C17-C18-C19-C20
7	A	406	P5S	C25-C26-C27-C28
7	A	404	P5S	C50-C51-C52-C53
7	C	403	P5S	O37-C38-C39-C40
7	C	403	P5S	C40-C41-C42-C43
8	E	1601	PTY	C12-C13-C14-C15
6	A	403	POV	C22-C21-O21-C2
7	B	402	P5S	C51-C52-C53-C54
7	D	402	P5S	C1-C2-C3-O16
7	B	402	P5S	C49-C50-C51-C52
8	E	1608	PTY	C15-C16-C17-C18
7	A	406	P5S	C43-C44-C45-C46
7	E	1609	P5S	C33-C34-C35-C36
8	E	1606	PTY	C3-O11-P1-O14
4	C	404	ATP	PB-O3B-PG-O1G
7	B	402	P5S	O37-C38-C39-C40
6	C	402	POV	C24-C25-C26-C27
7	D	402	P5S	O37-C38-C39-C40
6	C	402	POV	C23-C24-C25-C26
8	E	1601	PTY	O4-C30-C31-C32
4	A	401	ATP	PB-O3B-PG-O2G
7	A	406	P5S	O19-C1-C2-O37
4	A	401	ATP	C5'-O5'-PA-O3A
7	A	406	P5S	CA-CB-OG-P12
7	B	402	P5S	CA-CB-OG-P12
9	E	1602	BJX	C8-C5-C7-C6
4	A	401	ATP	PB-O3A-PA-O2A
7	A	404	P5S	O37-C38-C39-C40
7	C	403	P5S	C50-C51-C52-C53
7	B	402	P5S	O47-C38-C39-C40
8	E	1601	PTY	O30-C30-C31-C32
6	B	401	POV	C11-O12-P-O14

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Mol	Chain	Res	Type	Atoms
7	A	406	P5S	C3-O16-P12-O13
8	E	1601	PTY	C5-O14-P1-O13
9	E	1602	BJX	C10-C6-N-C1
7	D	402	P5S	O47-C38-C39-C40
8	E	1603	PTY	C2-C3-O11-P1
9	E	1602	BJX	N1-C5-C7-C6
6	E	1604	POV	O31-C31-C32-C33
6	D	401	POV	C34-C35-C36-C37
7	A	406	P5S	C29-C30-C31-C32
7	A	404	P5S	O47-C38-C39-C40
6	E	1604	POV	O32-C31-C32-C33

There are no ring outliers.

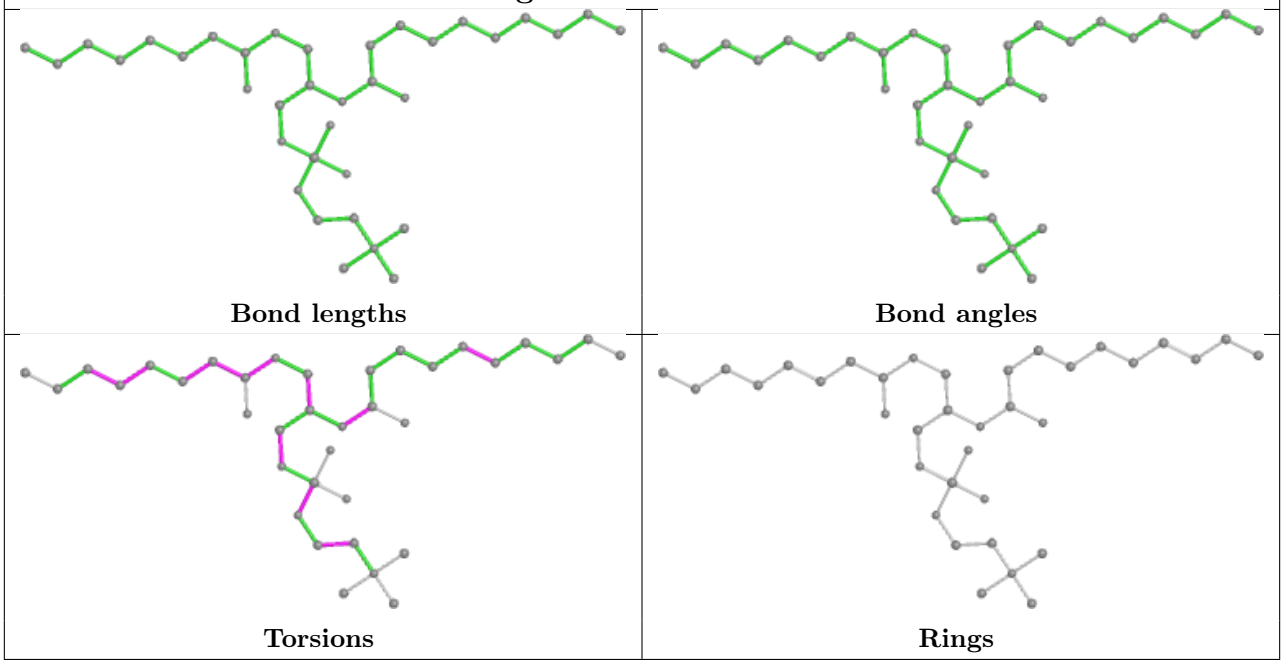
15 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	401	ATP	1	0
7	E	1609	P5S	4	0
8	E	1603	PTY	2	0
7	A	404	P5S	2	0
4	E	1610	ATP	1	0
7	B	402	P5S	5	0
7	A	406	P5S	6	0
6	B	401	POV	1	0
4	A	405	ATP	2	0
8	E	1607	PTY	1	0
8	E	1606	PTY	2	0
6	A	403	POV	3	0
7	D	402	P5S	4	0
8	E	1601	PTY	1	0
8	E	1605	PTY	2	0

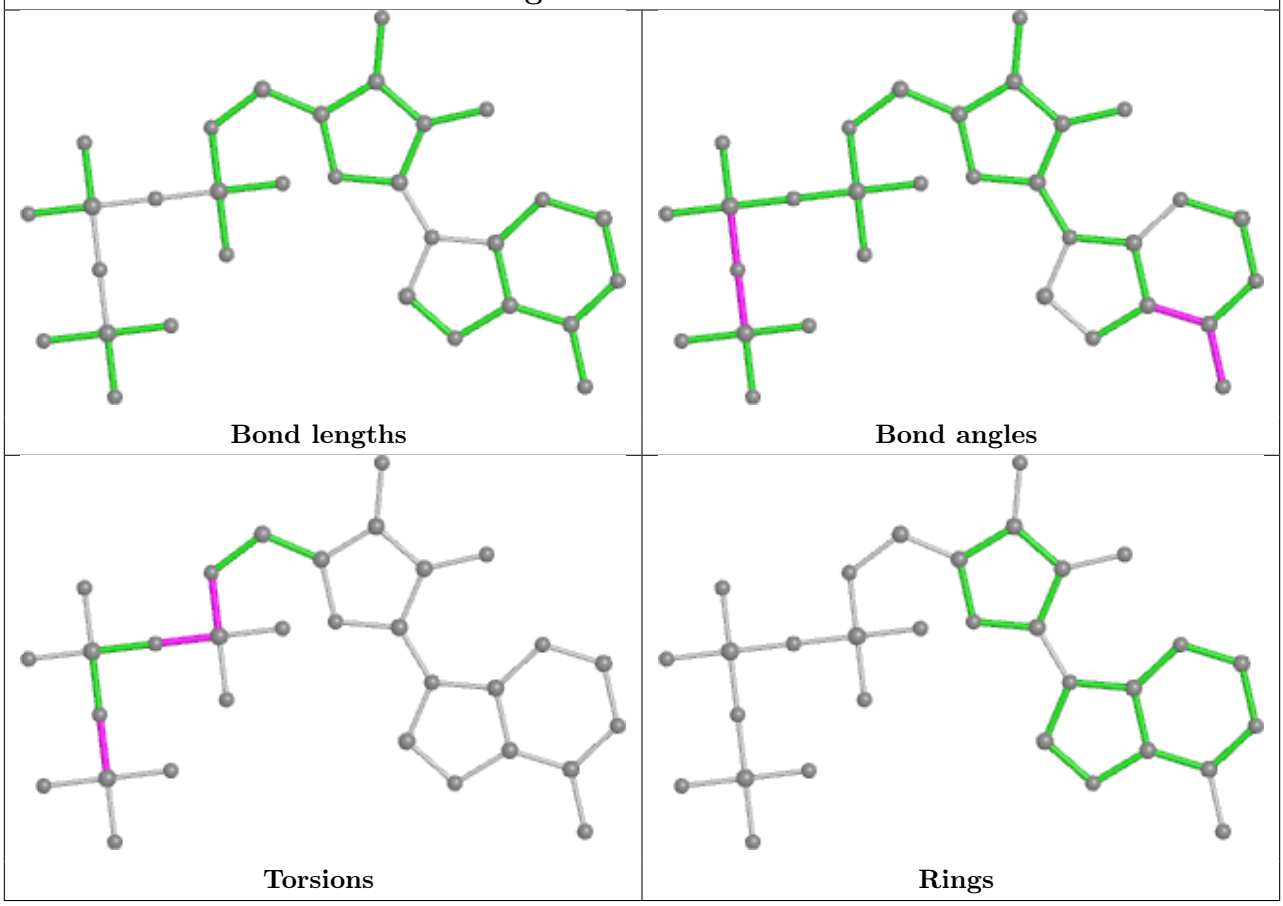
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

