Full wwPDB EM Validation Report ⓘ

Jan 5, 2025 – 10:42 PM EST

PDB ID	:	9CUK
EMDB ID	:	EMD-45936
Title	:	Structure of human full-length derived TRPV6 channel in Calmodulin-bound state
Authors	:	Neuberger, A.; Nadezhdin, K.D.; Sobolevsky, A.I.
Deposited on	:	2024-07-26
Resolution	:	3.26 Å(reported)

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

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

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

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

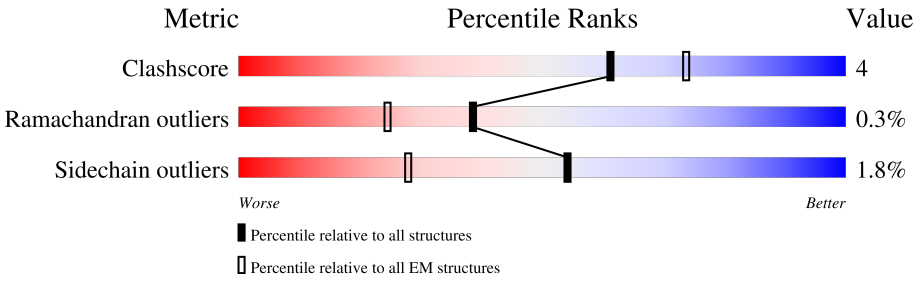
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 3.26 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	765	5% 70% 9% • 20%
1	B	765	6% 71% 10% • 19%
1	C	765	• 73% 10% • 16%
1	D	765	• 70% 10% • 20%
2	E	149	11% 87% 12% ••

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 22531 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.

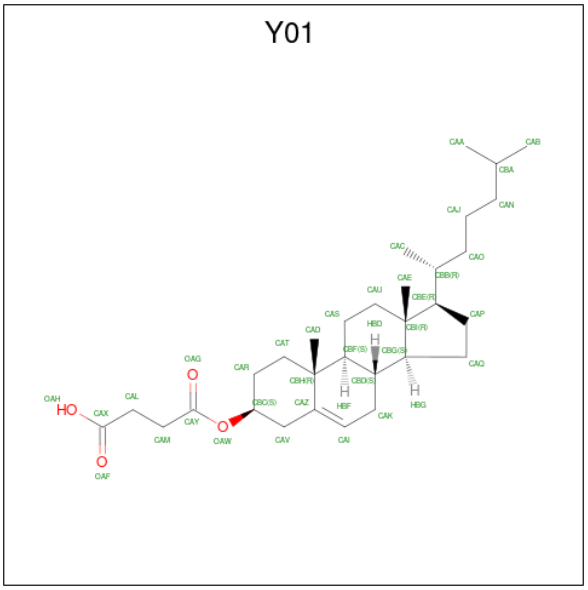
- Molecule 1 is a protein called Transient receptor potential cation channel subfamily V member 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	612	Total	C	N	O	S	0	0
			4912	3173	831	868	40		
1	B	619	Total	C	N	O	S	0	0
			4976	3211	847	878	40		
1	C	644	Total	C	N	O	S	0	0
			5182	3336	890	916	40		
1	D	612	Total	C	N	O	S	0	0
			4912	3173	831	868	40		

- Molecule 2 is a protein called Calmodulin-1.

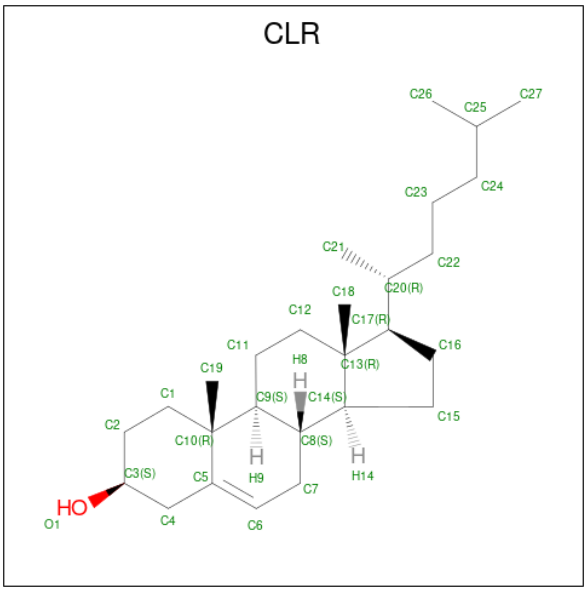
Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	148	Total	C	N	O	S	0	0
			1165	714	188	254	9		

- Molecule 3 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: $C_{31}H_{50}O_4$).



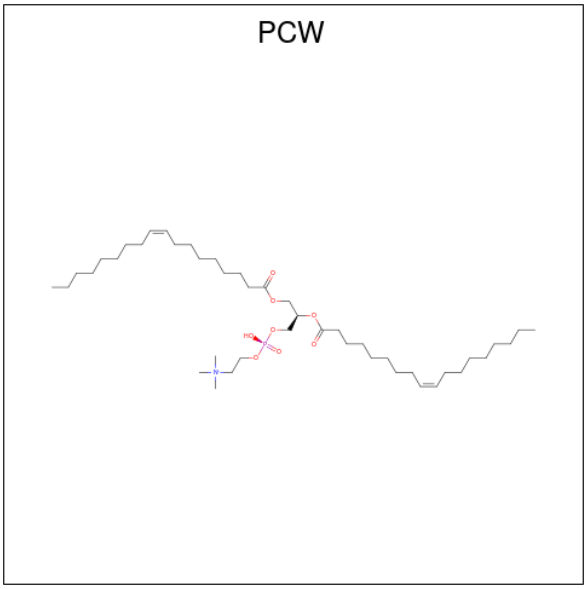
Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total C O 35 31 4	0
3	A	1	Total C O 35 31 4	0
3	B	1	Total C O 35 31 4	0
3	B	1	Total C O 35 31 4	0
3	C	1	Total C O 35 31 4	0
3	C	1	Total C O 35 31 4	0
3	C	1	Total C O 35 31 4	0
3	D	1	Total C O 35 31 4	0

- Molecule 4 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total C O 28 27 1	0
4	B	1	Total C O 28 27 1	0
4	C	1	Total C O 28 27 1	0
4	D	1	Total C O 28 27 1	0

- Molecule 5 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: $C_{44}H_{85}NO_8P$).



Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total C N O P 51 41 1 8 1	0
5	A	1	Total C 16 16	0
5	A	1	Total C 11 11	0
5	A	1	Total C 8 8	0
5	A	1	Total C 8 8	0
5	A	1	Total C 16 16	0
5	A	1	Total C 13 13	0
5	A	1	Total C N O P 43 33 1 8 1	0
5	A	1	Total C N O P 51 41 1 8 1	0
5	A	1	Total C 15 15	0
5	A	1	Total C 16 16	0
5	B	1	Total C 15 15	0

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Mol	Chain	Residues	Atoms	AltConf
5	B	1	Total C 16 16	0
5	B	1	Total C N O P 51 41 1 8 1	0
5	B	1	Total C 16 16	0
5	B	1	Total C 11 11	0
5	B	1	Total C 8 8	0
5	B	1	Total C 8 8	0
5	B	1	Total C 16 16	0
5	B	1	Total C 13 13	0
5	B	1	Total C N O P 43 33 1 8 1	0
5	B	1	Total C N O P 51 41 1 8 1	0
5	C	1	Total C 15 15	0
5	C	1	Total C 16 16	0
5	C	1	Total C N O P 51 41 1 8 1	0
5	C	1	Total C 16 16	0
5	C	1	Total C 11 11	0
5	C	1	Total C 8 8	0
5	C	1	Total C 16 16	0
5	C	1	Total C 13 13	0
5	C	1	Total C N O P 43 33 1 8 1	0
5	C	1	Total C N O P 51 41 1 8 1	0
5	D	1	Total C 13 13	0

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Mol	Chain	Residues	Atoms	AltConf
5	D	1	Total C N O P 43 33 1 8 1	0
5	D	1	Total C N O P 51 41 1 8 1	0
5	D	1	Total C 15 15	0
5	D	1	Total C 16 16	0
5	D	1	Total C N O P 51 41 1 8 1	0
5	D	1	Total C 16 16	0
5	D	1	Total C 11 11	0
5	D	1	Total C 8 8	0
5	D	1	Total C 8 8	0
5	D	1	Total C 16 16	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	AltConf
6	A	1	Total Ca 1 1	0
6	B	2	Total Ca 2 2	0
6	E	4	Total Ca 4 4	0

- Molecule 7 is water.

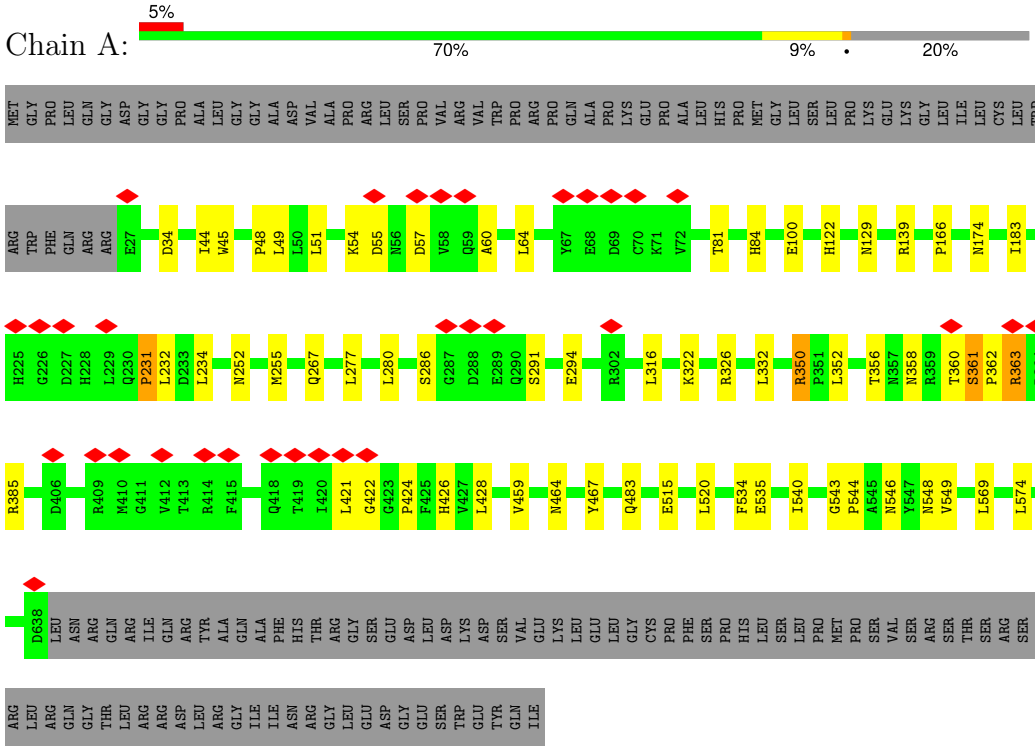
Mol	Chain	Residues	Atoms	AltConf
7	C	1	Total O 1 1	0

3 Residue-property plots (i)

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

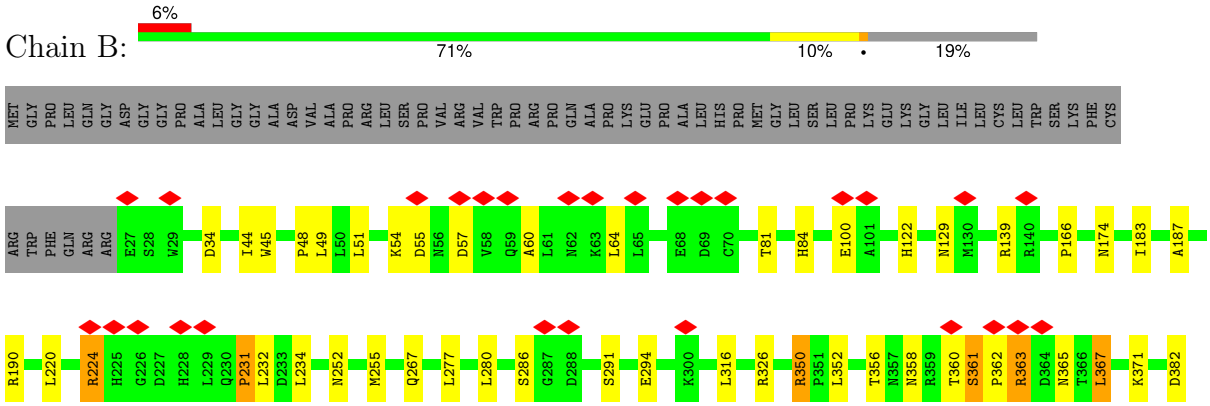
• Molecule 1: Transient receptor potential cation channel subfamily V member 6

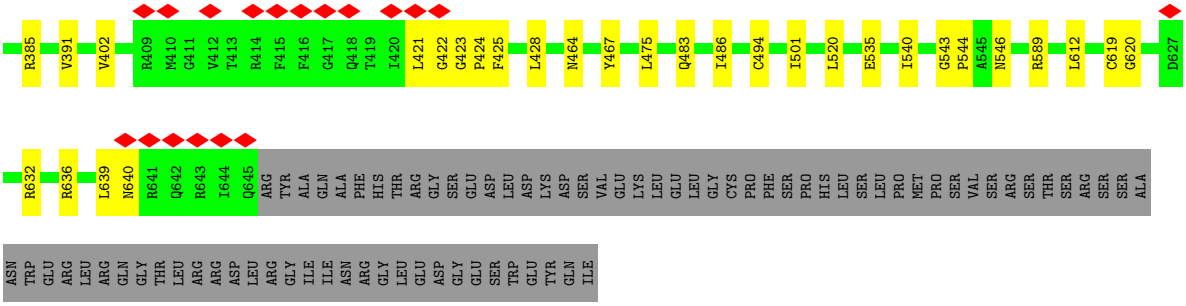
Chain A:



• Molecule 1: Transient receptor potential cation channel subfamily V member 6

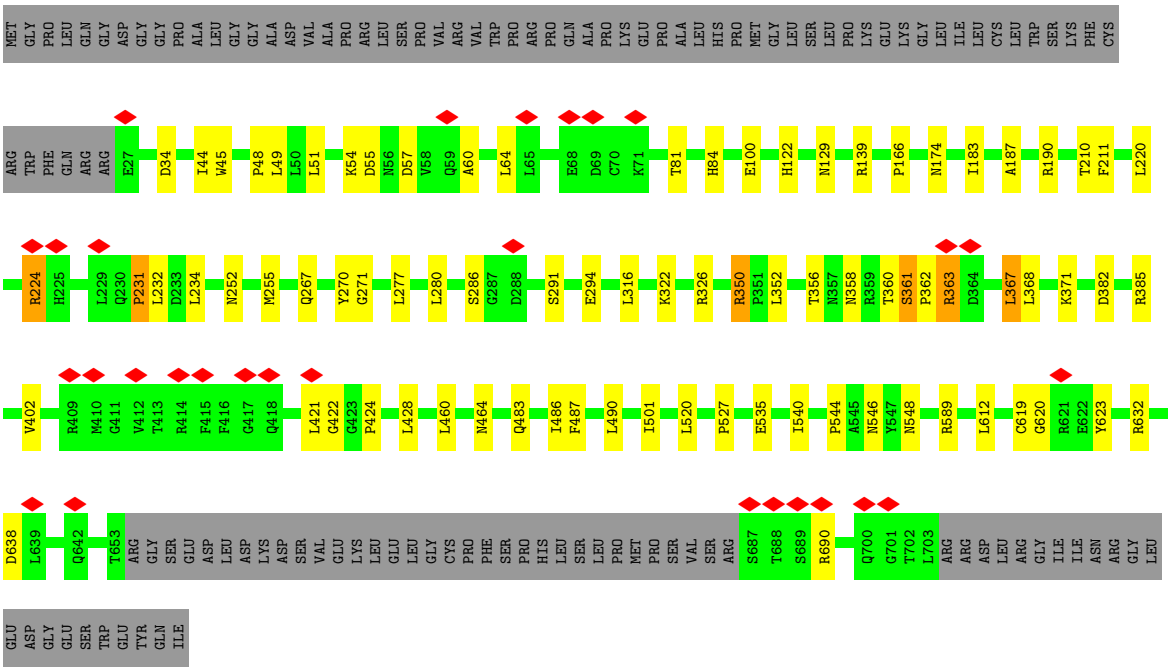
Chain B:





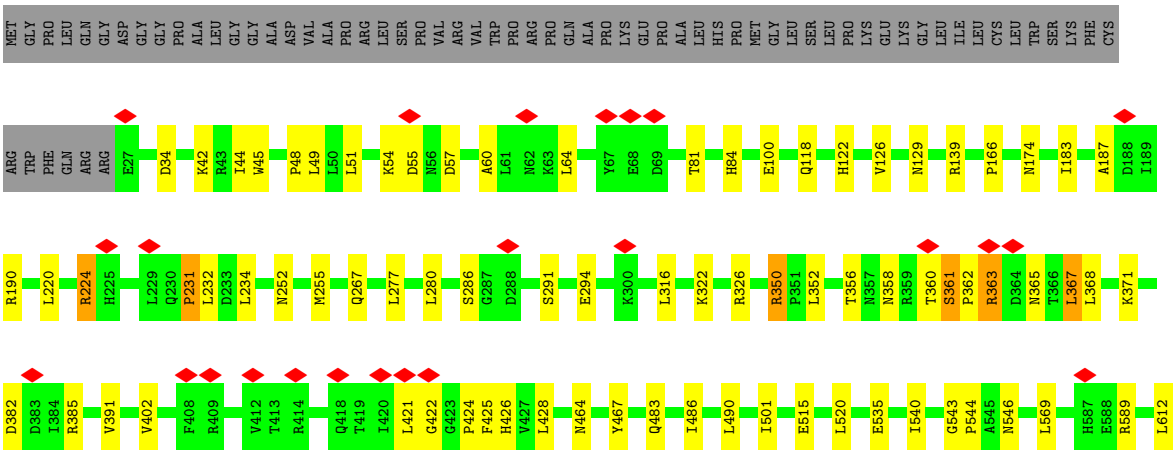
• Molecule 1: Transient receptor potential cation channel subfamily V member 6

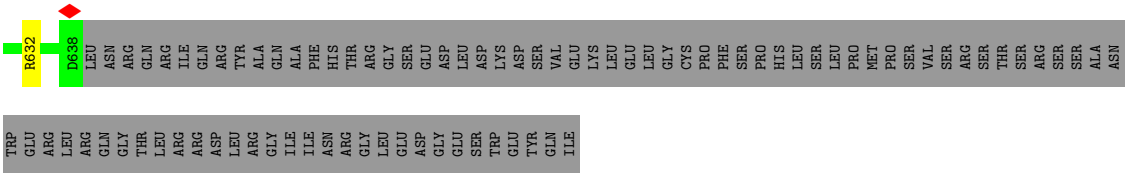
Chain C:



• Molecule 1: Transient receptor potential cation channel subfamily V member 6

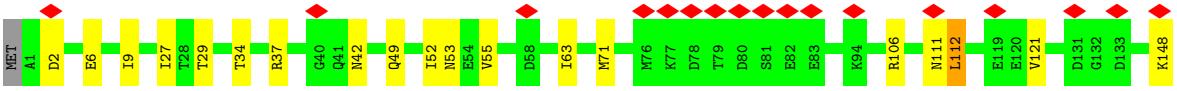
Chain D:





• Molecule 2: Calmodulin-1

Chain E:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	72482	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	58	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.956	Depositor
Minimum map value	-0.674	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.043	Depositor
Recommended contour level	0.109	Depositor
Map size (Å)	212.48, 212.48, 212.48	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PCW, Y01, CA, CLR

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	0.39	0/5025	0.56	3/6818 (0.0%)
1	B	0.38	0/5089	0.56	3/6903 (0.0%)
1	C	0.38	0/5299	0.56	3/7185 (0.0%)
1	D	0.39	0/5025	0.56	3/6818 (0.0%)
2	E	0.33	0/1177	0.61	2/1580 (0.1%)
All	All	0.38	0/21615	0.57	14/29304 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	5
1	C	0	6
1	D	0	5
All	All	0	21

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	112	LEU	CA-CB-CG	7.93	133.53	115.30
2	E	2	ASP	CB-CG-OD1	5.71	123.44	118.30
1	D	367	LEU	CA-CB-CG	5.49	127.93	115.30
1	C	367	LEU	CA-CB-CG	5.48	127.90	115.30
1	B	367	LEU	CA-CB-CG	5.48	127.89	115.30
1	A	367	LEU	CA-CB-CG	5.47	127.89	115.30
1	C	49	LEU	CA-CB-CG	5.15	127.14	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	49	LEU	CA-CB-CG	5.14	127.11	115.30
1	A	49	LEU	CA-CB-CG	5.13	127.09	115.30
1	D	49	LEU	CA-CB-CG	5.13	127.09	115.30
1	A	612	LEU	CA-CB-CG	5.09	127.01	115.30
1	D	612	LEU	CA-CB-CG	5.08	126.99	115.30
1	C	612	LEU	CA-CB-CG	5.08	126.99	115.30
1	B	612	LEU	CA-CB-CG	5.07	126.95	115.30

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	286	SER	Peptide
1	A	361	SER	Peptide
1	A	362	PRO	Peptide
1	A	422	GLY	Peptide
1	A	55	ASP	Peptide
1	B	286	SER	Peptide
1	B	361	SER	Peptide
1	B	362	PRO	Peptide
1	B	422	GLY	Peptide
1	B	55	ASP	Peptide
1	C	286	SER	Peptide
1	C	361	SER	Peptide
1	C	362	PRO	Peptide
1	C	422	GLY	Peptide
1	C	55	ASP	Peptide
1	C	638	ASP	Peptide
1	D	286	SER	Peptide
1	D	361	SER	Peptide
1	D	362	PRO	Peptide
1	D	422	GLY	Peptide
1	D	55	ASP	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4912	0	4964	40	0
1	B	4976	0	5034	41	0
1	C	5182	0	5229	45	0
1	D	4912	0	4964	48	0
2	E	1165	0	1096	9	0
3	A	70	0	98	4	0
3	B	70	0	98	5	0
3	C	105	0	147	6	0
3	D	35	0	49	7	0
4	A	28	0	46	3	0
4	B	28	0	46	5	0
4	C	28	0	46	4	0
4	D	28	0	46	3	0
5	A	248	0	368	3	0
5	B	248	0	368	11	0
5	C	240	0	356	9	0
5	D	248	0	368	7	0
6	A	1	0	0	0	0
6	B	2	0	0	0	0
6	E	4	0	0	0	0
7	C	1	0	0	0	0
All	All	22531	0	23323	194	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 4.

All (194) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:501:ILE:HD11	3:C:801:Y01:HAC2	1.76	0.68
2:E:55:VAL:HG21	2:E:71:MET:HB2	1.77	0.67
1:C:486:ILE:HD12	4:C:805:CLR:H191	1.80	0.64
1:D:467:TYR:CE1	3:D:806:Y01:HAM2	2.32	0.63
1:A:467:TYR:CE1	3:A:801:Y01:HAM2	2.35	0.62
1:C:190:ARG:NH2	1:C:231:PRO:O	2.33	0.61
1:C:501:ILE:HD11	3:C:806:Y01:HAC2	1.81	0.61
1:B:190:ARG:NH2	1:B:231:PRO:O	2.33	0.61
1:A:190:ARG:NH2	1:A:231:PRO:O	2.33	0.61
1:B:425:PHE:HB2	3:B:804:Y01:HAL1	1.83	0.60
1:D:190:ARG:NH2	1:D:231:PRO:O	2.33	0.60
1:C:421:LEU:O	1:C:483:GLN:NE2	2.37	0.57
1:D:361:SER:O	1:D:363:ARG:N	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:267:GLN:HE21	1:D:277:LEU:HD22	1.69	0.56
1:B:267:GLN:HE21	1:B:277:LEU:HD22	1.69	0.56
1:B:100:GLU:OE2	1:B:139:ARG:NH2	2.39	0.56
1:D:486:ILE:HD12	4:D:807:CLR:H191	1.87	0.56
1:C:267:GLN:HE21	1:C:277:LEU:HD22	1.70	0.56
1:C:361:SER:O	1:C:363:ARG:N	2.34	0.56
1:C:100:GLU:OE2	1:C:139:ARG:NH2	2.39	0.56
1:A:267:GLN:HE21	1:A:277:LEU:HD22	1.70	0.55
1:D:100:GLU:OE2	1:D:139:ARG:NH2	2.39	0.55
1:D:356:THR:HG23	1:D:371:LYS:HD3	1.89	0.55
1:C:356:THR:HG23	1:C:371:LYS:HD3	1.89	0.55
1:B:361:SER:O	1:B:363:ARG:N	2.34	0.55
1:A:100:GLU:OE2	1:A:139:ARG:NH2	2.39	0.55
1:A:361:SER:O	1:A:363:ARG:N	2.34	0.54
1:A:81:THR:H	1:A:84:HIS:HD2	1.56	0.54
1:A:356:THR:HG23	1:A:371:LYS:HD3	1.89	0.54
1:A:421:LEU:O	1:A:483:GLN:NE2	2.37	0.54
1:B:356:THR:HG23	1:B:371:LYS:HD3	1.88	0.54
1:B:365:ASN:ND2	1:C:548:ASN:O	2.41	0.54
1:D:421:LEU:O	1:D:483:GLN:NE2	2.37	0.54
1:D:81:THR:H	1:D:84:HIS:HD2	1.56	0.53
1:B:636:ARG:HH21	1:B:639:LEU:HD21	1.74	0.53
1:A:548:ASN:O	1:D:365:ASN:ND2	2.41	0.53
1:B:535:GLU:HG2	1:B:540:ILE:HD11	1.90	0.53
1:D:535:GLU:HG2	1:D:540:ILE:HD11	1.90	0.53
1:A:535:GLU:HG2	1:A:540:ILE:HD11	1.90	0.53
1:C:487:PHE:HZ	5:C:808:PCW:H182	1.74	0.52
1:C:81:THR:H	1:C:84:HIS:HD2	1.56	0.52
1:B:81:THR:H	1:B:84:HIS:HD2	1.56	0.52
1:C:535:GLU:HG2	1:C:540:ILE:HD11	1.90	0.52
1:C:632:ARG:NH1	1:D:34:ASP:OD1	2.35	0.52
1:B:391:VAL:HG11	5:B:814:PCW:H251	1.92	0.51
1:C:270:TYR:OH	1:D:118:GLN:NE2	2.43	0.51
1:D:220:LEU:HD23	1:D:232:LEU:HD23	1.93	0.51
1:B:421:LEU:O	1:B:483:GLN:NE2	2.37	0.51
1:B:428:LEU:HD11	4:B:805:CLR:H122	1.91	0.51
1:D:428:LEU:HD11	4:D:807:CLR:H122	1.92	0.51
1:C:231:PRO:HD2	1:C:234:LEU:HB2	1.93	0.51
2:E:49:GLN:OE1	2:E:53:ASN:ND2	2.44	0.51
1:B:382:ASP:OD1	1:B:385:ARG:NH2	2.44	0.51
1:D:382:ASP:OD1	1:D:385:ARG:NH2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:SER:OG	1:B:294:GLU:OE1	2.27	0.51
1:C:220:LEU:HD23	1:C:232:LEU:HD23	1.92	0.51
1:D:291:SER:OG	1:D:294:GLU:OE1	2.27	0.51
1:A:382:ASP:OD1	1:A:385:ARG:NH2	2.44	0.51
1:D:231:PRO:HD2	1:D:234:LEU:HB2	1.92	0.51
2:E:55:VAL:HG11	2:E:71:MET:HG3	1.92	0.51
1:B:231:PRO:HD2	1:B:234:LEU:HB2	1.93	0.50
1:C:291:SER:OG	1:C:294:GLU:OE1	2.27	0.50
1:A:220:LEU:HD23	1:A:232:LEU:HD23	1.93	0.50
2:E:106:ARG:HG2	2:E:121:VAL:HG21	1.93	0.50
1:B:220:LEU:HD23	1:B:232:LEU:HD23	1.93	0.50
1:C:382:ASP:OD1	1:C:385:ARG:NH2	2.44	0.50
1:C:520:LEU:HD21	1:C:544:PRO:HB3	1.94	0.50
1:A:520:LEU:HD21	1:A:544:PRO:HB3	1.94	0.50
1:A:231:PRO:HD2	1:A:234:LEU:HB2	1.93	0.49
1:B:57:ASP:HB3	1:B:60:ALA:HB3	1.95	0.49
1:C:460:LEU:HD21	5:C:808:PCW:H252	1.93	0.49
1:A:632:ARG:NH1	1:B:34:ASP:OD1	2.35	0.49
1:C:210:THR:HB	2:E:6:GLU:HG2	1.95	0.49
5:C:814:PCW:H152	5:C:814:PCW:H121	1.64	0.49
2:E:27:ILE:HB	2:E:63:ILE:HB	1.94	0.49
1:D:57:ASP:HB3	1:D:60:ALA:HB3	1.95	0.49
1:D:520:LEU:HD21	1:D:544:PRO:HB3	1.94	0.48
1:B:486:ILE:HD12	4:B:805:CLR:H191	1.95	0.48
1:A:332:LEU:HD23	3:A:801:Y01:HAD2	1.95	0.48
1:C:211:PHE:HE1	2:E:9:ILE:HG13	1.79	0.48
1:A:57:ASP:HB3	1:A:60:ALA:HB3	1.95	0.48
5:B:806:PCW:H212	3:C:801:Y01:HAE2	1.95	0.48
1:C:57:ASP:HB3	1:C:60:ALA:HB3	1.95	0.47
1:C:623:TYR:HA	1:D:42:LYS:HD2	1.95	0.47
1:B:520:LEU:HD21	1:B:544:PRO:HB3	1.94	0.47
1:D:467:TYR:CE2	3:D:806:Y01:HAR2	2.50	0.47
5:D:803:PCW:H272	3:D:806:Y01:HAB3	1.97	0.47
1:A:424:PRO:HB2	4:A:802:CLR:H11	1.96	0.47
1:B:632:ARG:NH1	1:C:34:ASP:OD1	2.44	0.47
1:C:368:LEU:HA	1:D:515:GLU:HG2	1.97	0.47
1:C:428:LEU:HD11	4:C:805:CLR:H122	1.98	0.46
1:B:424:PRO:HB2	4:B:805:CLR:H11	1.98	0.46
1:A:459:VAL:HG21	4:A:802:CLR:H241	1.98	0.46
1:B:326:ARG:HD3	5:B:813:PCW:H132	1.97	0.46
1:A:291:SER:OG	1:A:294:GLU:OE1	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:467:TYR:CE2	3:B:804:Y01:HAR2	2.51	0.46
1:B:402:VAL:HG21	3:B:804:Y01:HAK1	1.98	0.45
5:C:807:PCW:H82	5:C:807:PCW:H42	1.76	0.45
1:C:402:VAL:HG21	3:C:804:Y01:HAK1	1.98	0.45
5:C:808:PCW:H132	5:C:808:PCW:H162	1.77	0.45
1:D:391:VAL:HG11	5:D:803:PCW:H261	1.99	0.45
1:B:48:PRO:HB2	1:B:64:LEU:HD21	1.99	0.45
1:C:527:PRO:HB2	3:C:806:Y01:HAL2	1.99	0.45
1:C:490:LEU:HD22	1:D:569:LEU:HD13	1.98	0.44
1:A:44:ILE:HG21	1:A:54:LYS:HD2	1.99	0.44
1:A:280:LEU:HD21	1:A:316:LEU:HD13	1.99	0.44
1:D:425:PHE:HB2	3:D:806:Y01:HAM1	1.99	0.44
1:A:428:LEU:HD11	4:A:802:CLR:H122	1.99	0.44
1:D:48:PRO:HB2	1:D:64:LEU:HD21	1.99	0.44
5:D:808:PCW:H42	5:D:808:PCW:H62	1.81	0.44
1:A:549:VAL:HA	1:D:365:ASN:HA	1.99	0.44
3:A:812:Y01:HAC1	1:D:501:ILE:HD11	2.00	0.44
1:B:44:ILE:HG21	1:B:54:LYS:HD2	1.98	0.44
1:B:494:CYS:HB3	3:C:801:Y01:HAN2	1.99	0.44
5:C:802:PCW:H152	5:C:803:PCW:H121	1.99	0.44
1:C:350:ARG:HE	1:C:352:LEU:HD11	1.83	0.44
5:C:814:PCW:H261	5:C:814:PCW:H231	1.85	0.44
1:B:280:LEU:HD21	1:B:316:LEU:HD13	1.99	0.44
5:D:810:PCW:H211	5:D:810:PCW:H182	1.72	0.44
1:A:34:ASP:OD1	1:D:632:ARG:NH1	2.44	0.43
1:A:48:PRO:HB2	1:A:64:LEU:HD21	1.99	0.43
5:A:811:PCW:H40	5:A:811:PCW:H432	1.78	0.43
1:D:350:ARG:HE	1:D:352:LEU:HD11	1.83	0.43
1:A:350:ARG:HE	1:A:352:LEU:HD11	1.83	0.43
1:B:350:ARG:HE	1:B:352:LEU:HD11	1.83	0.43
1:C:44:ILE:HG21	1:C:54:LYS:HD2	1.99	0.43
1:C:48:PRO:HB2	1:C:64:LEU:HD21	1.99	0.43
1:C:280:LEU:HD21	1:C:316:LEU:HD13	1.99	0.43
1:C:632:ARG:HD3	1:D:34:ASP:HA	2.01	0.43
5:B:814:PCW:H212	5:B:814:PCW:H182	1.78	0.43
1:D:44:ILE:HG21	1:D:54:LYS:HD2	1.99	0.43
1:C:358:ASN:HB3	1:C:360:THR:HG23	2.01	0.43
1:D:280:LEU:HD21	1:D:316:LEU:HD13	1.99	0.43
1:D:81:THR:H	1:D:84:HIS:CD2	2.36	0.43
1:A:515:GLU:HG2	1:D:368:LEU:HA	2.01	0.42
1:D:402:VAL:HG21	3:D:806:Y01:HAK1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:HIS:CD2	1:A:166:PRO:HG3	2.54	0.42
1:C:122:HIS:CD2	1:C:166:PRO:HG3	2.55	0.42
1:C:252:ASN:HB3	1:C:255:MET:HB2	2.02	0.42
1:B:358:ASN:HB3	1:B:360:THR:HG23	2.01	0.42
5:B:814:PCW:H122	5:B:814:PCW:H31	1.84	0.42
2:E:34:THR:HG22	2:E:37:ARG:HH21	1.85	0.42
1:C:81:THR:H	1:C:84:HIS:CD2	2.36	0.42
1:A:426:HIS:HD2	3:A:801:Y01:OAG	2.03	0.42
3:D:806:Y01:HAB1	3:D:806:Y01:HAJ2	1.73	0.42
1:B:183:ILE:HD13	1:B:187:ALA:HB3	2.02	0.42
1:B:475:LEU:HD13	5:B:812:PCW:H161	2.02	0.42
5:B:806:PCW:H152	5:B:806:PCW:H182	1.78	0.42
1:D:122:HIS:CD2	1:D:166:PRO:HG3	2.55	0.42
1:A:252:ASN:HB3	1:A:255:MET:HB2	2.01	0.41
5:D:804:PCW:H221	5:D:805:PCW:H171	2.02	0.41
1:A:358:ASN:HB3	1:A:360:THR:HG23	2.01	0.41
1:B:543:GLY:HA2	1:B:544:PRO:HD3	1.90	0.41
1:D:426:HIS:NE2	3:D:806:Y01:HAL2	2.35	0.41
1:B:122:HIS:CD2	1:B:166:PRO:HG3	2.55	0.41
3:B:804:Y01:HAO1	3:B:804:Y01:HAP1	1.75	0.41
1:C:183:ILE:HD13	1:C:187:ALA:HB3	2.02	0.41
5:B:813:PCW:H73	5:B:813:PCW:H41	1.94	0.41
1:C:271:GLY:HA3	1:D:126:VAL:HG12	2.01	0.41
1:A:543:GLY:HA2	1:A:544:PRO:HD3	1.90	0.41
1:C:45:TRP:HD1	1:C:51:LEU:HD13	1.85	0.41
1:D:358:ASN:HB3	1:D:360:THR:HG23	2.01	0.41
1:A:45:TRP:HD1	1:A:51:LEU:HD13	1.85	0.41
1:A:183:ILE:HD13	1:A:187:ALA:HB3	2.02	0.41
1:A:569:LEU:HD13	1:D:490:LEU:HD22	2.02	0.41
1:C:424:PRO:HG2	4:C:805:CLR:H11	2.01	0.41
1:A:81:THR:H	1:A:84:HIS:CD2	2.36	0.41
1:D:45:TRP:HD1	1:D:51:LEU:HD13	1.85	0.41
1:D:424:PRO:HB2	4:D:807:CLR:H11	2.03	0.41
2:E:29:THR:HG22	2:E:52:ILE:HG13	2.02	0.41
1:B:45:TRP:HD1	1:B:51:LEU:HD13	1.85	0.41
1:B:252:ASN:HB3	1:B:255:MET:HB2	2.02	0.41
4:C:805:CLR:H211	4:C:805:CLR:H232	1.83	0.41
5:C:807:PCW:H222	5:C:807:PCW:H422	2.02	0.41
1:D:252:ASN:HB3	1:D:255:MET:HB2	2.01	0.41
5:B:813:PCW:H341	5:B:813:PCW:H372	1.89	0.41
5:C:813:PCW:H211	5:C:813:PCW:H181	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:810:PCW:H142	5:B:810:PCW:H171	1.88	0.40
1:A:322:LYS:NZ	1:A:326:ARG:HH12	2.19	0.40
5:A:811:PCW:H162	5:A:811:PCW:H131	1.81	0.40
1:B:423:GLY:HA3	1:B:424:PRO:HD3	1.90	0.40
1:C:322:LYS:NZ	1:C:326:ARG:HH12	2.19	0.40
1:D:183:ILE:HD13	1:D:187:ALA:HB3	2.02	0.40
1:D:322:LYS:NZ	1:D:326:ARG:HH12	2.19	0.40
5:A:810:PCW:H211	5:A:810:PCW:H181	1.89	0.40
5:D:803:PCW:H181	5:D:803:PCW:H211	1.85	0.40
1:A:534:PHE:HB2	3:B:801:Y01:HAC2	2.03	0.40
1:D:543:GLY:HA2	1:D:544:PRO:HD3	1.90	0.40
5:D:802:PCW:H121	5:D:802:PCW:H31	1.82	0.40
1:A:574:LEU:HA	1:A:574:LEU:HD23	1.89	0.40
1:B:619:CYS:SG	1:B:620:GLY:N	2.95	0.40
4:B:805:CLR:H212	5:B:807:PCW:H19	2.04	0.40
4:B:805:CLR:H222	4:B:805:CLR:H162	1.93	0.40
1:C:619:CYS:SG	1:C:620:GLY:N	2.95	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	610/765 (80%)	547 (90%)	61 (10%)	2 (0%)	37	66
1	B	617/765 (81%)	551 (89%)	64 (10%)	2 (0%)	37	66
1	C	640/765 (84%)	575 (90%)	63 (10%)	2 (0%)	37	66
1	D	610/765 (80%)	547 (90%)	61 (10%)	2 (0%)	37	66
2	E	146/149 (98%)	132 (90%)	14 (10%)	0	100	100
All	All	2623/3209 (82%)	2352 (90%)	263 (10%)	8 (0%)	38	66