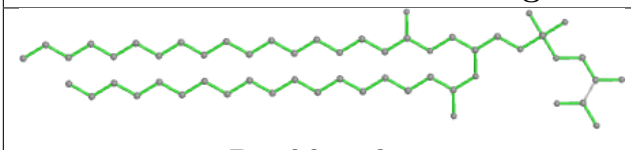
Ligand POV E 1604



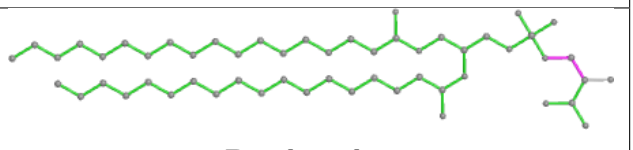
Ligand ATP A 401



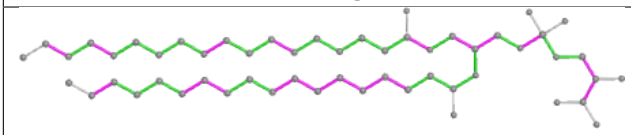
Ligand P5S E 1609



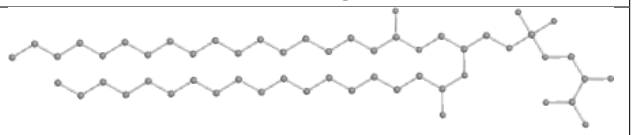
Bond lengths



Bond angles

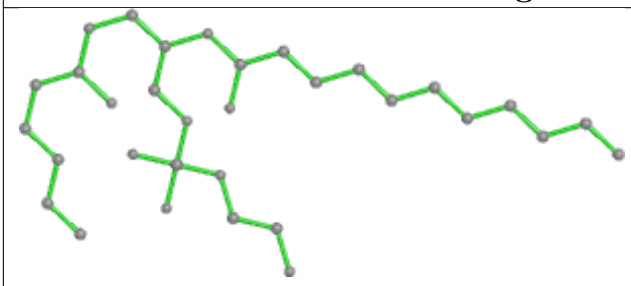


Torsions

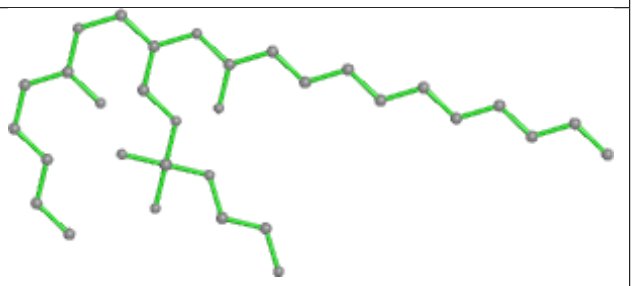


Rings

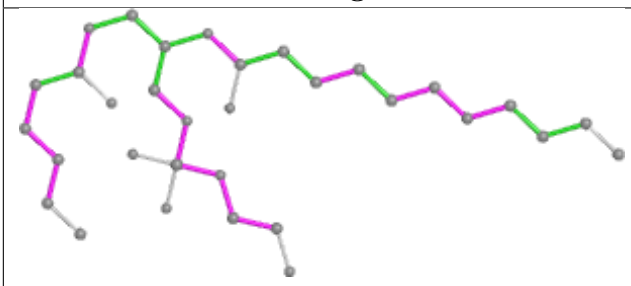
Ligand PTY E 1603



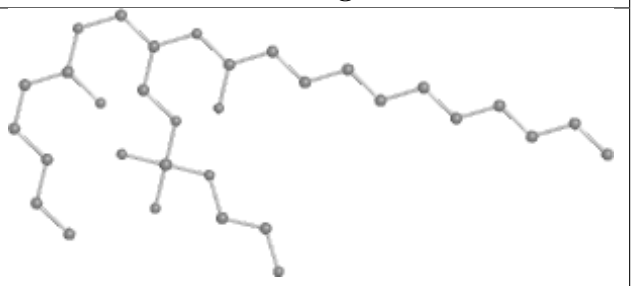
Bond lengths



Bond angles

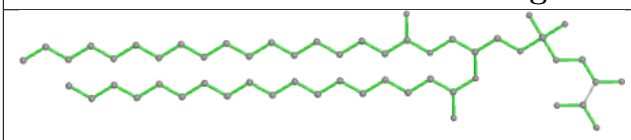


Torsions

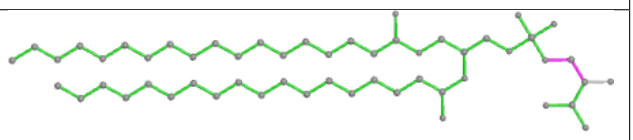


Rings

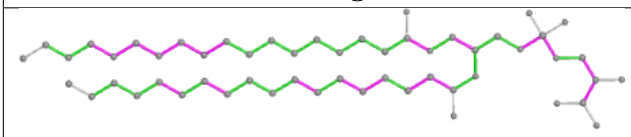
Ligand P5S A 404



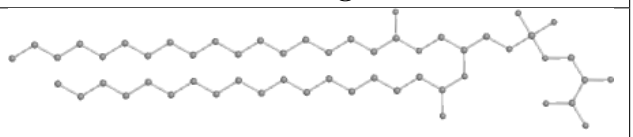
Bond lengths



Bond angles

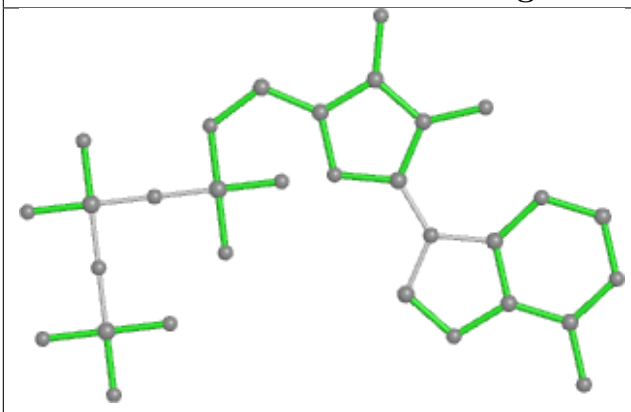


Torsions

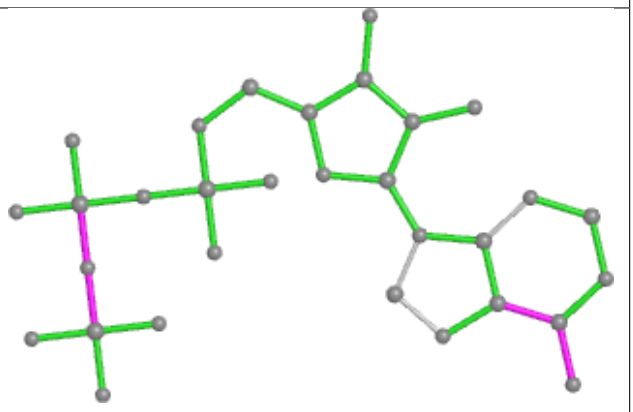


Rings

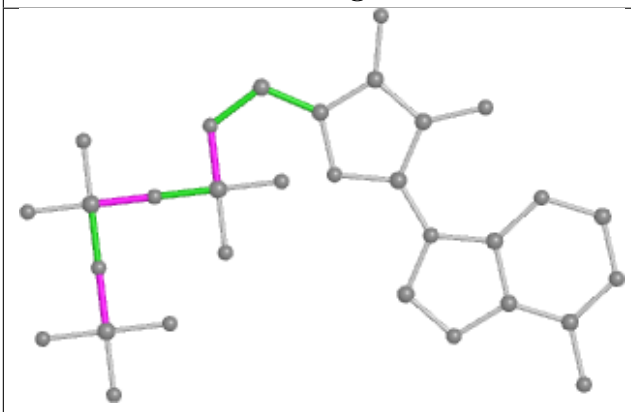
Ligand ATP E 1610



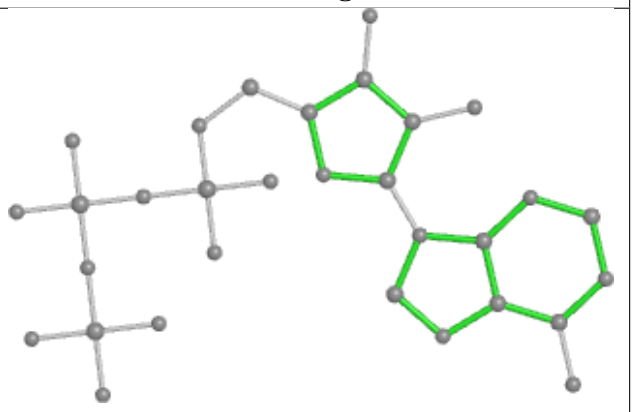
Bond lengths



Bond angles

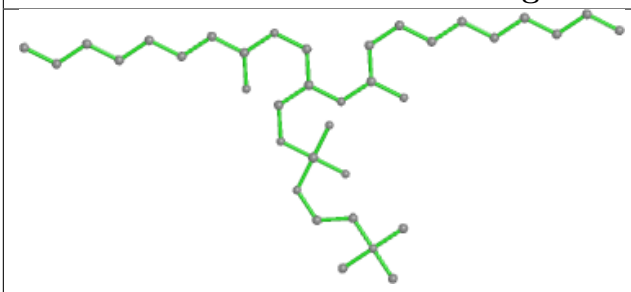


Torsions

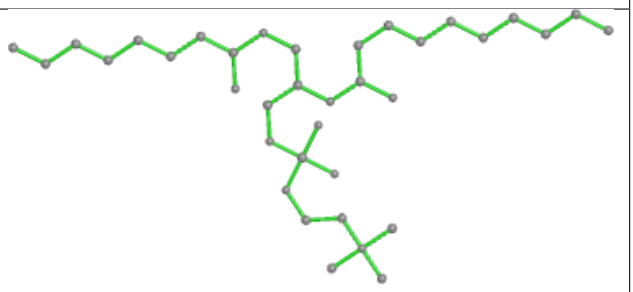


Rings

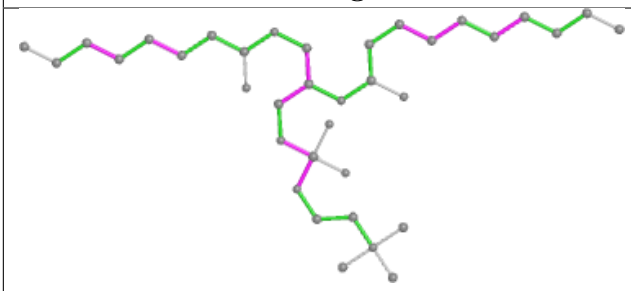
Ligand POV D 401



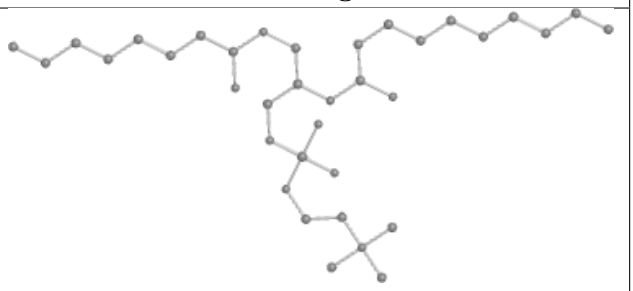
Bond lengths



Bond angles

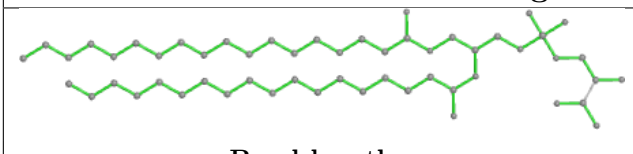


Torsions

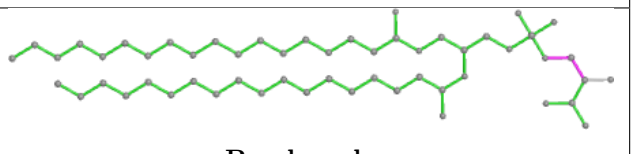


Rings

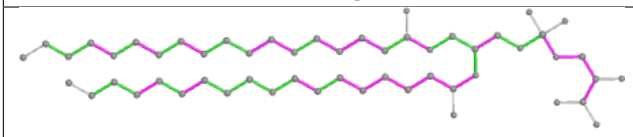
Ligand P5S B 402



Bond lengths



Bond angles



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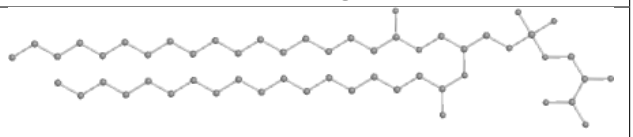
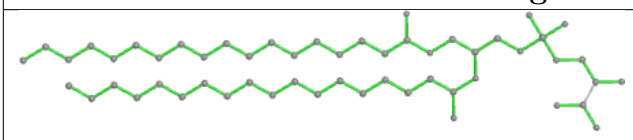
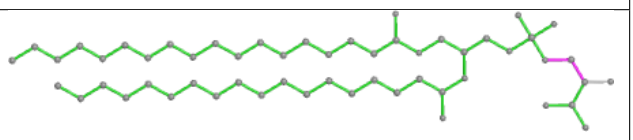