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	ARG
1	A	231	PRO
1	B	224	ARG
1	B	231	PRO
1	C	224	ARG
1	C	231	PRO
1	D	224	ARG
1	D	231	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	A	531/662 (80%)	522 (98%)	9 (2%)	56	73
1	B	538/662 (81%)	528 (98%)	10 (2%)	52	71
1	C	559/662 (84%)	549 (98%)	10 (2%)	54	72
1	D	531/662 (80%)	522 (98%)	9 (2%)	56	73
2	E	126/127 (99%)	122 (97%)	4 (3%)	34	59
All	All	2285/2775 (82%)	2243 (98%)	42 (2%)	54	72

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	ASN
1	A	174	ASN
1	A	224	ARG
1	A	350	ARG
1	A	363	ARG
1	A	367	LEU
1	A	464	ASN
1	A	546	ASN
1	A	589	ARG
1	B	129	ASN

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Mol	Chain	Res	Type
1	B	174	ASN
1	B	224	ARG
1	B	350	ARG
1	B	363	ARG
1	B	367	LEU
1	B	464	ASN
1	B	546	ASN
1	B	589	ARG
1	B	640	ASN
1	C	129	ASN
1	C	174	ASN
1	C	224	ARG
1	C	350	ARG
1	C	363	ARG
1	C	367	LEU
1	C	464	ASN
1	C	546	ASN
1	C	589	ARG
1	C	690	ARG
1	D	129	ASN
1	D	174	ASN
1	D	224	ARG
1	D	350	ARG
1	D	363	ARG
1	D	367	LEU
1	D	464	ASN
1	D	546	ASN
1	D	589	ARG
2	E	42	ASN
2	E	111	ASN
2	E	112	LEU
2	E	148	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	HIS
1	A	84	HIS
1	A	118	GLN
1	A	129	ASN
1	A	174	ASN
1	A	206	GLN

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Mol	Chain	Res	Type
1	A	217	ASN
1	A	228	HIS
1	A	230	GLN
1	A	252	ASN
1	A	267	GLN
1	A	365	ASN
1	A	426	HIS
1	B	73	HIS
1	B	84	HIS
1	B	118	GLN
1	B	129	ASN
1	B	174	ASN
1	B	206	GLN
1	B	217	ASN
1	B	228	HIS
1	B	230	GLN
1	B	252	ASN
1	B	267	GLN
1	B	365	ASN
1	B	640	ASN
1	C	73	HIS
1	C	84	HIS
1	C	118	GLN
1	C	129	ASN
1	C	174	ASN
1	C	206	GLN
1	C	217	ASN
1	C	228	HIS
1	C	230	GLN
1	C	252	ASN
1	C	267	GLN
1	C	652	HIS
1	D	31	GLN
1	D	73	HIS
1	D	84	HIS
1	D	118	GLN
1	D	129	ASN
1	D	174	ASN
1	D	206	GLN
1	D	217	ASN
1	D	228	HIS
1	D	230	GLN

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Mol	Chain	Res	Type
1	D	252	ASN
1	D	267	GLN
1	D	365	ASN
2	E	42	ASN
2	E	49	GLN
2	E	53	ASN
2	E	111	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

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 62 ligands modelled in this entry, 7 are monoatomic - leaving 55 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	$\#\|Z\| > 2$
5	PCW	A	805	-	10,10,53	0.91	0	9,9,61	0.50	0
5	PCW	C	807	-	50,50,53	1.30	6 (12%)	56,58,61	0.89	3 (5%)
5	PCW	D	811	-	7,7,53	0.91	0	6,6,61	0.28	0
5	PCW	D	809	-	15,15,53	1.51	2 (13%)	14,14,61	0.74	0
4	CLR	C	805	-	31,31,31	0.35	0	48,48,48	0.75	0
5	PCW	C	814	-	50,50,53	1.32	6 (12%)	56,58,61	0.87	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	PCW	D	810	-	10,10,53	0.90	0	9,9,61	0.49	0
5	PCW	C	802	-	14,14,53	0.87	0	13,13,61	0.33	0
5	PCW	A	807	-	7,7,53	0.92	0	6,6,61	0.27	0
5	PCW	A	804	-	15,15,53	1.50	2 (13%)	14,14,61	0.72	0
5	PCW	B	806	-	50,50,53	1.31	6 (12%)	56,58,61	0.95	3 (5%)
5	PCW	B	811	-	15,15,53	1.49	2 (13%)	14,14,61	0.70	0
5	PCW	A	810	-	42,42,53	1.41	6 (14%)	48,50,61	0.90	3 (6%)
5	PCW	B	814	-	50,50,53	1.32	6 (12%)	56,58,61	0.90	3 (5%)
5	PCW	C	809	-	10,10,53	0.93	0	9,9,61	0.42	0
5	PCW	D	804	-	14,14,53	0.85	0	13,13,61	0.39	0
3	Y01	D	806	-	38,38,38	0.49	0	57,57,57	0.58	0
5	PCW	C	803	-	15,15,53	1.52	2 (13%)	14,14,61	0.69	0
3	Y01	B	804	-	38,38,38	0.49	0	57,57,57	0.58	0
5	PCW	D	801	-	12,12,53	0.81	0	11,11,61	0.38	0
5	PCW	A	813	-	14,14,53	0.86	0	13,13,61	0.37	0
5	PCW	B	809	-	7,7,53	0.92	0	6,6,61	0.27	0
5	PCW	D	805	-	15,15,53	1.52	2 (13%)	14,14,61	0.69	0
5	PCW	B	807	-	15,15,53	1.51	2 (13%)	14,14,61	0.68	0
5	PCW	D	812	-	7,7,53	0.91	0	6,6,61	0.30	0
3	Y01	C	801	-	38,38,38	0.50	0	57,57,57	0.73	0
5	PCW	B	810	-	7,7,53	0.90	0	6,6,61	0.29	0
5	PCW	A	811	-	50,50,53	1.35	8 (16%)	56,58,61	0.93	3 (5%)
5	PCW	A	803	-	50,50,53	1.30	6 (12%)	56,58,61	1.00	3 (5%)
5	PCW	C	813	-	42,42,53	1.40	7 (16%)	48,50,61	0.97	3 (6%)
5	PCW	C	810	-	7,7,53	0.91	0	6,6,61	0.26	0
3	Y01	C	806	-	38,38,38	0.47	0	57,57,57	0.52	0
5	PCW	C	811	-	15,15,53	1.49	2 (13%)	14,14,61	0.71	0
5	PCW	D	813	-	15,15,53	1.50	2 (13%)	14,14,61	0.71	0
3	Y01	A	812	-	38,38,38	0.50	0	57,57,57	0.79	1 (1%)
5	PCW	D	802	-	42,42,53	1.38	6 (14%)	48,50,61	1.00	3 (6%)
5	PCW	A	808	-	15,15,53	1.51	2 (13%)	14,14,61	0.68	0
4	CLR	B	805	-	31,31,31	0.35	0	48,48,48	0.67	0
3	Y01	A	801	-	38,38,38	0.48	0	57,57,57	0.62	0
5	PCW	B	813	-	42,42,53	1.40	6 (14%)	48,50,61	1.02	3 (6%)
5	PCW	C	812	-	12,12,53	0.83	0	11,11,61	0.38	0
4	CLR	A	802	-	31,31,31	0.37	0	48,48,48	0.76	0
3	Y01	C	804	-	38,38,38	0.46	0	57,57,57	0.52	0
5	PCW	A	814	-	15,15,53	1.52	2 (13%)	14,14,61	0.71	0
5	PCW	B	802	-	14,14,53	0.87	0	13,13,61	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	PCW	C	808	-	15,15,53	1.48	2 (13%)	14,14,61	0.78	0
5	PCW	B	803	-	15,15,53	1.53	2 (13%)	14,14,61	0.66	0
5	PCW	D	808	-	50,50,53	1.30	6 (12%)	56,58,61	0.91	3 (5%)
5	PCW	A	806	-	7,7,53	0.92	0	6,6,61	0.25	0
5	PCW	B	812	-	12,12,53	0.76	0	11,11,61	0.48	0
5	PCW	D	803	-	50,50,53	1.32	7 (14%)	56,58,61	0.95	3 (5%)
5	PCW	B	808	-	10,10,53	0.92	0	9,9,61	0.43	0
3	Y01	B	801	-	38,38,38	0.46	0	57,57,57	0.51	0
5	PCW	A	809	-	12,12,53	0.84	0	11,11,61	0.38	0
4	CLR	D	807	-	31,31,31	0.32	0	48,48,48	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
5	PCW	A	805	-	-	4/8/8/57	-
5	PCW	C	807	-	-	24/54/54/57	-
5	PCW	D	811	-	-	3/5/5/57	-
5	PCW	D	809	-	-	10/13/13/57	-
4	CLR	C	805	-	-	7/10/68/68	0/4/4/4
5	PCW	C	814	-	-	29/54/54/57	-
5	PCW	D	810	-	-	4/8/8/57	-
5	PCW	C	802	-	-	7/12/12/57	-
5	PCW	A	807	-	-	3/5/5/57	-
5	PCW	A	804	-	-	9/13/13/57	-
5	PCW	B	806	-	-	31/54/54/57	-
5	PCW	B	811	-	-	8/13/13/57	-
5	PCW	A	810	-	-	27/46/46/57	-
5	PCW	B	814	-	-	26/54/54/57	-
5	PCW	C	809	-	-	4/8/8/57	-
5	PCW	D	804	-	-	7/12/12/57	-
3	Y01	D	806	-	-	16/19/77/77	0/4/4/4
5	PCW	C	803	-	-	10/13/13/57	-
3	Y01	B	804	-	-	9/19/77/77	0/4/4/4
5	PCW	D	801	-	-	4/10/10/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PCW	A	813	-	-	4/12/12/57	-
5	PCW	B	809	-	-	3/5/5/57	-
5	PCW	D	805	-	-	6/13/13/57	-
5	PCW	B	807	-	-	6/13/13/57	-
5	PCW	D	812	-	-	3/5/5/57	-
3	Y01	C	801	-	-	10/19/77/77	0/4/4/4
5	PCW	B	810	-	-	4/5/5/57	-
5	PCW	A	811	-	-	25/54/54/57	-
5	PCW	A	803	-	-	25/54/54/57	-
5	PCW	C	813	-	-	17/46/46/57	-
5	PCW	C	810	-	-	2/5/5/57	-
3	Y01	C	806	-	-	6/19/77/77	0/4/4/4
5	PCW	C	811	-	-	8/13/13/57	-
5	PCW	D	813	-	-	8/13/13/57	-
3	Y01	A	812	-	-	13/19/77/77	0/4/4/4
5	PCW	D	802	-	-	26/46/46/57	-
5	PCW	A	808	-	-	4/13/13/57	-
4	CLR	B	805	-	-	5/10/68/68	0/4/4/4
3	Y01	A	801	-	-	11/19/77/77	0/4/4/4
5	PCW	B	813	-	-	23/46/46/57	-
5	PCW	C	812	-	-	6/10/10/57	-
4	CLR	A	802	-	-	8/10/68/68	0/4/4/4
3	Y01	C	804	-	-	9/19/77/77	0/4/4/4
5	PCW	A	814	-	-	7/13/13/57	-
5	PCW	B	802	-	-	6/12/12/57	-
5	PCW	C	808	-	-	8/13/13/57	-
5	PCW	B	803	-	-	10/13/13/57	-
5	PCW	D	808	-	-	24/54/54/57	-
5	PCW	A	806	-	-	2/5/5/57	-
5	PCW	B	812	-	-	6/10/10/57	-
5	PCW	D	803	-	-	27/54/54/57	-
5	PCW	B	808	-	-	4/8/8/57	-
3	Y01	B	801	-	-	9/19/77/77	0/4/4/4
5	PCW	A	809	-	-	5/10/10/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CLR	D	807	-	-	8/10/68/68	0/4/4/4

All (100) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	805	PCW	C20-C19	4.16	1.55	1.31
5	B	803	PCW	C20-C19	4.15	1.55	1.31
5	A	804	PCW	C20-C19	4.14	1.55	1.31
5	C	803	PCW	C20-C19	4.14	1.55	1.31
5	B	807	PCW	C20-C19	4.13	1.55	1.31
5	A	808	PCW	C20-C19	4.13	1.55	1.31
5	A	814	PCW	C20-C19	4.10	1.55	1.31
5	D	813	PCW	C20-C19	4.08	1.54	1.31
5	D	809	PCW	C20-C19	4.08	1.54	1.31
5	B	811	PCW	C20-C19	4.07	1.54	1.31
5	C	811	PCW	C20-C19	4.04	1.54	1.31
5	C	808	PCW	C20-C19	4.02	1.54	1.31
5	A	811	PCW	O3-C11	3.90	1.44	1.33
5	D	803	PCW	O3-C11	3.77	1.44	1.33
5	A	810	PCW	O3-C11	3.76	1.44	1.33
5	B	814	PCW	O3-C11	3.73	1.44	1.33
5	D	802	PCW	O3-C11	3.70	1.44	1.33
5	C	814	PCW	O3-C11	3.70	1.44	1.33
5	B	813	PCW	O3-C11	3.69	1.44	1.33
5	D	808	PCW	O3-C11	3.69	1.44	1.33
5	B	806	PCW	O3-C11	3.68	1.44	1.33
5	C	807	PCW	O3-C11	3.66	1.44	1.33
5	A	803	PCW	O3-C11	3.64	1.44	1.33
5	C	813	PCW	O3-C11	3.63	1.43	1.33
5	B	813	PCW	O2-C31	3.57	1.44	1.34
5	C	813	PCW	O2-C31	3.48	1.44	1.34
5	A	811	PCW	O2-C31	3.44	1.44	1.34
5	C	814	PCW	O2-C31	3.44	1.44	1.34
5	A	810	PCW	O2-C31	3.42	1.44	1.34
5	D	803	PCW	O2-C31	3.39	1.43	1.34
5	C	807	PCW	O2-C31	3.38	1.43	1.34
5	A	803	PCW	O2-C31	3.37	1.43	1.34
5	D	808	PCW	O2-C31	3.32	1.43	1.34
5	B	814	PCW	O2-C31	3.31	1.43	1.34
5	D	802	PCW	O2-C31	3.29	1.43	1.34
5	B	806	PCW	O2-C31	3.23	1.43	1.34
5	D	808	PCW	O2-C2	-3.11	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	806	PCW	O2-C2	-3.11	1.39	1.46
5	C	807	PCW	O2-C2	-3.08	1.39	1.46
5	D	803	PCW	O2-C2	-2.97	1.39	1.46
5	A	803	PCW	O2-C2	-2.96	1.39	1.46
5	A	811	PCW	O2-C2	-2.96	1.39	1.46
5	B	814	PCW	O2-C2	-2.95	1.39	1.46
5	C	814	PCW	O2-C2	-2.92	1.39	1.46
5	D	802	PCW	O2-C2	-2.91	1.39	1.46
5	C	813	PCW	O2-C2	-2.86	1.39	1.46
5	C	811	PCW	C18-C19	-2.80	1.34	1.50
5	A	804	PCW	C18-C19	-2.78	1.34	1.50
5	A	810	PCW	O2-C2	-2.78	1.40	1.46
5	B	811	PCW	C18-C19	-2.77	1.34	1.50
5	C	808	PCW	C18-C19	-2.76	1.34	1.50
5	B	803	PCW	C18-C19	-2.75	1.34	1.50
5	A	814	PCW	C18-C19	-2.74	1.35	1.50
5	D	813	PCW	C18-C19	-2.73	1.35	1.50
5	C	803	PCW	C18-C19	-2.71	1.35	1.50
5	A	808	PCW	C18-C19	-2.71	1.35	1.50
5	D	809	PCW	C18-C19	-2.68	1.35	1.50
5	D	805	PCW	C18-C19	-2.64	1.35	1.50
5	B	807	PCW	C18-C19	-2.63	1.35	1.50
5	B	813	PCW	O2-C2	-2.63	1.40	1.46
5	B	814	PCW	P-O3P	2.52	1.69	1.59
5	C	814	PCW	P-O4P	2.49	1.69	1.59
5	B	814	PCW	P-O4P	2.48	1.69	1.59
5	C	813	PCW	P-O4P	2.47	1.69	1.59
5	A	811	PCW	P-O3P	2.47	1.69	1.59
5	B	813	PCW	P-O3P	2.44	1.68	1.59
5	D	803	PCW	P-O3P	2.44	1.68	1.59
5	A	811	PCW	P-O4P	2.43	1.68	1.59
5	D	803	PCW	P-O4P	2.42	1.68	1.59
5	A	803	PCW	P-O3P	2.40	1.68	1.59
5	D	802	PCW	P-O3P	2.40	1.68	1.59
5	B	813	PCW	P-O4P	2.39	1.68	1.59
5	C	814	PCW	P-O3P	2.38	1.68	1.59
5	D	802	PCW	P-O4P	2.38	1.68	1.59
5	B	806	PCW	P-O4P	2.37	1.68	1.59
5	B	806	PCW	P-O3P	2.37	1.68	1.59
5	A	810	PCW	C12-C11	2.36	1.57	1.50
5	C	813	PCW	P-O3P	2.35	1.68	1.59
5	D	808	PCW	P-O3P	2.34	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	807	PCW	C12-C11	2.33	1.57	1.50
5	A	810	PCW	P-O3P	2.32	1.68	1.59
5	A	811	PCW	C12-C11	2.32	1.57	1.50
5	D	808	PCW	P-O4P	2.30	1.68	1.59
5	C	807	PCW	P-O3P	2.30	1.68	1.59
5	A	803	PCW	P-O4P	2.30	1.68	1.59
5	A	810	PCW	P-O4P	2.27	1.68	1.59
5	C	807	PCW	P-O4P	2.22	1.68	1.59
5	B	813	PCW	C12-C11	2.19	1.57	1.50
5	C	813	PCW	C12-C11	2.13	1.56	1.50
5	A	803	PCW	C12-C11	2.13	1.56	1.50
5	D	803	PCW	C12-C11	2.13	1.56	1.50
5	C	814	PCW	C12-C11	2.13	1.56	1.50
5	B	806	PCW	C12-C11	2.13	1.56	1.50
5	B	814	PCW	C12-C11	2.12	1.56	1.50
5	D	802	PCW	C12-C11	2.10	1.56	1.50
5	C	813	PCW	C32-C31	2.08	1.56	1.50
5	D	803	PCW	C32-C31	2.06	1.56	1.50
5	A	811	PCW	C5-C4	2.04	1.57	1.51
5	A	811	PCW	C32-C31	2.03	1.56	1.50
5	D	808	PCW	C12-C11	2.02	1.56	1.50

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	803	PCW	O2-C31-C32	4.26	120.70	111.48
5	B	806	PCW	O2-C31-C32	4.20	120.56	111.48
5	D	803	PCW	O2-C31-C32	4.00	120.14	111.48
5	B	813	PCW	O2-C31-C32	3.97	120.06	111.48
5	A	811	PCW	O2-C31-C32	3.89	119.91	111.48
5	B	814	PCW	O2-C31-C32	3.79	119.68	111.48
5	C	813	PCW	O2-C31-C32	3.78	119.65	111.48
5	D	808	PCW	O2-C31-C32	3.72	119.52	111.48
5	C	814	PCW	O2-C31-C32	3.58	119.23	111.48
5	D	802	PCW	O2-C31-C32	3.57	119.21	111.48
5	C	807	PCW	O2-C31-C32	3.37	118.78	111.48
5	A	810	PCW	O2-C31-C32	3.05	118.07	111.48
5	D	802	PCW	O3-C11-C12	2.89	120.66	111.83
5	A	811	PCW	O3-C11-C12	2.83	120.48	111.83
5	B	814	PCW	O3-C11-C12	2.79	120.33	111.83
3	A	812	Y01	CBG-CBI-CBE	2.76	103.26	100.10
5	A	810	PCW	O3-C11-C12	2.74	120.19	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	808	PCW	O3-C11-C12	2.73	120.16	111.83
5	A	803	PCW	O3-C11-C12	2.72	120.12	111.83
5	D	803	PCW	O3-C11-C12	2.61	119.81	111.83
5	A	803	PCW	C7-N-C5	2.57	120.13	109.91
5	B	806	PCW	O3-C11-C12	2.56	119.64	111.83
5	C	813	PCW	O3-C11-C12	2.52	119.52	111.83
5	B	813	PCW	C7-N-C5	2.50	119.86	109.91
5	B	813	PCW	O3-C11-C12	2.50	119.45	111.83
5	D	803	PCW	C7-N-C5	2.49	119.80	109.91
5	C	807	PCW	O3-C11-C12	2.47	119.37	111.83
5	C	814	PCW	O3-C11-C12	2.46	119.33	111.83
5	D	802	PCW	C7-N-C5	2.37	119.33	109.91
5	A	810	PCW	C7-N-C5	2.28	118.97	109.91
5	D	808	PCW	C7-N-C5	2.22	118.72	109.91
5	C	813	PCW	C7-N-C5	2.22	118.72	109.91
5	A	811	PCW	C7-N-C5	2.18	118.57	109.91
5	B	806	PCW	C7-N-C5	2.14	118.42	109.91
5	C	814	PCW	C7-N-C5	2.13	118.36	109.91
5	C	807	PCW	C7-N-C5	2.08	118.19	109.91
5	B	814	PCW	C7-N-C5	2.08	118.18	109.91

There are no chirality outliers.

All (590) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	801	Y01	CAX-CAL-CAM-CAY
3	A	812	Y01	CAO-CBB-CBE-CAP
3	A	812	Y01	CAO-CBB-CBE-CBI
3	A	812	Y01	CAC-CBB-CBE-CBI
3	A	812	Y01	CAM-CAY-OAW-CBC
3	C	801	Y01	CAR-CBC-OAW-CAY
3	C	801	Y01	CAM-CAY-OAW-CBC
3	C	806	Y01	CAM-CAY-OAW-CBC
4	D	807	CLR	C13-C17-C20-C21
5	A	803	PCW	C1-O3P-P-O1P
5	A	803	PCW	C1-O3P-P-O2P
5	A	803	PCW	C1-O3P-P-O4P
5	A	803	PCW	C4-O4P-P-O2P
5	A	803	PCW	C4-O4P-P-O3P
5	A	810	PCW	O4P-C4-C5-N
5	A	810	PCW	C39-C40-C41-C42
5	A	811	PCW	C4-O4P-P-O1P