Rings

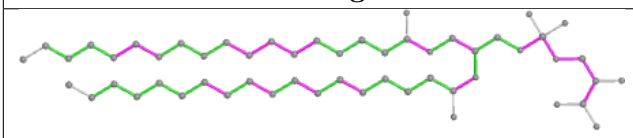
Ligand P5S A 406



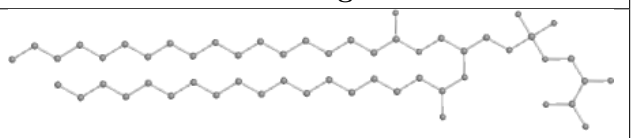
Bond lengths



Bond angles

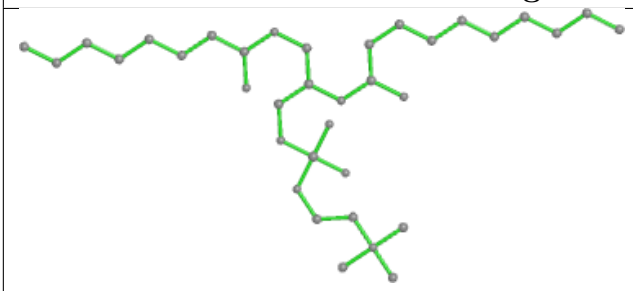


Torsions

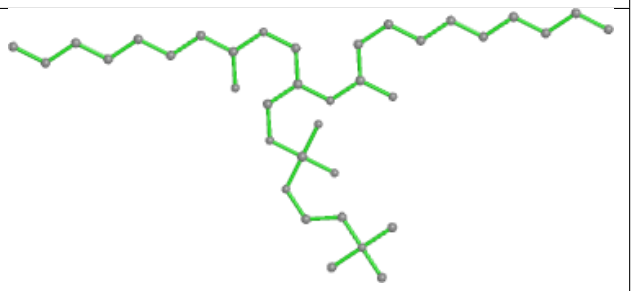


Rings

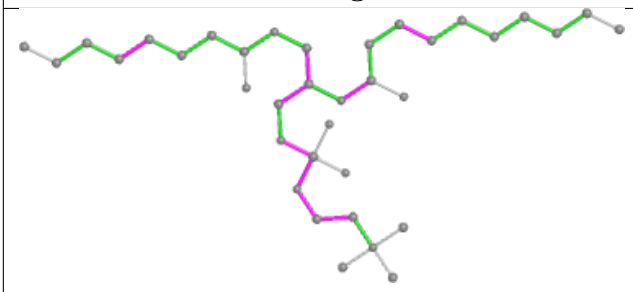
Ligand POV B 401



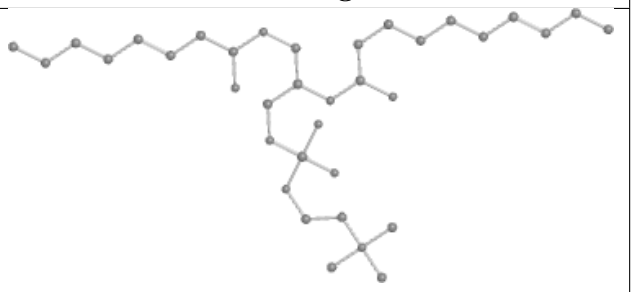
Bond lengths



Bond angles

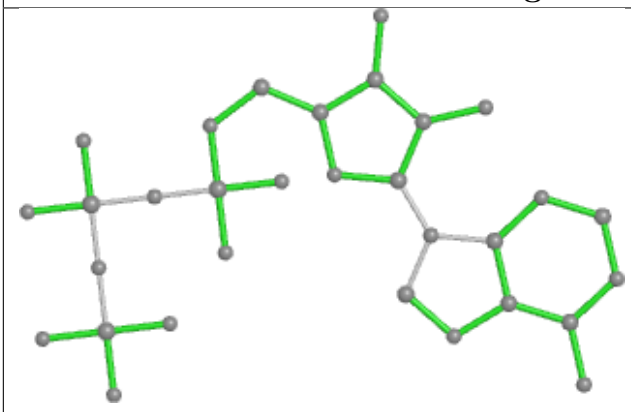


Torsions

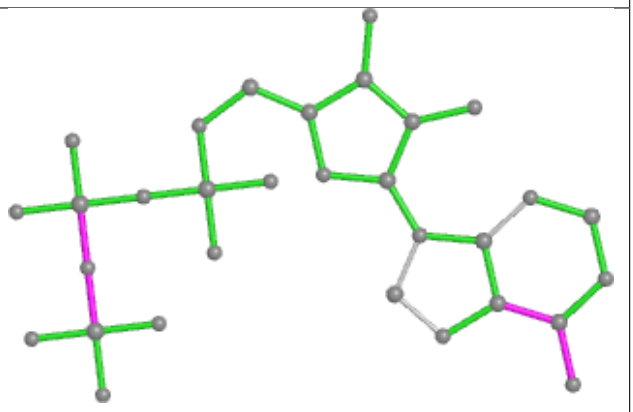


Rings

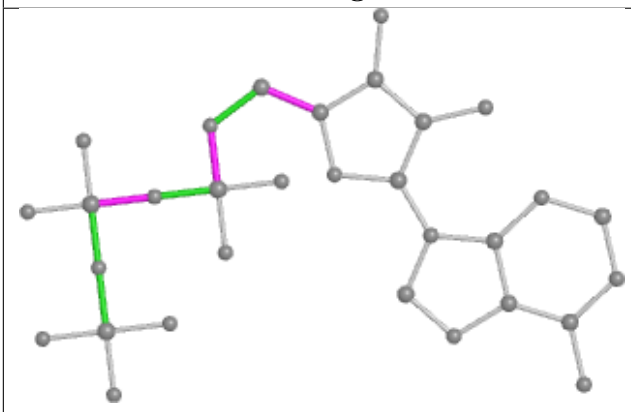
Ligand ATP A 405



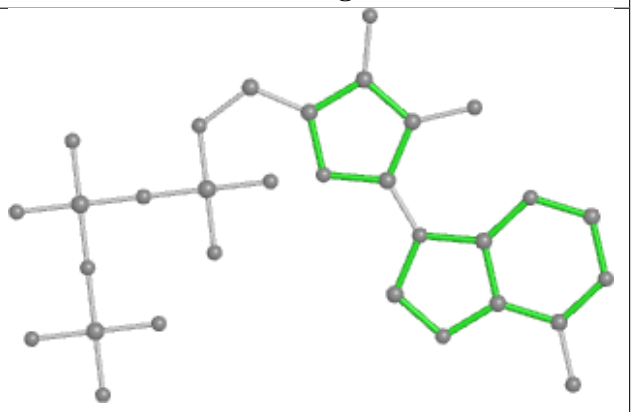
Bond lengths



Bond angles

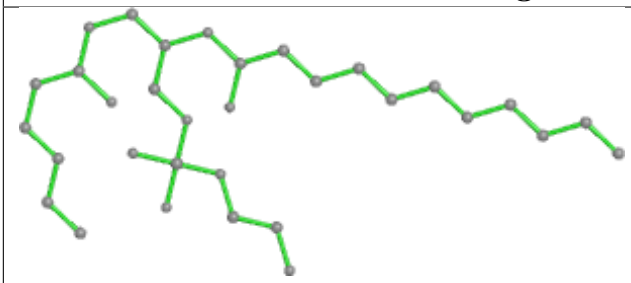


Torsions

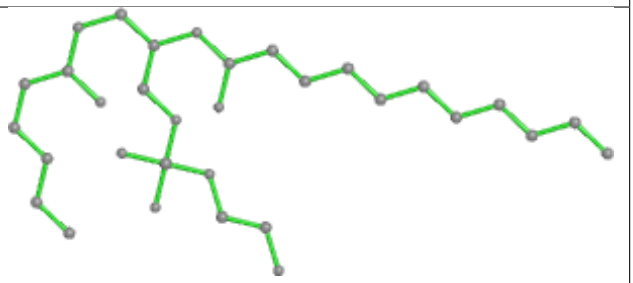


Rings

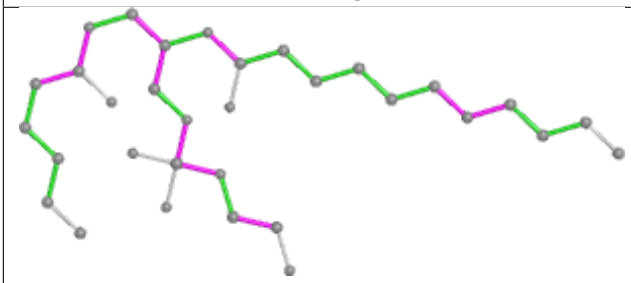