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Mol	Chain	Res	Type	Atoms
5	A	811	PCW	C4-O4P-P-O3P
5	B	806	PCW	O4P-C4-C5-N
5	B	806	PCW	C1-O3P-P-O1P
5	B	806	PCW	C1-O3P-P-O4P
5	B	806	PCW	C4-O4P-P-O2P
5	B	806	PCW	C4-O4P-P-O3P
5	B	813	PCW	O31-C31-O2-C2
5	B	813	PCW	C4-O4P-P-O1P
5	B	813	PCW	C4-O4P-P-O3P
5	C	807	PCW	C1-O3P-P-O1P
5	C	807	PCW	C1-O3P-P-O2P
5	C	807	PCW	C4-O4P-P-O2P
5	C	807	PCW	C4-O4P-P-O3P
5	C	814	PCW	O4P-C4-C5-N
5	C	814	PCW	C1-O3P-P-O1P
5	C	814	PCW	C1-O3P-P-O2P
5	C	814	PCW	C1-O3P-P-O4P
5	C	814	PCW	C4-O4P-P-O1P
5	C	814	PCW	C4-O4P-P-O3P
5	D	802	PCW	C12-C11-O3-C3
5	D	802	PCW	O11-C11-O3-C3
5	D	802	PCW	C1-O3P-P-O1P
5	D	802	PCW	C1-O3P-P-O2P
5	D	802	PCW	C1-O3P-P-O4P
5	D	802	PCW	C4-O4P-P-O1P
5	D	802	PCW	C4-O4P-P-O2P
5	D	802	PCW	C4-O4P-P-O3P
5	D	803	PCW	O4P-C4-C5-N
5	D	803	PCW	C32-C31-O2-C2
5	D	803	PCW	O31-C31-O2-C2
5	D	803	PCW	C1-O3P-P-O1P
5	D	803	PCW	C1-O3P-P-O2P
5	D	803	PCW	C1-O3P-P-O4P
5	D	803	PCW	C4-O4P-P-O1P
5	D	803	PCW	C4-O4P-P-O3P
5	D	808	PCW	C1-O3P-P-O1P
5	D	808	PCW	C1-O3P-P-O2P
5	D	808	PCW	C1-O3P-P-O4P
5	D	808	PCW	C4-O4P-P-O1P
5	D	808	PCW	C4-O4P-P-O2P
5	D	808	PCW	C4-O4P-P-O3P
5	D	809	PCW	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
5	B	814	PCW	O11-C11-O3-C3
5	C	814	PCW	O11-C11-O3-C3
5	B	814	PCW	C12-C11-O3-C3
5	C	814	PCW	C12-C11-O3-C3
5	A	803	PCW	O11-C11-O3-C3
5	A	811	PCW	O11-C11-O3-C3
5	B	813	PCW	O11-C11-O3-C3
5	C	807	PCW	O11-C11-O3-C3
5	D	803	PCW	O11-C11-O3-C3
3	A	801	Y01	CAC-CBB-CBE-CAP
3	A	812	Y01	CAC-CBB-CBE-CAP
4	D	807	CLR	C16-C17-C20-C21
3	A	801	Y01	CAC-CBB-CBE-CBI
3	C	804	Y01	CAC-CBB-CBE-CBI
3	A	812	Y01	OAG-CAY-OAW-CBC
3	C	801	Y01	OAG-CAY-OAW-CBC
3	C	806	Y01	OAG-CAY-OAW-CBC
5	B	813	PCW	C12-C11-O3-C3
5	C	807	PCW	C12-C11-O3-C3
5	D	803	PCW	C12-C11-O3-C3
3	B	801	Y01	CAM-CAY-OAW-CBC
5	B	813	PCW	C32-C31-O2-C2
3	A	801	Y01	CAJ-CAO-CBB-CAC
3	A	812	Y01	CAJ-CAO-CBB-CAC
3	D	806	Y01	CAJ-CAO-CBB-CAC
4	A	802	CLR	C21-C20-C22-C23
4	D	807	CLR	C21-C20-C22-C23
3	C	804	Y01	CAC-CBB-CBE-CAP
3	D	806	Y01	CAC-CBB-CBE-CAP
4	C	805	CLR	C16-C17-C20-C21
3	C	804	Y01	CAO-CBB-CBE-CAP
4	D	807	CLR	C16-C17-C20-C22
3	A	801	Y01	CAO-CBB-CBE-CBI
3	C	804	Y01	CAO-CBB-CBE-CBI
3	D	806	Y01	CAO-CBB-CBE-CBI
4	C	805	CLR	C13-C17-C20-C22
4	D	807	CLR	C13-C17-C20-C22
3	D	806	Y01	CAX-CAL-CAM-CAY
5	A	803	PCW	C12-C11-O3-C3
5	A	811	PCW	C12-C11-O3-C3
5	B	803	PCW	C18-C19-C20-C21
3	C	804	Y01	CAJ-CAO-CBB-CAC

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Mol	Chain	Res	Type	Atoms
3	B	801	Y01	OAG-CAY-OAW-CBC
3	D	806	Y01	CAC-CBB-CBE-CBI
4	C	805	CLR	C13-C17-C20-C21
5	D	808	PCW	C12-C11-O3-C3
3	A	801	Y01	CAO-CBB-CBE-CAP
4	D	807	CLR	C17-C20-C22-C23
5	D	808	PCW	O11-C11-O3-C3
4	C	805	CLR	C21-C20-C22-C23
3	C	801	Y01	CAJ-CAO-CBB-CBE
5	A	804	PCW	C18-C19-C20-C21
4	B	805	CLR	C21-C20-C22-C23
3	A	812	Y01	CAJ-CAO-CBB-CBE
3	D	806	Y01	CAJ-CAO-CBB-CBE
5	D	802	PCW	C32-C31-O2-C2
5	B	806	PCW	O2-C2-C3-O3
3	B	801	Y01	CAO-CAJ-CAN-CBA
3	C	801	Y01	CAJ-CAO-CBB-CAC
5	B	811	PCW	C18-C19-C20-C21
3	A	801	Y01	CAJ-CAO-CBB-CBE
3	A	812	Y01	CAN-CAJ-CAO-CBB
5	C	814	PCW	C31-C32-C33-C34
3	D	806	Y01	CAO-CBB-CBE-CAP
4	C	805	CLR	C16-C17-C20-C22
3	C	806	Y01	CAN-CAJ-CAO-CBB
3	D	806	Y01	CAO-CAJ-CAN-CBA
5	A	806	PCW	C15-C16-C17-C18
5	A	814	PCW	C14-C15-C16-C17
5	D	811	PCW	C13-C14-C15-C16
3	A	801	Y01	CAO-CAJ-CAN-CBA
3	B	801	Y01	CAN-CAJ-CAO-CBB
5	A	811	PCW	C31-C32-C33-C34
5	B	813	PCW	C31-C32-C33-C34
5	D	802	PCW	O31-C31-O2-C2
4	B	805	CLR	C13-C17-C20-C22
3	C	801	Y01	CAN-CAJ-CAO-CBB
3	C	801	Y01	CAX-CAL-CAM-CAY
3	C	806	Y01	CAX-CAL-CAM-CAY
5	A	810	PCW	C32-C31-O2-C2
3	C	804	Y01	CAJ-CAO-CBB-CBE
5	A	810	PCW	O31-C31-O2-C2
5	B	814	PCW	C15-C16-C17-C18
3	B	804	Y01	CAX-CAL-CAM-CAY

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Mol	Chain	Res	Type	Atoms
5	B	807	PCW	C18-C19-C20-C21
5	D	803	PCW	C13-C14-C15-C16
3	B	801	Y01	CAJ-CAN-CBA-CAB
5	B	806	PCW	C15-C16-C17-C18
5	B	814	PCW	C32-C31-O2-C2
3	A	812	Y01	CAJ-CAN-CBA-CAA
5	D	802	PCW	C15-C16-C17-C18
5	D	813	PCW	C12-C13-C14-C15
5	A	809	PCW	C22-C23-C24-C25
5	B	803	PCW	C14-C15-C16-C17
5	C	814	PCW	C15-C16-C17-C18
5	C	808	PCW	C18-C19-C20-C21
4	B	805	CLR	C16-C17-C20-C21
5	B	810	PCW	C15-C16-C17-C18
5	B	813	PCW	C11-C12-C13-C14
5	A	813	PCW	C15-C16-C17-C18
5	A	814	PCW	C13-C14-C15-C16
5	D	803	PCW	C22-C23-C24-C25
3	A	812	Y01	CAJ-CAN-CBA-CAB
3	B	801	Y01	CAJ-CAN-CBA-CAA
3	C	801	Y01	CAJ-CAN-CBA-CAB
5	A	808	PCW	C14-C15-C16-C17
5	D	805	PCW	C14-C15-C16-C17
5	A	805	PCW	C14-C15-C16-C17
5	A	809	PCW	C21-C22-C23-C24
5	A	810	PCW	C34-C35-C36-C37
5	B	810	PCW	C13-C14-C15-C16
5	B	814	PCW	C12-C13-C14-C15
5	B	814	PCW	C35-C36-C37-C38
5	C	807	PCW	C33-C34-C35-C36
5	C	813	PCW	C12-C13-C14-C15
4	B	805	CLR	C13-C17-C20-C21
5	B	814	PCW	O31-C31-O2-C2
5	B	803	PCW	C12-C13-C14-C15
5	B	806	PCW	C24-C25-C26-C27
5	C	814	PCW	C22-C23-C24-C25
5	D	802	PCW	C13-C14-C15-C16
5	D	804	PCW	C15-C16-C17-C18
5	B	814	PCW	C14-C15-C16-C17
5	A	803	PCW	C12-C13-C14-C15
5	A	807	PCW	C13-C14-C15-C16
5	C	807	PCW	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
5	A	804	PCW	C14-C15-C16-C17
5	A	810	PCW	C13-C14-C15-C16
5	C	808	PCW	C14-C15-C16-C17
5	D	808	PCW	C15-C16-C17-C18
5	B	807	PCW	C16-C17-C18-C19
5	B	811	PCW	C20-C21-C22-C23
5	C	807	PCW	C16-C17-C18-C19
5	C	814	PCW	C16-C17-C18-C19
5	C	814	PCW	C36-C37-C38-C39
5	C	811	PCW	C18-C19-C20-C21
5	A	811	PCW	C24-C25-C26-C27
5	B	813	PCW	C15-C16-C17-C18
5	A	803	PCW	C31-C32-C33-C34
5	D	802	PCW	C11-C12-C13-C14
5	A	803	PCW	C33-C34-C35-C36
5	C	814	PCW	C33-C34-C35-C36
5	C	808	PCW	C21-C22-C23-C24
3	C	801	Y01	CAO-CAJ-CAN-CBA
3	B	801	Y01	CAX-CAL-CAM-CAY
5	A	813	PCW	C14-C15-C16-C17
5	B	814	PCW	C23-C24-C25-C26
5	B	814	PCW	C33-C34-C35-C36
5	D	809	PCW	C15-C16-C17-C18
5	B	806	PCW	C32-C33-C34-C35
5	C	803	PCW	C14-C15-C16-C17
5	D	808	PCW	C21-C22-C23-C24
5	A	807	PCW	C15-C16-C17-C18
5	D	808	PCW	C13-C14-C15-C16
5	A	810	PCW	C35-C36-C37-C38
5	B	808	PCW	C19-C20-C21-C22
5	C	802	PCW	C15-C16-C17-C18
5	D	810	PCW	C13-C14-C15-C16
4	D	807	CLR	C23-C24-C25-C27
3	D	806	Y01	CAM-CAY-OAW-CBC
5	A	811	PCW	C32-C31-O2-C2
5	C	813	PCW	C32-C31-O2-C2
5	C	813	PCW	O31-C31-O2-C2
5	B	803	PCW	C15-C16-C17-C18
5	A	803	PCW	C16-C17-C18-C19
5	B	803	PCW	C16-C17-C18-C19
5	B	814	PCW	C40-C41-C42-C43
5	C	807	PCW	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
5	D	809	PCW	C12-C13-C14-C15
3	D	806	Y01	CAJ-CAN-CBA-CAA
5	A	805	PCW	C15-C16-C17-C18
5	B	813	PCW	C12-C13-C14-C15
5	C	810	PCW	C14-C15-C16-C17
5	D	808	PCW	C34-C35-C36-C37
5	C	814	PCW	C32-C33-C34-C35
5	B	803	PCW	C21-C22-C23-C24
5	D	802	PCW	C31-C32-C33-C34
5	D	803	PCW	C11-C12-C13-C14
5	C	807	PCW	C24-C25-C26-C27
5	B	806	PCW	C16-C17-C18-C19
5	B	806	PCW	C36-C37-C38-C39
5	D	802	PCW	C36-C37-C38-C39
5	B	811	PCW	C15-C16-C17-C18
5	B	812	PCW	C17-C18-C19-C20
5	C	807	PCW	C37-C38-C39-C40
5	D	801	PCW	C21-C22-C23-C24
5	C	808	PCW	C13-C14-C15-C16
5	D	802	PCW	C32-C33-C34-C35
5	A	811	PCW	O31-C31-O2-C2
5	A	810	PCW	C33-C34-C35-C36
4	B	805	CLR	C16-C17-C20-C22
5	C	811	PCW	C22-C23-C24-C25
5	A	803	PCW	C19-C20-C21-C22
5	A	810	PCW	C36-C37-C38-C39
5	B	812	PCW	C20-C21-C22-C23
5	C	814	PCW	C20-C21-C22-C23
5	D	803	PCW	C16-C17-C18-C19
5	D	813	PCW	C20-C21-C22-C23
5	D	803	PCW	C33-C34-C35-C36
5	B	813	PCW	O3P-C1-C2-C3
5	C	814	PCW	O3P-C1-C2-C3
5	A	803	PCW	C15-C16-C17-C18
5	A	810	PCW	C31-C32-C33-C34
5	D	803	PCW	C15-C16-C17-C18
5	C	803	PCW	C23-C24-C25-C26
5	D	808	PCW	C22-C23-C24-C25
5	C	814	PCW	C23-C24-C25-C26
5	A	813	PCW	C17-C18-C19-C20
5	A	814	PCW	C18-C19-C20-C21
5	C	807	PCW	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
5	C	813	PCW	C1-C2-C3-O3
5	D	805	PCW	C21-C22-C23-C24
5	A	811	PCW	C16-C17-C18-C19
5	C	814	PCW	C35-C36-C37-C38
4	D	807	CLR	C23-C24-C25-C26
5	D	801	PCW	C22-C23-C24-C25
5	C	813	PCW	C11-C12-C13-C14
5	B	802	PCW	C15-C16-C17-C18
5	D	808	PCW	C12-C13-C14-C15
5	B	811	PCW	C12-C13-C14-C15
5	B	809	PCW	C15-C16-C17-C18
5	B	813	PCW	C20-C21-C22-C23
5	C	813	PCW	C20-C21-C22-C23
5	D	802	PCW	C20-C21-C22-C23
3	B	804	Y01	CAC-CBB-CBE-CAP
4	A	802	CLR	C16-C17-C20-C21
5	A	809	PCW	C15-C16-C17-C18
5	A	803	PCW	C22-C23-C24-C25
5	C	809	PCW	C16-C17-C18-C19
5	D	810	PCW	C16-C17-C18-C19
5	B	810	PCW	C14-C15-C16-C17
5	C	808	PCW	C15-C16-C17-C18
3	B	804	Y01	CAJ-CAN-CBA-CAA
5	D	808	PCW	C35-C36-C37-C38
5	D	808	PCW	C37-C38-C39-C40
5	C	814	PCW	C12-C13-C14-C15
5	A	803	PCW	C24-C25-C26-C27
5	B	802	PCW	C22-C23-C24-C25
5	B	814	PCW	C32-C33-C34-C35
5	A	806	PCW	C12-C13-C14-C15
5	B	808	PCW	C15-C16-C17-C18
5	D	813	PCW	C23-C24-C25-C26
5	B	806	PCW	C21-C22-C23-C24
5	B	814	PCW	C42-C43-C44-C45
5	C	811	PCW	C16-C17-C18-C19
5	C	812	PCW	C16-C17-C18-C19
5	C	812	PCW	C20-C21-C22-C23
5	C	814	PCW	C40-C41-C42-C43
5	B	802	PCW	C13-C14-C15-C16
5	B	803	PCW	C22-C23-C24-C25
3	B	804	Y01	CAC-CBB-CBE-CBI
5	D	801	PCW	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
5	D	803	PCW	C21-C22-C23-C24
5	B	813	PCW	C33-C34-C35-C36
5	D	813	PCW	C13-C14-C15-C16
5	A	811	PCW	C40-C41-C42-C43
5	C	802	PCW	C23-C24-C25-C26
5	B	812	PCW	C15-C16-C17-C18
5	C	812	PCW	C15-C16-C17-C18
5	A	809	PCW	C17-C18-C19-C20
5	D	803	PCW	C32-C33-C34-C35
4	A	802	CLR	C13-C17-C20-C21
5	C	811	PCW	C12-C13-C14-C15
5	D	812	PCW	C12-C13-C14-C15
5	B	806	PCW	C1-C2-C3-O3
5	D	803	PCW	C1-C2-C3-O3
5	A	811	PCW	C15-C16-C17-C18
3	B	804	Y01	CAJ-CAN-CBA-CAB
4	A	802	CLR	C23-C24-C25-C27
4	A	802	CLR	C16-C17-C20-C22
5	B	803	PCW	C20-C21-C22-C23
3	B	804	Y01	CAO-CBB-CBE-CBI
4	A	802	CLR	C13-C17-C20-C22
5	D	802	PCW	C35-C36-C37-C38
5	A	810	PCW	O2-C2-C3-O3
5	C	813	PCW	O2-C2-C3-O3
5	C	809	PCW	C15-C16-C17-C18
3	B	804	Y01	CAO-CBB-CBE-CAP
5	B	809	PCW	C13-C14-C15-C16
5	C	811	PCW	C14-C15-C16-C17
5	C	814	PCW	C41-C42-C43-C44
5	B	803	PCW	C23-C24-C25-C26
5	D	805	PCW	C19-C20-C21-C22
3	D	806	Y01	CAJ-CAN-CBA-CAB
5	B	806	PCW	C25-C26-C27-C28
5	B	813	PCW	C35-C36-C37-C38
5	B	807	PCW	C15-C16-C17-C18
3	C	801	Y01	CAJ-CAN-CBA-CAA
5	D	802	PCW	C39-C40-C41-C42
5	C	811	PCW	C13-C14-C15-C16
5	D	809	PCW	C14-C15-C16-C17
5	B	814	PCW	C41-C42-C43-C44
5	C	807	PCW	O3P-C1-C2-C3
5	D	808	PCW	O3P-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
5	A	804	PCW	C13-C14-C15-C16
5	C	803	PCW	C12-C13-C14-C15
5	C	803	PCW	C22-C23-C24-C25
5	B	806	PCW	C12-C11-O3-C3
5	A	814	PCW	C12-C13-C14-C15
5	D	813	PCW	C14-C15-C16-C17
5	B	814	PCW	C31-C32-C33-C34
3	D	806	Y01	OAG-CAY-OAW-CBC
5	B	806	PCW	C13-C14-C15-C16
5	A	810	PCW	C1-C2-O2-C31
5	D	802	PCW	C3-C2-O2-C31
5	B	808	PCW	C16-C17-C18-C19
5	D	808	PCW	C40-C41-C42-C43
4	A	802	CLR	C23-C24-C25-C26
5	C	814	PCW	C34-C35-C36-C37
5	D	805	PCW	C12-C13-C14-C15
5	C	802	PCW	C24-C25-C26-C27
5	B	813	PCW	O3P-C1-C2-O2
5	D	802	PCW	O3P-C1-C2-O2
5	D	808	PCW	O3P-C1-C2-O2
4	C	805	CLR	C23-C24-C25-C26
5	B	811	PCW	C14-C15-C16-C17
5	D	811	PCW	C15-C16-C17-C18
5	B	806	PCW	C5-C4-O4P-P
5	B	813	PCW	C5-C4-O4P-P
5	C	814	PCW	C5-C4-O4P-P
5	B	814	PCW	O2-C2-C3-O3
5	D	803	PCW	O2-C2-C3-O3
5	A	811	PCW	C21-C22-C23-C24
5	A	808	PCW	C12-C13-C14-C15
5	B	806	PCW	C35-C36-C37-C38
5	D	810	PCW	C15-C16-C17-C18
5	B	806	PCW	O11-C11-O3-C3
5	C	811	PCW	C11-C12-C13-C14
5	A	803	PCW	C21-C22-C23-C24
5	A	803	PCW	C4-C5-N-C7
5	B	808	PCW	C13-C14-C15-C16
5	C	807	PCW	C42-C43-C44-C45
5	A	811	PCW	O4P-C4-C5-N
5	B	814	PCW	O4P-C4-C5-N
5	C	813	PCW	O4P-C4-C5-N
5	D	802	PCW	O4P-C4-C5-N

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Mol	Chain	Res	Type	Atoms
5	A	811	PCW	C33-C34-C35-C36
5	D	803	PCW	C31-C32-C33-C34
5	A	814	PCW	C22-C23-C24-C25
5	D	809	PCW	C21-C22-C23-C24
5	D	804	PCW	C22-C23-C24-C25
5	C	813	PCW	C12-C11-O3-C3
5	D	804	PCW	C21-C22-C23-C24
5	A	810	PCW	O3P-C1-C2-C3
5	B	806	PCW	O3P-C1-C2-C3
5	C	807	PCW	C22-C23-C24-C25
3	A	801	Y01	CAJ-CAN-CBA-CAB
5	A	805	PCW	C13-C14-C15-C16
5	A	804	PCW	C11-C12-C13-C14
5	B	807	PCW	C19-C20-C21-C22
5	C	811	PCW	C17-C18-C19-C20
5	C	807	PCW	O3P-C1-C2-O2
5	A	814	PCW	C16-C17-C18-C19
5	D	809	PCW	C13-C14-C15-C16
5	B	813	PCW	C13-C14-C15-C16
5	A	804	PCW	C17-C18-C19-C20
5	B	802	PCW	C19-C20-C21-C22
5	C	813	PCW	O11-C11-O3-C3
5	C	807	PCW	O2-C2-C3-O3
5	C	802	PCW	C22-C23-C24-C25
5	A	804	PCW	C23-C24-C25-C26
5	D	803	PCW	C34-C35-C36-C37
5	A	803	PCW	C4-C5-N-C6
5	A	803	PCW	C4-O4P-P-O1P
5	A	810	PCW	C4-O4P-P-O1P
5	A	810	PCW	C4-O4P-P-O2P
5	A	810	PCW	C4-O4P-P-O3P
5	A	811	PCW	C1-O3P-P-O1P
5	A	811	PCW	C4-O4P-P-O2P
5	B	806	PCW	C4-O4P-P-O1P
5	B	814	PCW	C4-O4P-P-O1P
5	B	814	PCW	C4-O4P-P-O3P
5	C	807	PCW	C1-O3P-P-O4P
5	C	807	PCW	C4-O4P-P-O1P
5	C	813	PCW	C1-O3P-P-O2P
5	C	813	PCW	C4-O4P-P-O2P
5	A	811	PCW	C34-C35-C36-C37
5	C	803	PCW	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
5	C	807	PCW	C32-C33-C34-C35
5	D	812	PCW	C13-C14-C15-C16
5	C	803	PCW	C15-C16-C17-C18
5	B	806	PCW	C31-C32-C33-C34
5	A	803	PCW	C4-C5-N-C8
5	A	810	PCW	C12-C13-C14-C15
5	C	803	PCW	C19-C20-C21-C22
5	C	813	PCW	C37-C38-C39-C40
5	A	810	PCW	O3P-C1-C2-O2
5	B	806	PCW	O3P-C1-C2-O2
5	C	814	PCW	O3P-C1-C2-O2
5	C	813	PCW	C34-C35-C36-C37
5	C	808	PCW	C23-C24-C25-C26
5	C	809	PCW	C19-C20-C21-C22
5	C	813	PCW	C39-C40-C41-C42
5	D	812	PCW	C15-C16-C17-C18
5	A	807	PCW	C12-C13-C14-C15
5	D	805	PCW	C13-C14-C15-C16
5	D	808	PCW	C14-C15-C16-C17
5	D	808	PCW	C36-C37-C38-C39
5	A	810	PCW	C1-C2-C3-O3
5	A	810	PCW	C15-C16-C17-C18
5	C	810	PCW	C15-C16-C17-C18
5	C	803	PCW	C20-C21-C22-C23
5	D	804	PCW	C16-C17-C18-C19
5	B	812	PCW	C21-C22-C23-C24
5	C	809	PCW	C12-C13-C14-C15
5	B	812	PCW	C19-C20-C21-C22
5	C	814	PCW	C39-C40-C41-C42
5	D	801	PCW	C17-C18-C19-C20
5	D	802	PCW	O3P-C1-C2-C3
5	A	809	PCW	C24-C25-C26-C27
5	D	802	PCW	C34-C35-C36-C37
5	A	811	PCW	C37-C38-C39-C40
5	D	804	PCW	C17-C18-C19-C20
5	D	804	PCW	C24-C25-C26-C27
5	A	811	PCW	C35-C36-C37-C38
5	D	802	PCW	C14-C15-C16-C17
5	C	812	PCW	C22-C23-C24-C25
5	D	808	PCW	C11-C12-C13-C14
5	A	810	PCW	C20-C21-C22-C23
3	C	806	Y01	CAM-CAL-CAX-OAH

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Mol	Chain	Res	Type	Atoms
3	C	806	Y01	CAM-CAL-CAX-OAF
3	D	806	Y01	CAM-CAL-CAX-OAH
3	B	804	Y01	CAM-CAL-CAX-OAF
5	B	806	PCW	C42-C43-C44-C45
5	B	806	PCW	O3-C11-C12-C13
3	C	804	Y01	CAM-CAL-CAX-OAH
4	A	802	CLR	C17-C20-C22-C23
3	D	806	Y01	CAM-CAL-CAX-OAF
5	A	810	PCW	C37-C38-C39-C40
5	D	804	PCW	C19-C20-C21-C22
5	A	803	PCW	C36-C37-C38-C39
5	C	814	PCW	C2-C1-O3P-P
3	B	804	Y01	CAM-CAL-CAX-OAH
3	C	804	Y01	CAM-CAL-CAX-OAF
5	A	804	PCW	C12-C13-C14-C15
4	C	805	CLR	C23-C24-C25-C27
5	A	803	PCW	C37-C38-C39-C40
5	B	811	PCW	C21-C22-C23-C24
5	B	814	PCW	C22-C23-C24-C25
5	C	807	PCW	C41-C42-C43-C44
5	B	802	PCW	C21-C22-C23-C24
5	D	809	PCW	C22-C23-C24-C25
5	C	813	PCW	C13-C14-C15-C16
5	C	802	PCW	C21-C22-C23-C24
5	D	802	PCW	C2-C1-O3P-P
5	D	803	PCW	C41-C42-C43-C44
5	C	802	PCW	C14-C15-C16-C17
5	C	813	PCW	C16-C17-C18-C19
5	D	809	PCW	C20-C21-C22-C23
5	B	807	PCW	C11-C12-C13-C14
3	B	801	Y01	CAM-CAL-CAX-OAH
5	A	804	PCW	C15-C16-C17-C18
5	B	806	PCW	C39-C40-C41-C42
5	D	813	PCW	C18-C19-C20-C21
3	B	801	Y01	CAM-CAL-CAX-OAF
5	A	813	PCW	C22-C23-C24-C25
5	B	814	PCW	O3P-C1-C2-C3
5	D	808	PCW	C32-C33-C34-C35
5	C	812	PCW	C17-C18-C19-C20
5	A	811	PCW	C13-C14-C15-C16
5	A	805	PCW	C17-C18-C19-C20
5	A	811	PCW	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
5	B	814	PCW	C39-C40-C41-C42
5	C	814	PCW	C21-C22-C23-C24
5	B	806	PCW	C41-C42-C43-C44
5	A	811	PCW	C17-C18-C19-C20
5	B	813	PCW	C19-C20-C21-C22
5	C	802	PCW	C17-C18-C19-C20
5	C	807	PCW	C17-C18-C19-C20
5	D	813	PCW	C19-C20-C21-C22
5	C	814	PCW	C13-C14-C15-C16
5	D	803	PCW	C24-C25-C26-C27
5	B	810	PCW	C12-C13-C14-C15
5	B	814	PCW	C34-C35-C36-C37
5	B	813	PCW	C37-C38-C39-C40
5	A	808	PCW	C20-C21-C22-C23
5	A	811	PCW	O2-C2-C3-O3
5	A	803	PCW	C39-C40-C41-C42
5	C	812	PCW	C19-C20-C21-C22
3	D	806	Y01	CAL-CAM-CAY-OAW
5	B	806	PCW	O31-C31-O2-C2
5	A	810	PCW	C32-C33-C34-C35
5	A	810	PCW	O3-C11-C12-C13
5	B	806	PCW	C23-C24-C25-C26
5	A	804	PCW	C19-C20-C21-C22
5	C	808	PCW	C19-C20-C21-C22
5	D	808	PCW	C23-C24-C25-C26
3	C	804	Y01	CAN-CAJ-CAO-CBB
3	A	812	Y01	CAL-CAM-CAY-OAW
5	D	811	PCW	C12-C13-C14-C15
5	D	803	PCW	C4-C5-N-C7
5	D	810	PCW	C12-C13-C14-C15
5	A	811	PCW	C1-C2-C3-O3
5	B	814	PCW	C1-C2-C3-O3
5	A	810	PCW	O2-C31-C32-C33
3	A	801	Y01	CAL-CAM-CAY-OAW
5	C	803	PCW	C16-C17-C18-C19
5	B	811	PCW	C11-C12-C13-C14
5	B	812	PCW	C22-C23-C24-C25
5	B	813	PCW	C39-C40-C41-C42
5	B	806	PCW	C33-C34-C35-C36
5	B	813	PCW	C34-C35-C36-C37
5	B	809	PCW	C14-C15-C16-C17
5	B	813	PCW	O2-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
5	C	807	PCW	C23-C24-C25-C26
3	A	812	Y01	CAL-CAM-CAY-OAG
5	B	814	PCW	O3P-C1-C2-O2
5	B	802	PCW	C17-C18-C19-C20
5	A	810	PCW	O11-C11-C12-C13
5	A	808	PCW	C17-C18-C19-C20
5	A	814	PCW	C17-C18-C19-C20
5	B	803	PCW	C17-C18-C19-C20
5	B	807	PCW	C17-C18-C19-C20
5	B	811	PCW	C17-C18-C19-C20
5	C	803	PCW	C17-C18-C19-C20
5	C	808	PCW	C17-C18-C19-C20
5	D	805	PCW	C17-C18-C19-C20
5	D	813	PCW	C17-C18-C19-C20
3	A	801	Y01	CAL-CAM-CAY-OAG
5	A	810	PCW	O31-C31-C32-C33
5	A	811	PCW	C36-C37-C38-C39
3	D	806	Y01	CAL-CAM-CAY-OAG
5	A	803	PCW	O3-C11-C12-C13
5	D	809	PCW	C17-C18-C19-C20
5	D	803	PCW	C25-C26-C27-C28
5	B	813	PCW	O31-C31-C32-C33
5	D	803	PCW	O2-C31-C32-C33
5	B	806	PCW	C32-C31-O2-C2
5	D	809	PCW	C19-C20-C21-C22
5	A	803	PCW	O2-C31-C32-C33
5	B	814	PCW	O3-C11-C12-C13

There are no ring outliers.