Ligand PTY E 1607



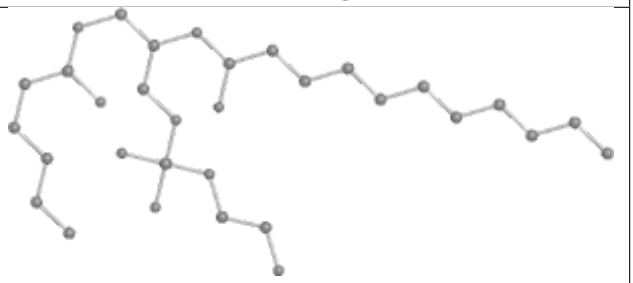
Bond lengths



Bond angles

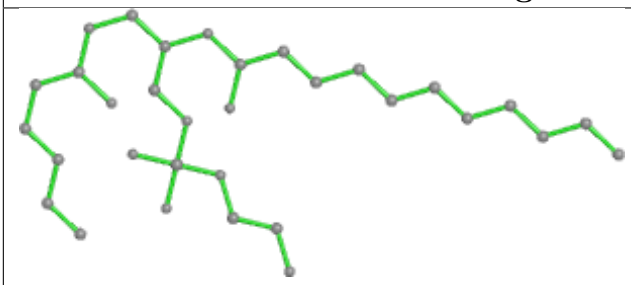


Torsions

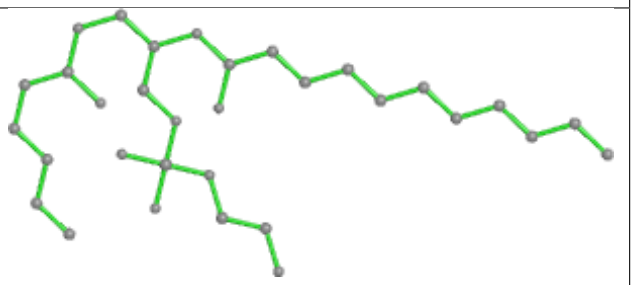


Rings

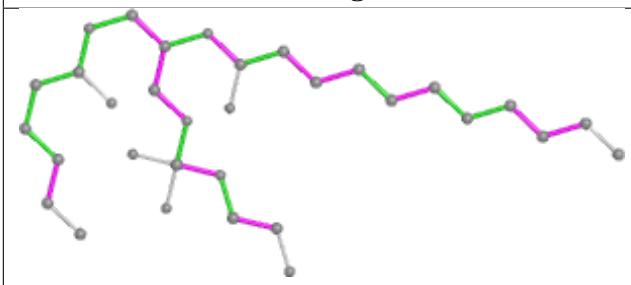
Ligand PTY E 1606



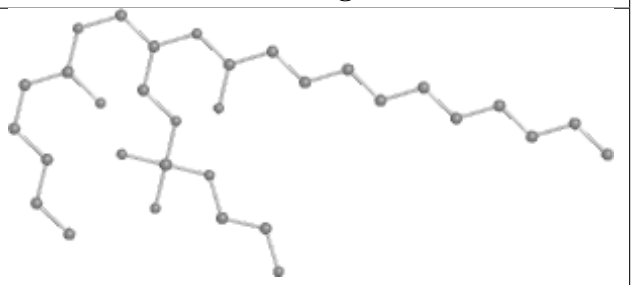
Bond lengths



Bond angles

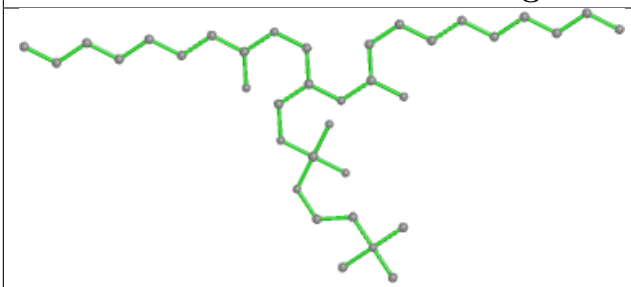


Torsions

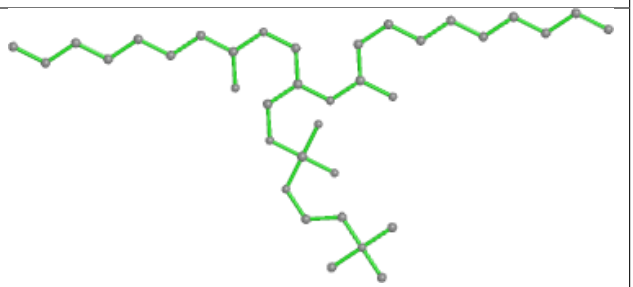


Rings

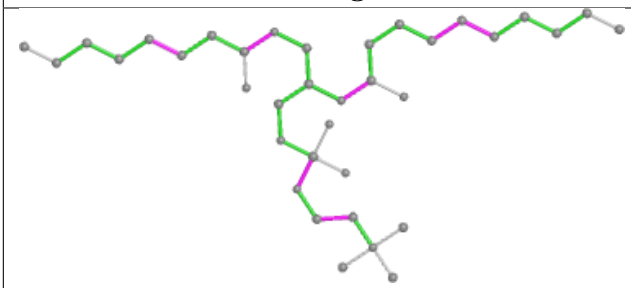
Ligand POV A 403



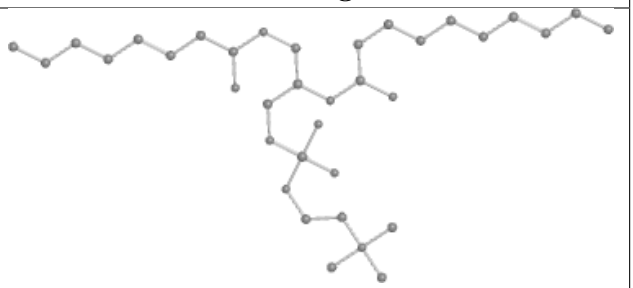
Bond lengths



Bond angles

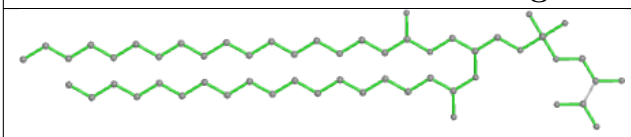


Torsions

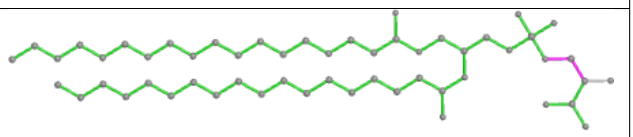


Rings

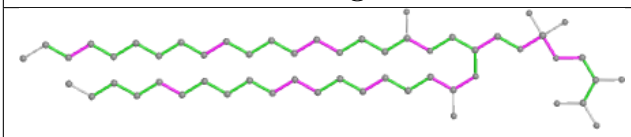
Ligand P5S C 403



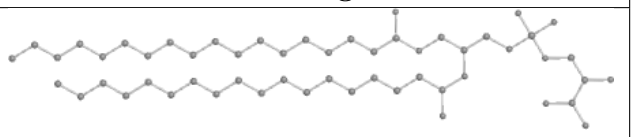
Bond lengths



Bond angles

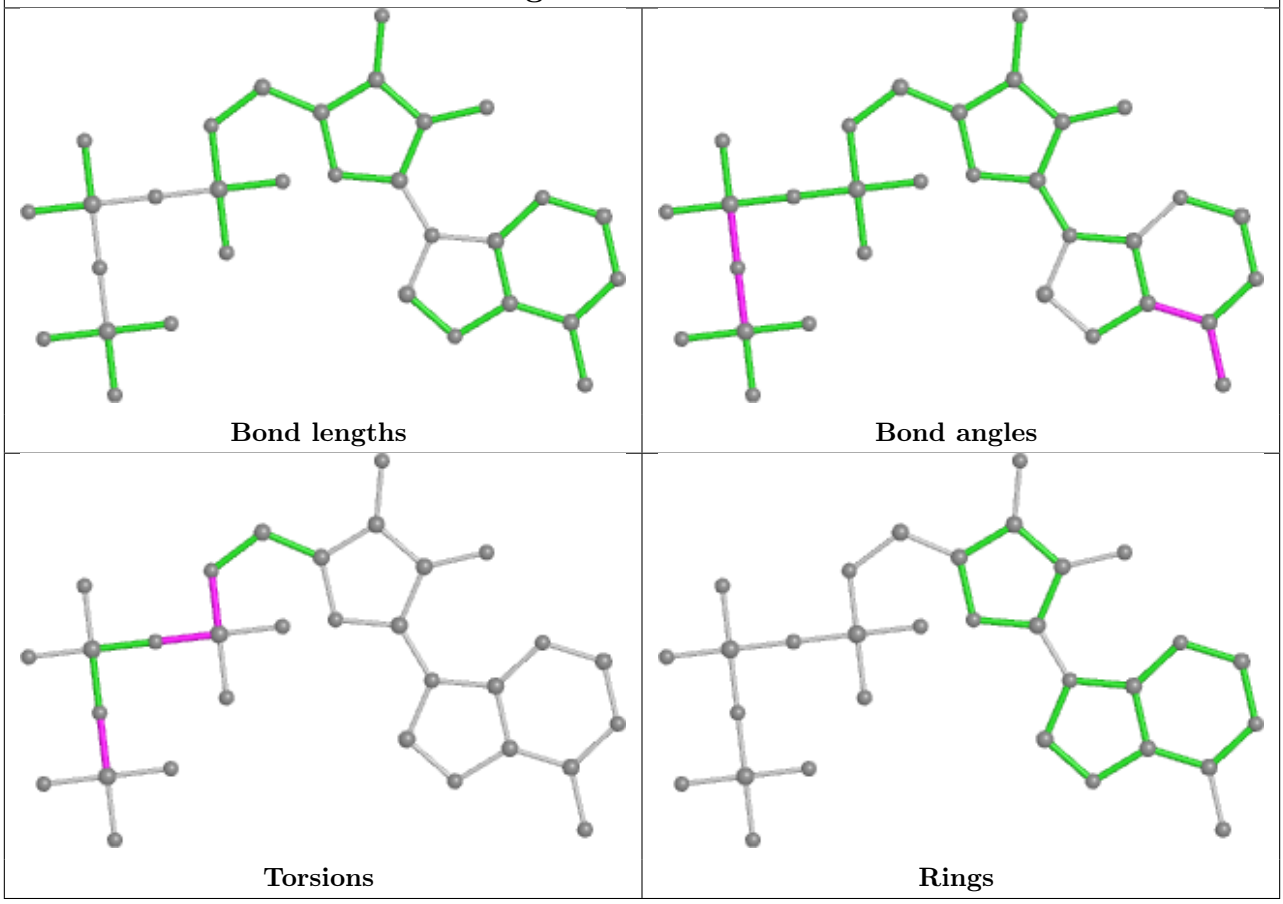


Torsions

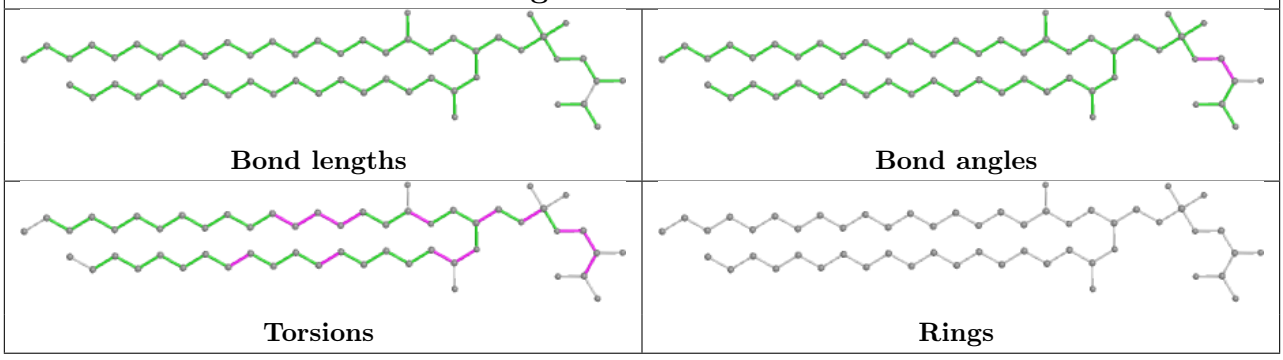


Rings

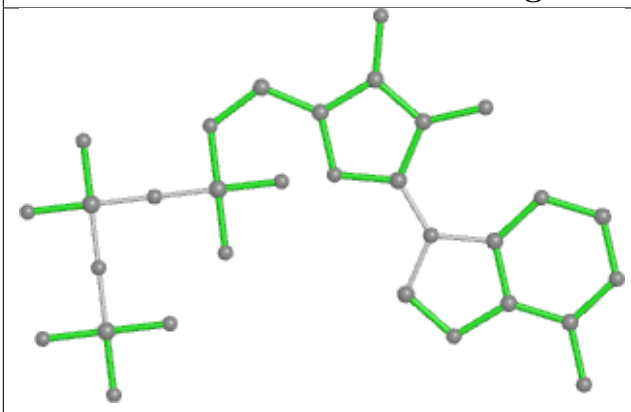
Ligand ATP C 404



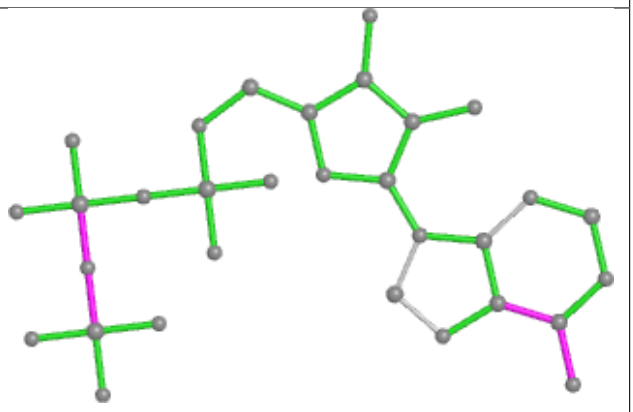
Ligand P5S D 402



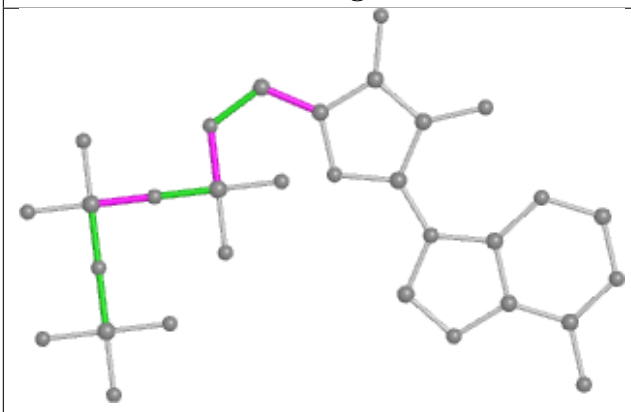
Ligand ATP C 401



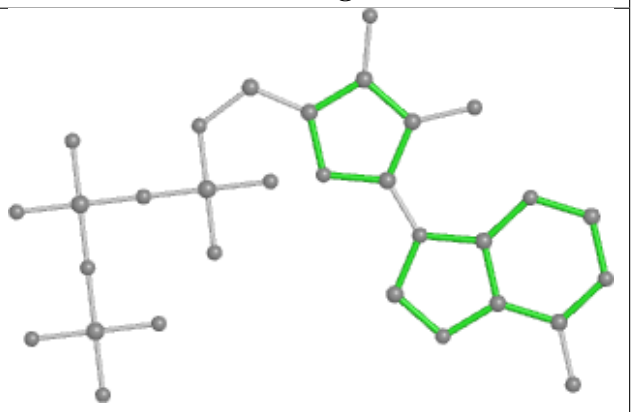
Bond lengths



Bond angles

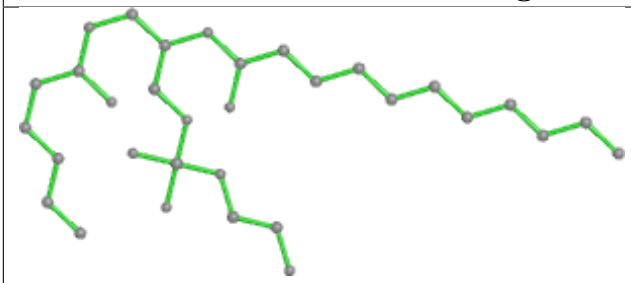


Torsions

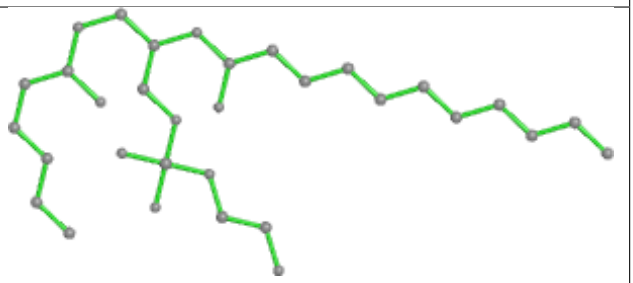


Rings

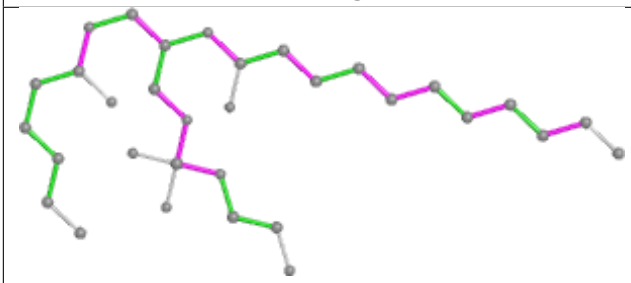
Ligand PTY E 1608



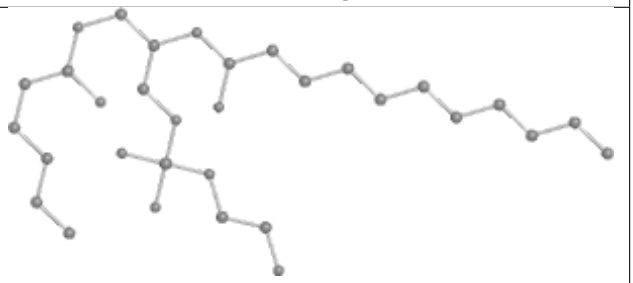
Bond lengths



Bond angles

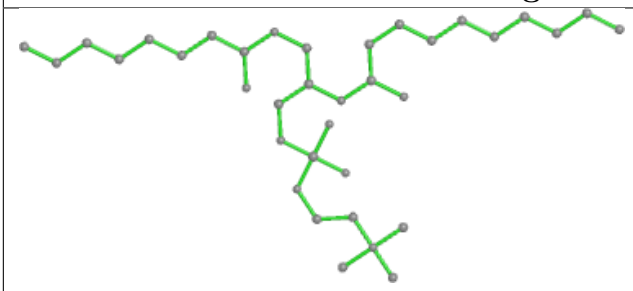


Torsions

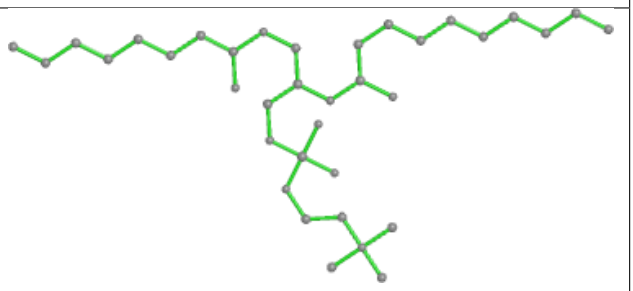


Rings