32 monomers are involved in 64 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	807	PCW	2	0
4	C	805	CLR	4	0
5	C	814	PCW	2	0
5	D	810	PCW	1	0
5	C	802	PCW	1	0
5	B	806	PCW	2	0
5	A	810	PCW	1	0
5	B	814	PCW	3	0
5	D	804	PCW	1	0
3	D	806	Y01	7	0

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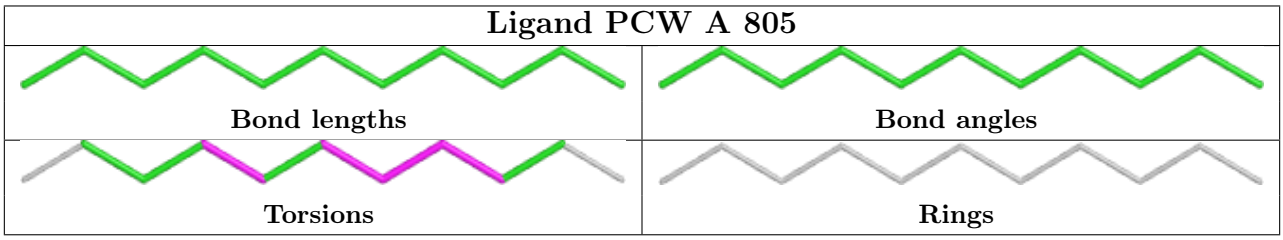
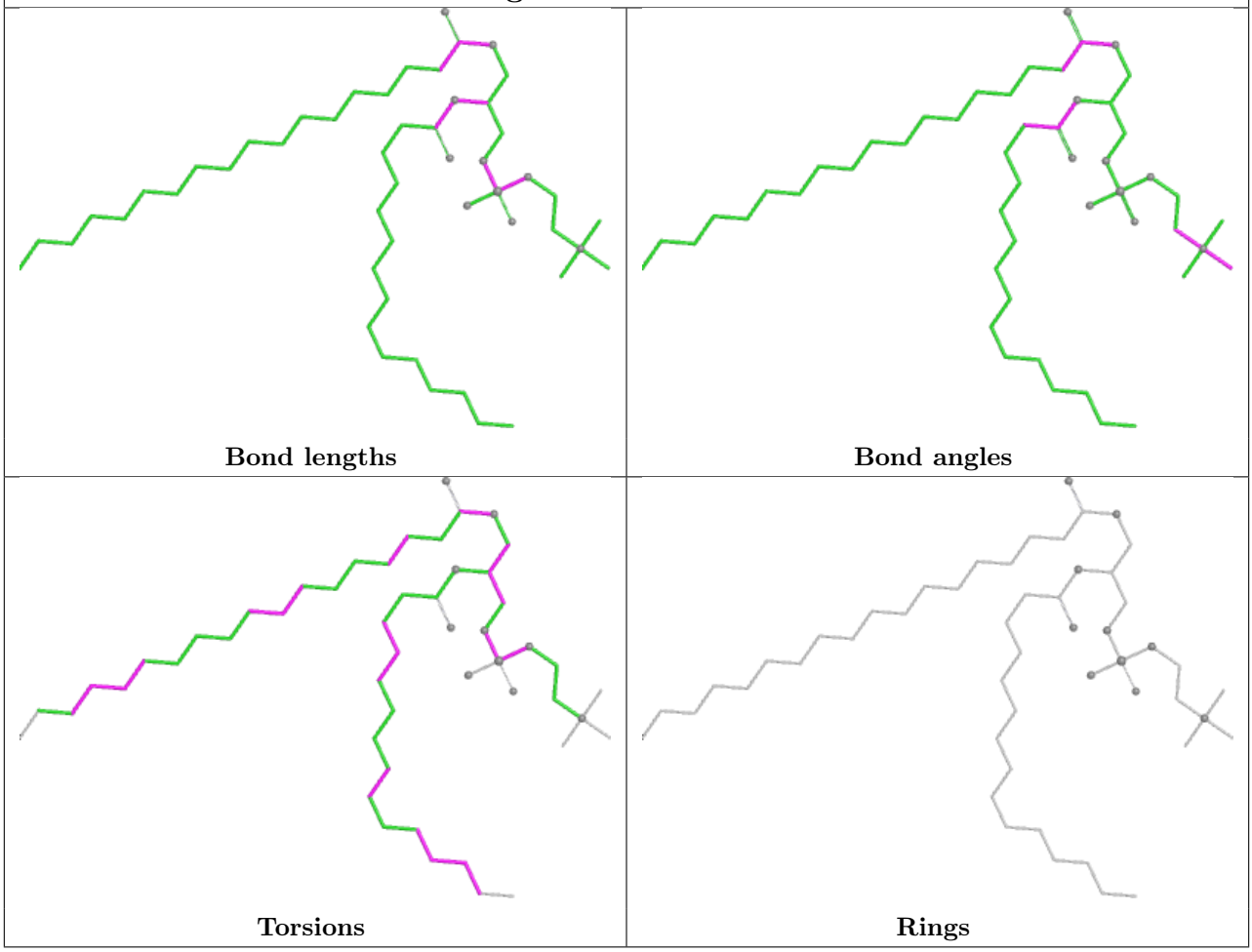
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	803	PCW	1	0
3	B	804	Y01	4	0
5	D	805	PCW	1	0
5	B	807	PCW	1	0
3	C	801	Y01	3	0
5	B	810	PCW	1	0
5	A	811	PCW	2	0
5	C	813	PCW	1	0
3	C	806	Y01	2	0
3	A	812	Y01	1	0
5	D	802	PCW	1	0
4	B	805	CLR	5	0
3	A	801	Y01	3	0
5	B	813	PCW	3	0
4	A	802	CLR	3	0
3	C	804	Y01	1	0
5	C	808	PCW	3	0
5	D	808	PCW	1	0
5	B	812	PCW	1	0
5	D	803	PCW	3	0
3	B	801	Y01	1	0
4	D	807	CLR	3	0

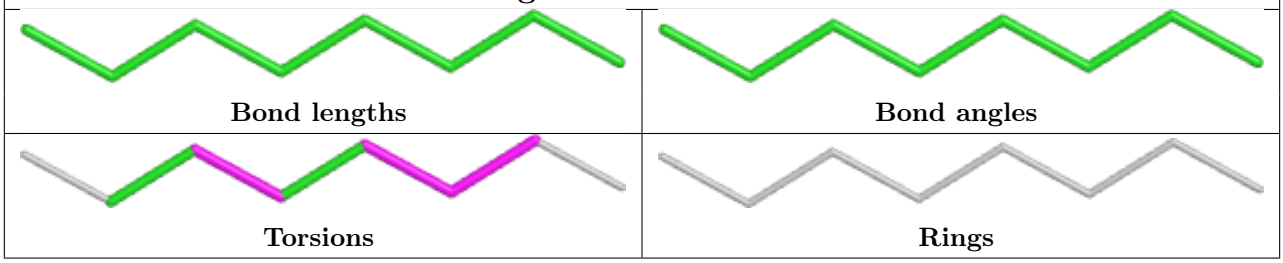
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



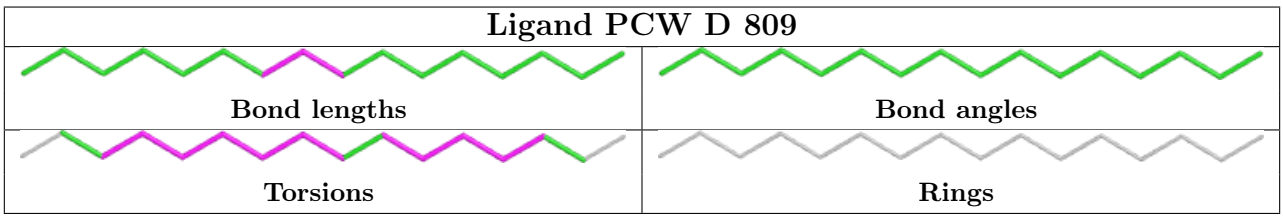
Ligand PCW C 807



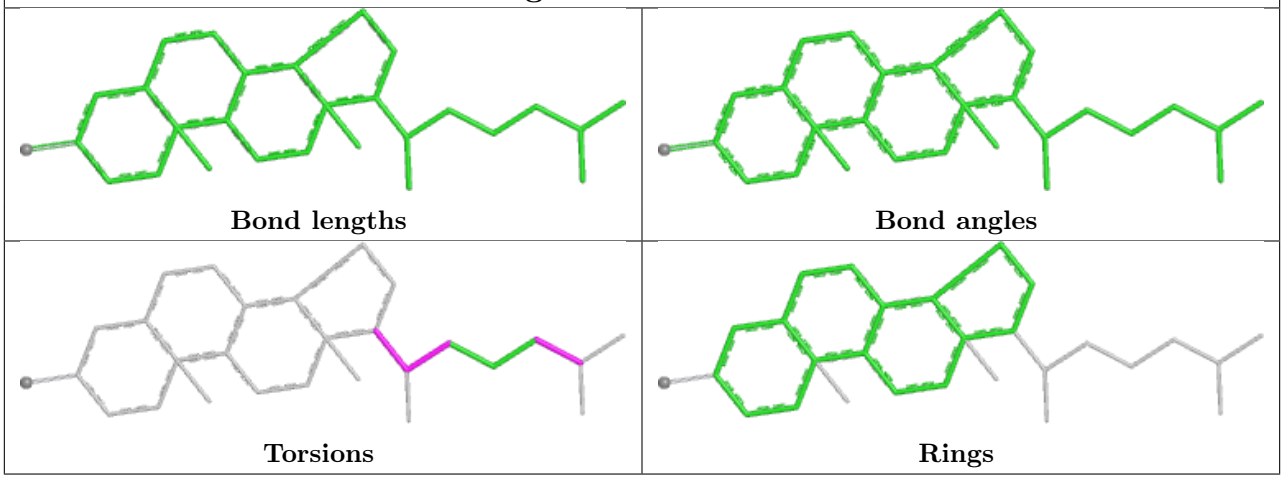
Ligand PCW D 811



Ligand PCW D 809



Ligand CLR C 805



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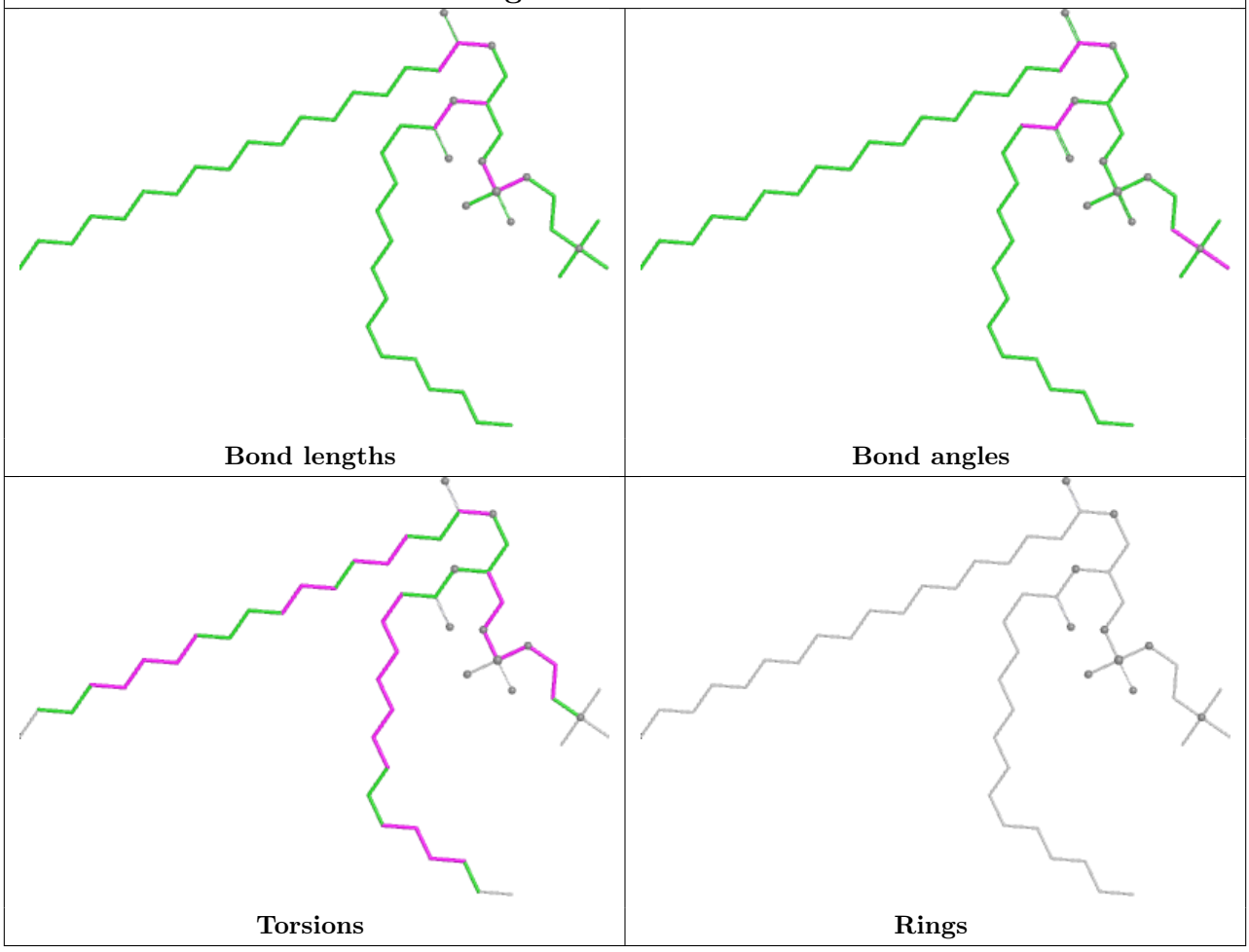

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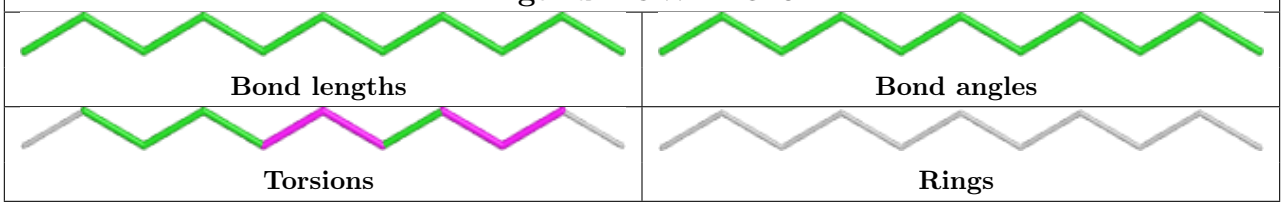

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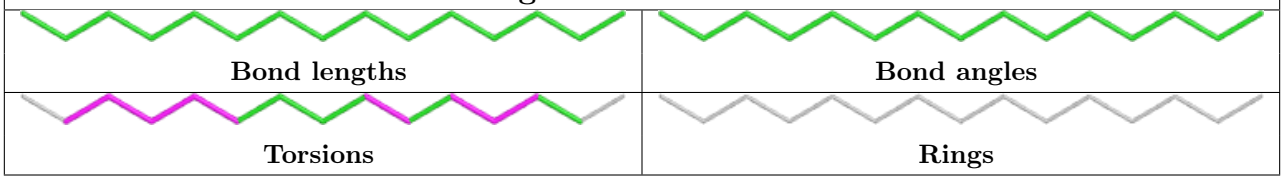
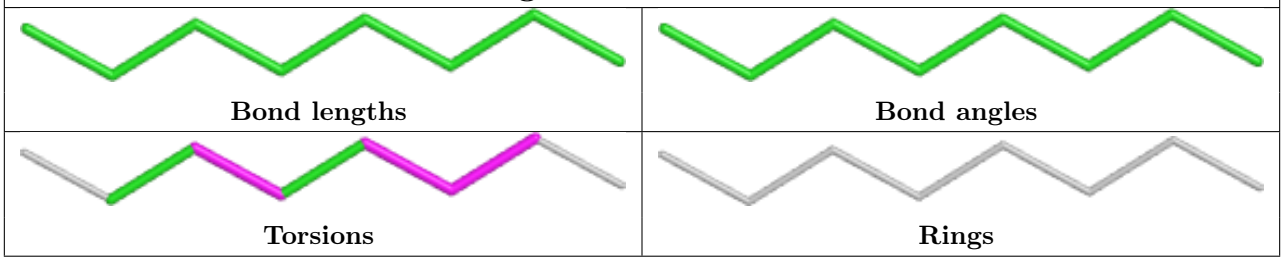
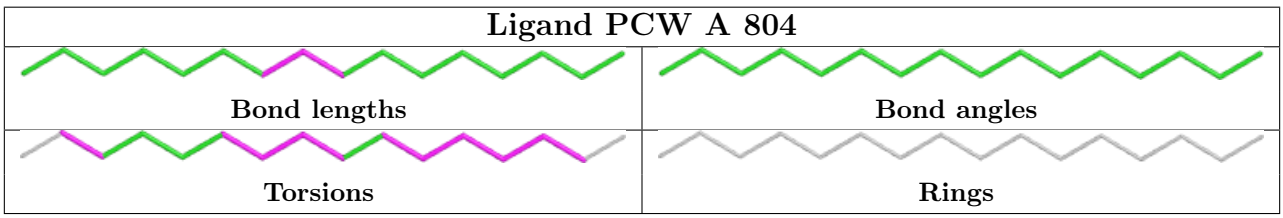