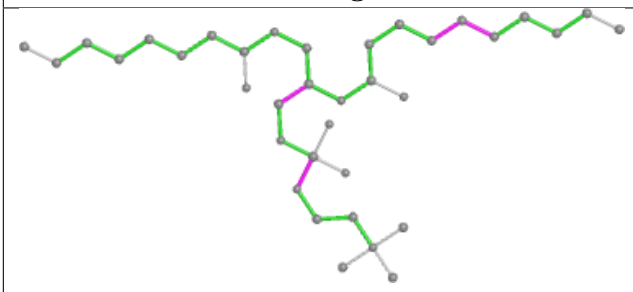
Ligand POV C 402



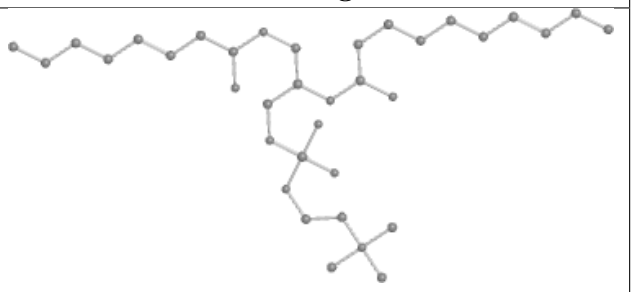
Bond lengths



Bond angles

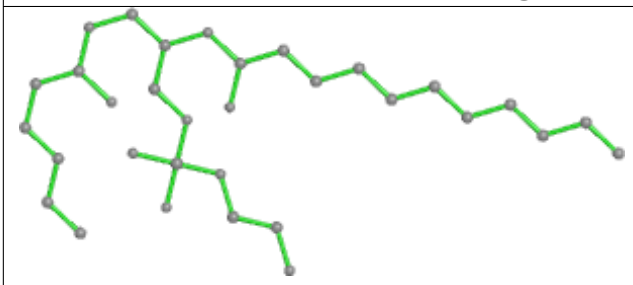


Torsions

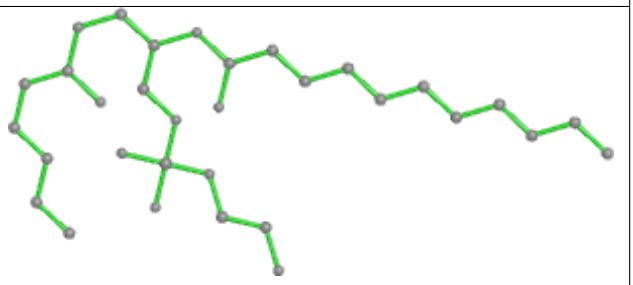


Rings

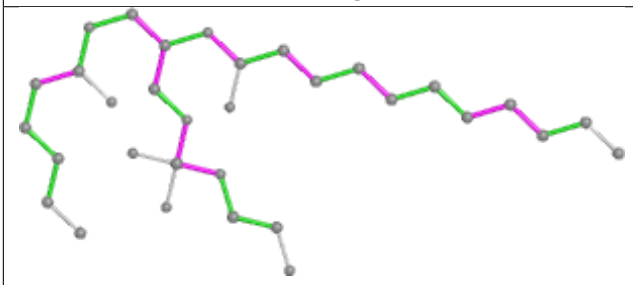
Ligand PTY E 1601



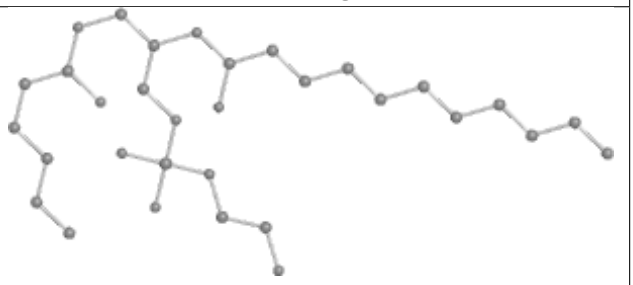
Bond lengths



Bond angles

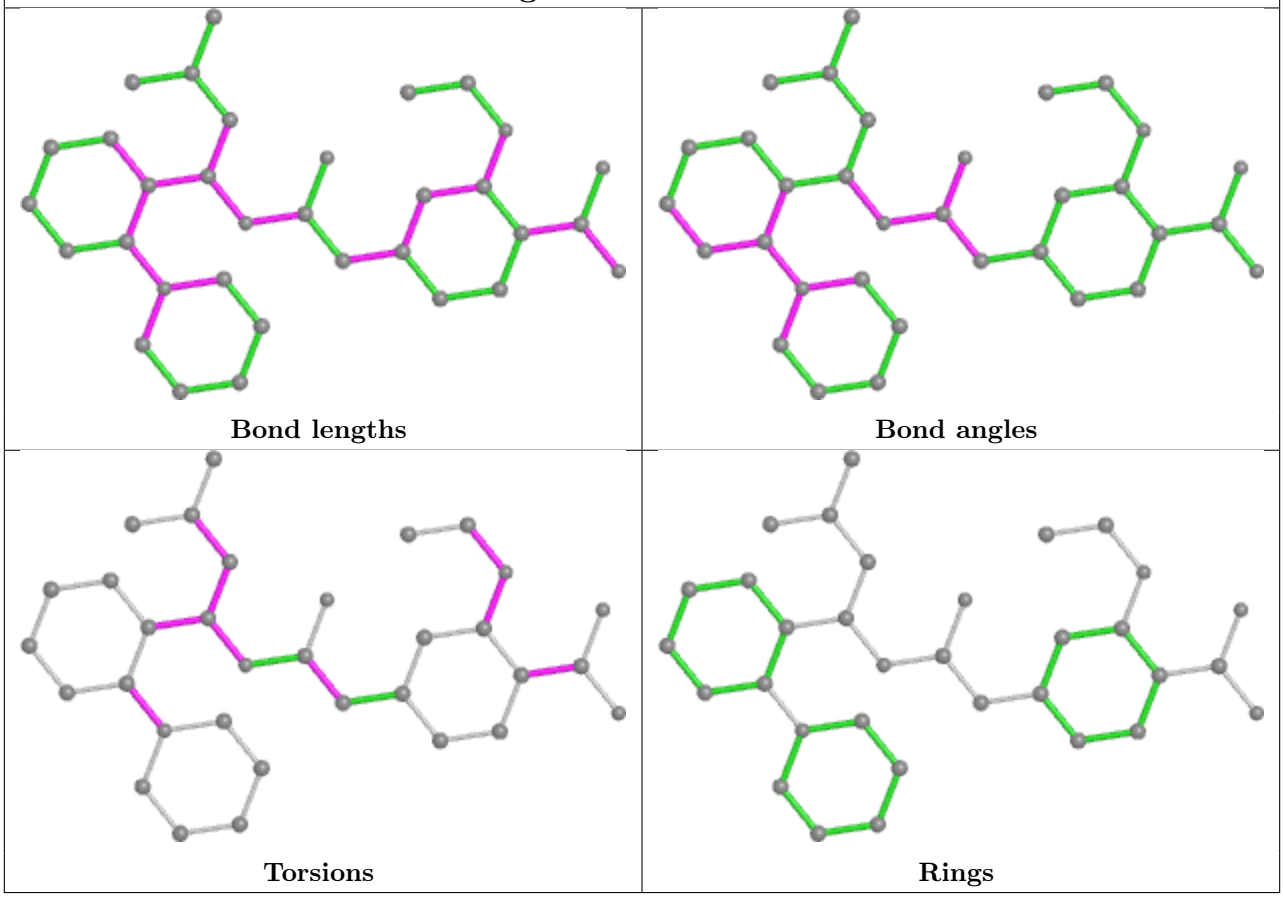


Torsions

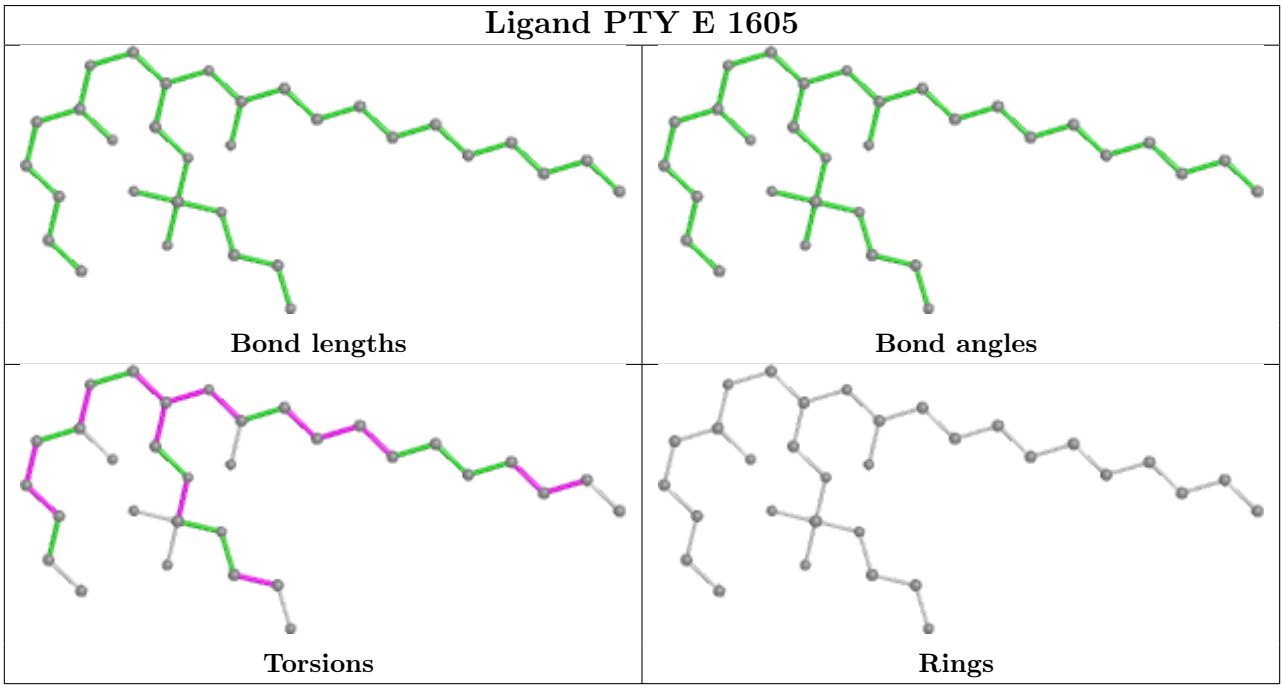


Rings

Ligand BJX E 1602



Ligand PTY E 1605



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.

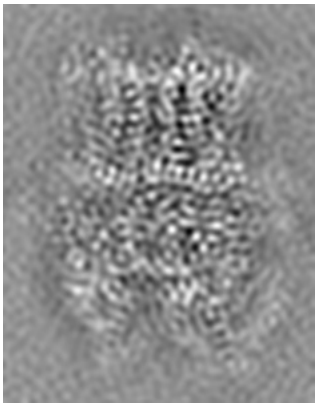
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-26304. These allow visual inspection of the internal detail of the map and identification of artifacts.

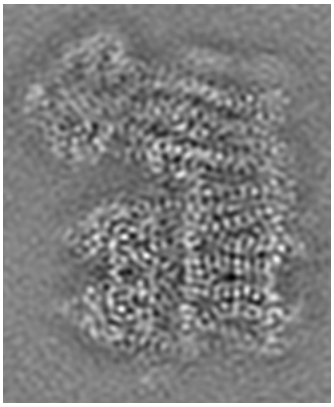
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

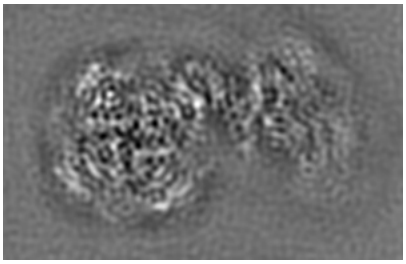
6.1.1 Primary map



X



Y

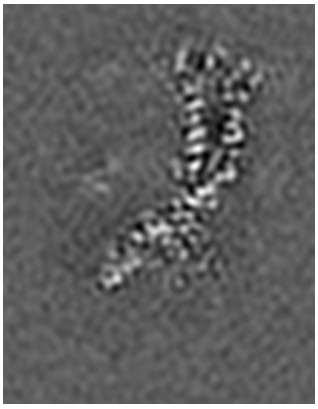


Z

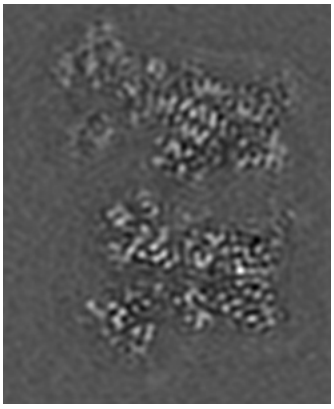
The images above show the map projected in three orthogonal directions.

6.2 Central slices

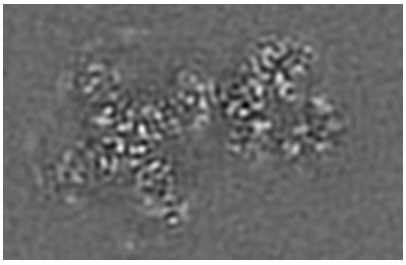
6.2.1 Primary map



X Index: 85



Y Index: 54

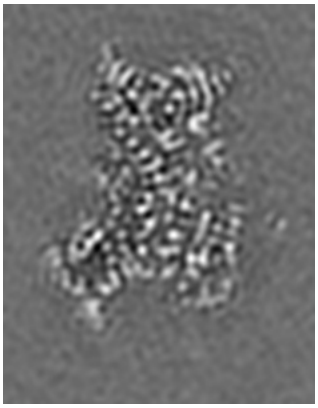


Z Index: 70

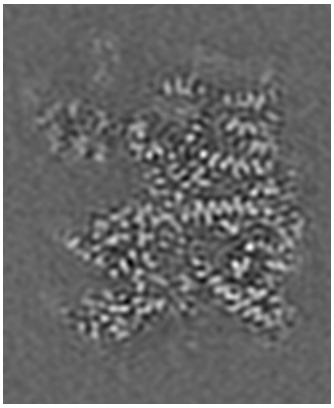
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

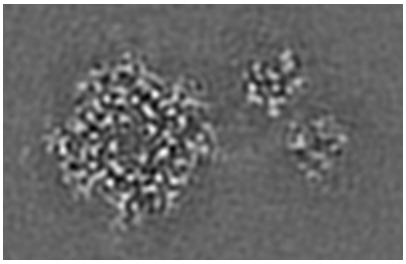
6.3.1 Primary map



X Index: 45



Y Index: 67

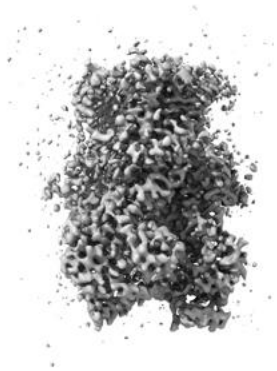


Z Index: 58

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 1.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

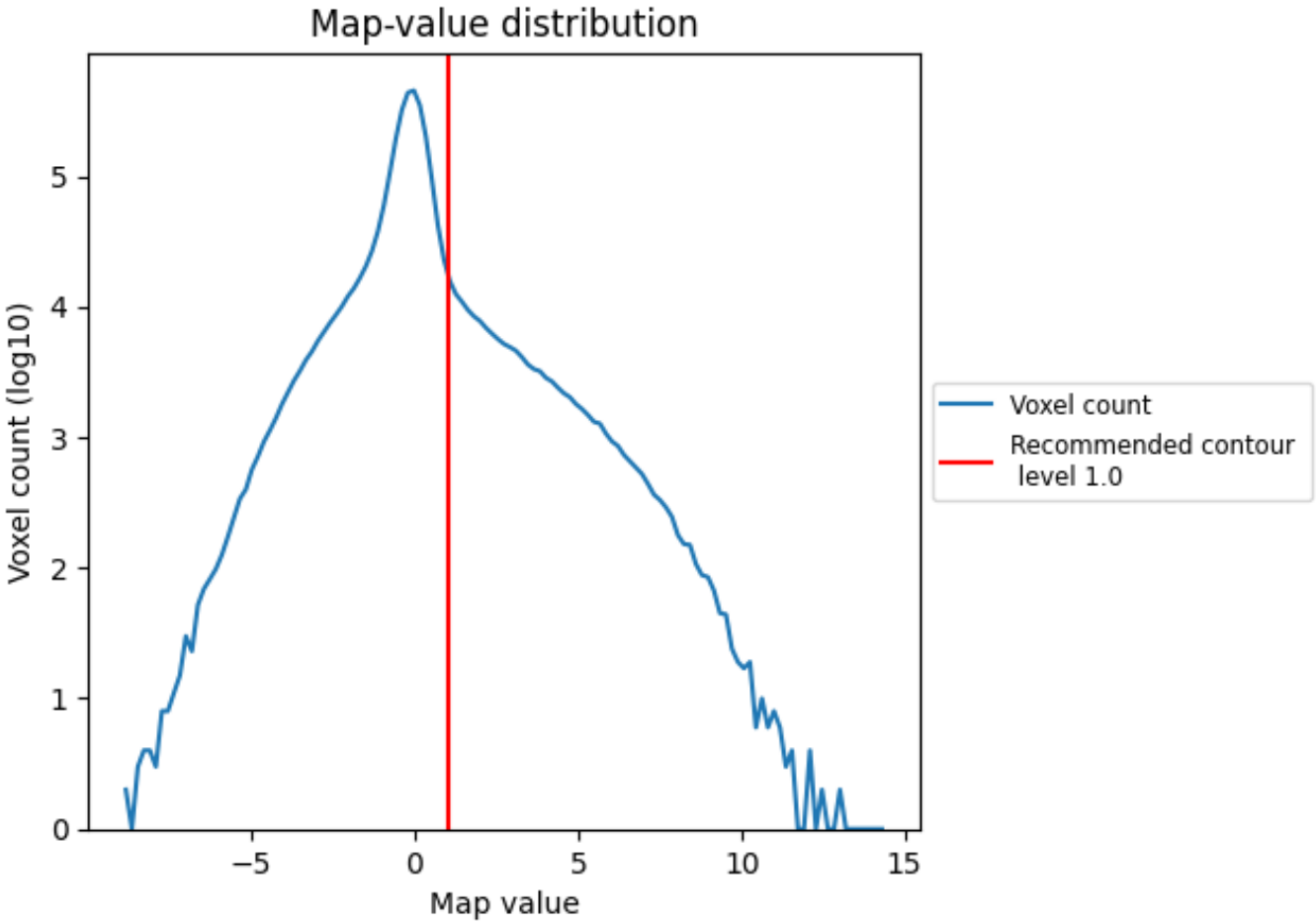
6.5 Mask visualisation (i)

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

7 Map analysis

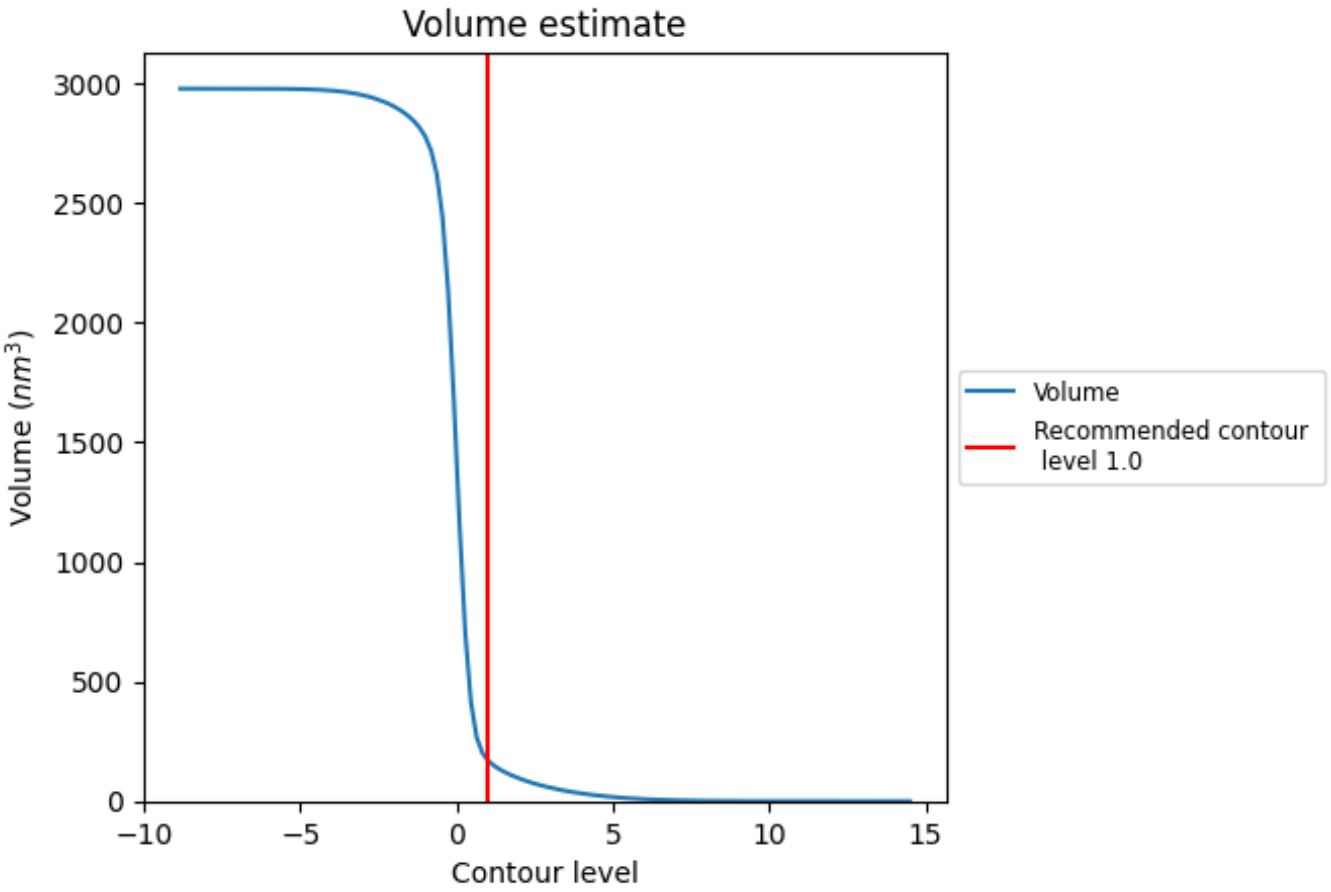
This section contains the results of statistical analysis of the map.

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 170 nm^3; this corresponds to an approximate mass of 154 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)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

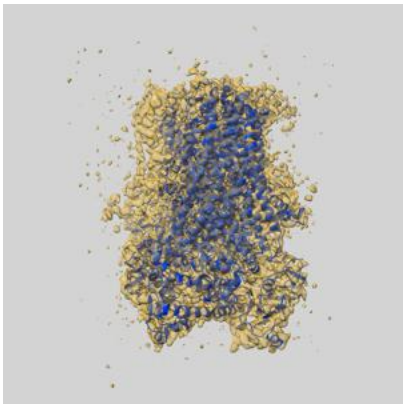
8 Fourier-Shell correlation (i)

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

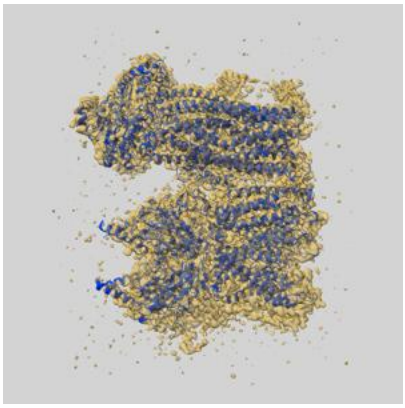
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-26304 and PDB model 7U1S. Per-residue inclusion information can be found in section 3 on page 9.

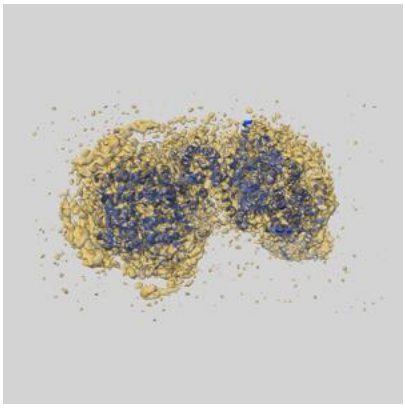
9.1 Map-model overlay



X



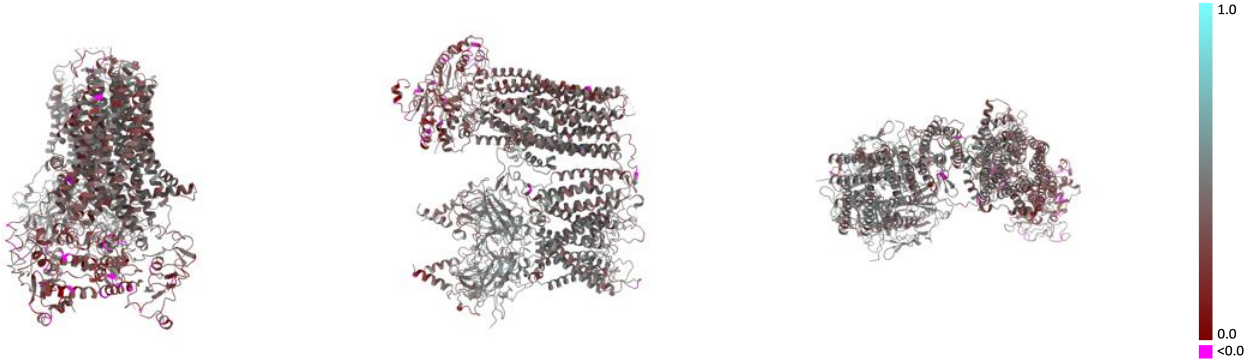
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.0 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.

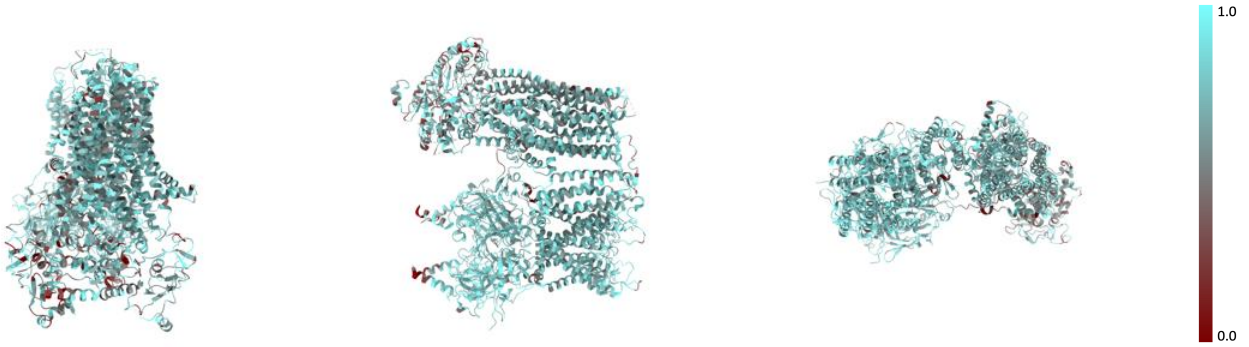
9.2 Q-score mapped to coordinate model



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.

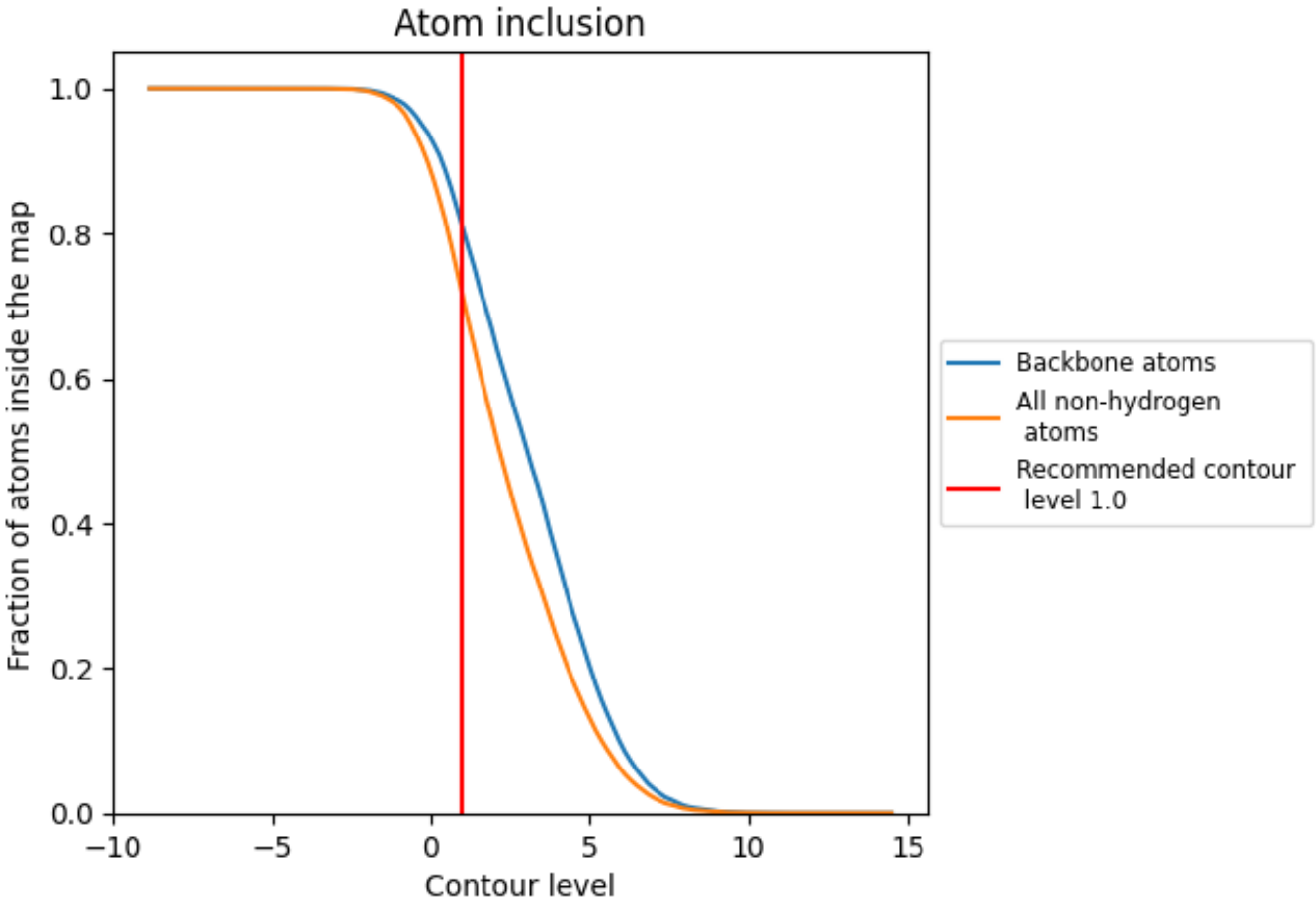
9.3 Atom inclusion mapped to coordinate model



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 (1.0).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 71% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (1.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7133	0.4040
A	0.7393	0.4420
B	0.7529	0.4420
C	0.7746	0.4460
D	0.7702	0.4440
E	0.6688	0.3650
F	0.1429	0.2030