Ligand PCW A 807



Ligand PCW A 804



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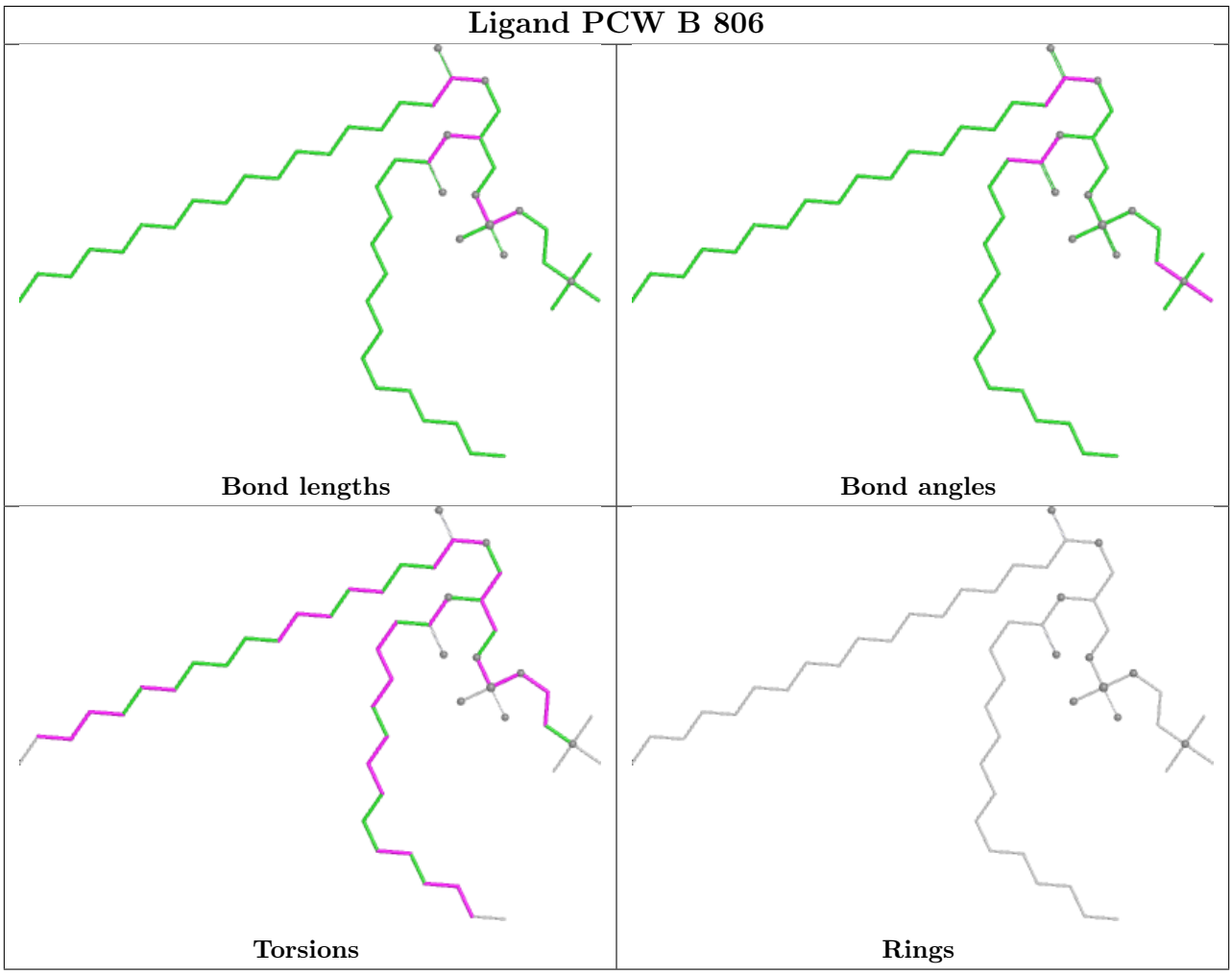

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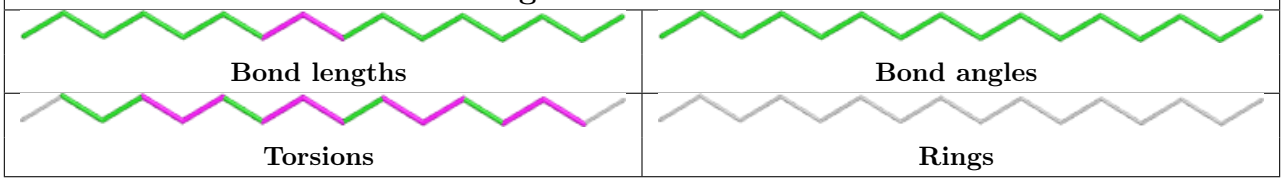
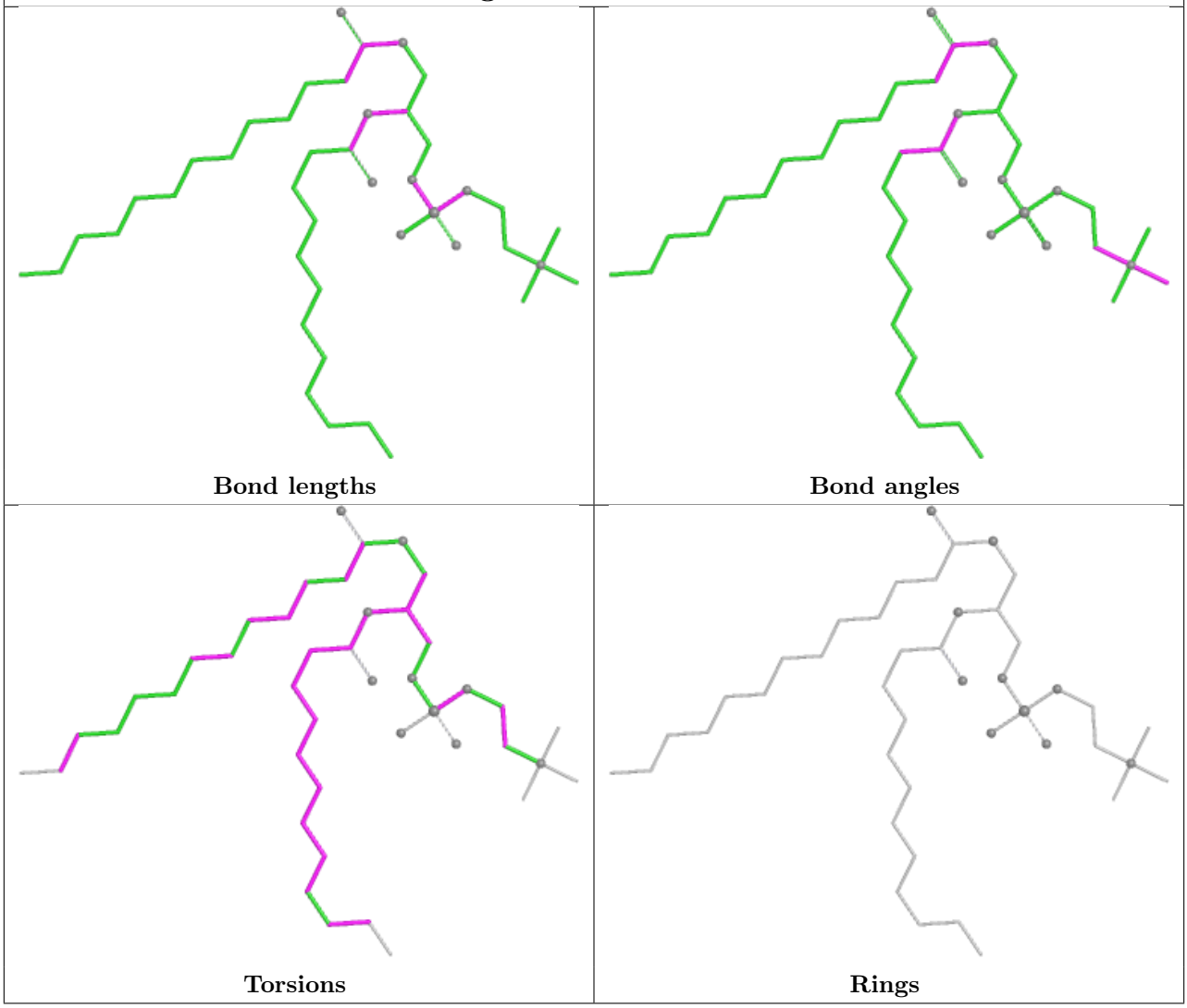


Ligand PCW A 810



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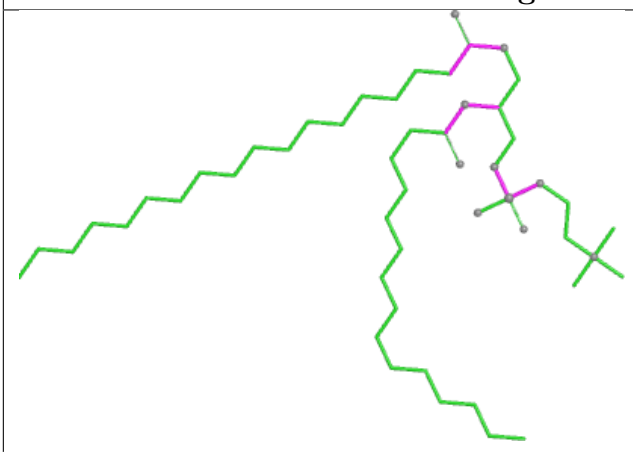
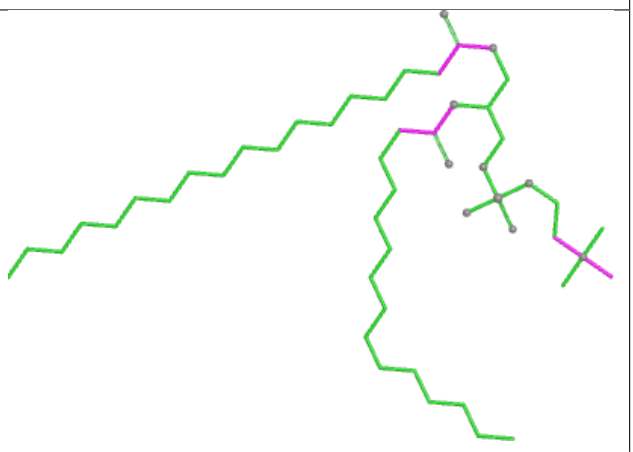
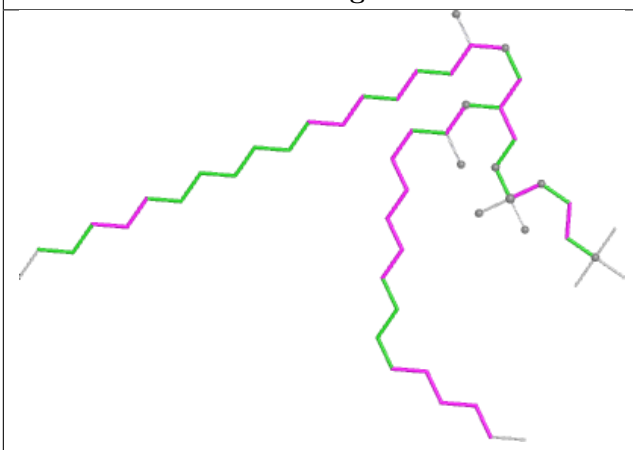


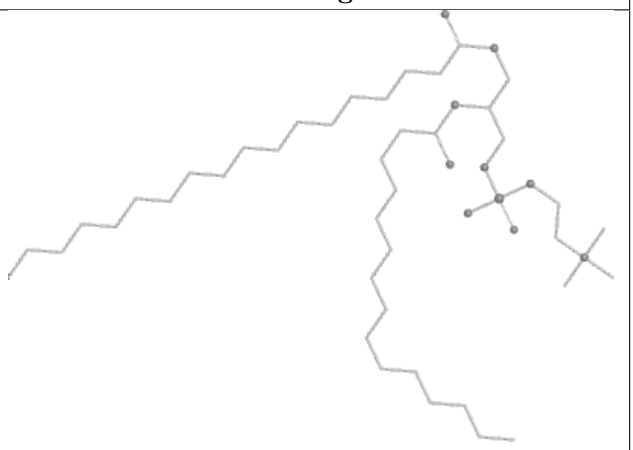
Bond lengths



Bond angles



Torsions



Rings

Ligand PCW C 809

Bond lengths

Bond angles

Torsions

Rings

Ligand PCW D 804

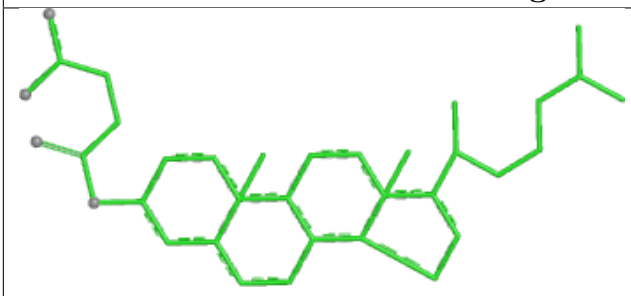
Bond lengths

Bond angles

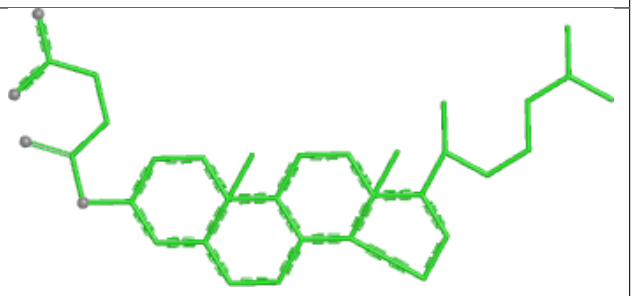
Torsions

Rings

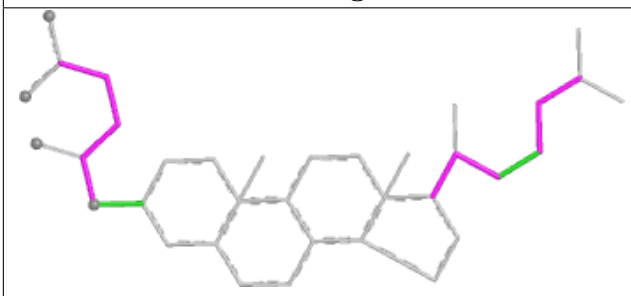
Ligand Y01 D 806



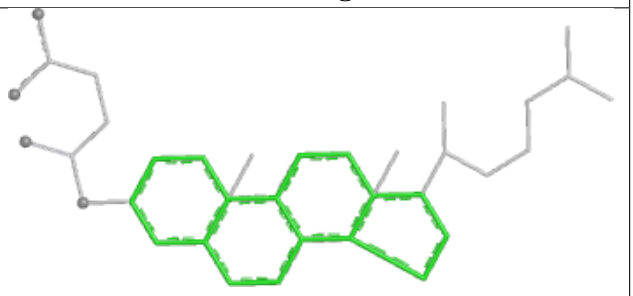
Bond lengths



Bond angles



Torsions

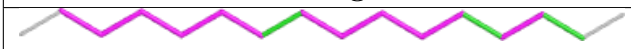


Rings

Ligand PCW C 803

Bond lengths

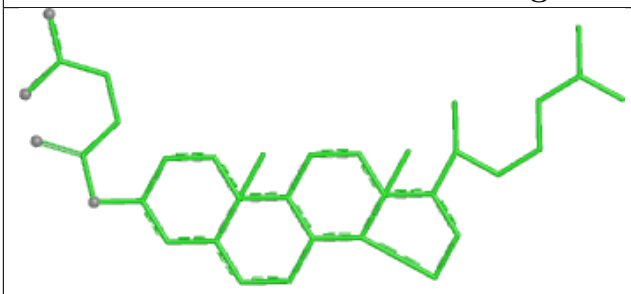
Bond angles



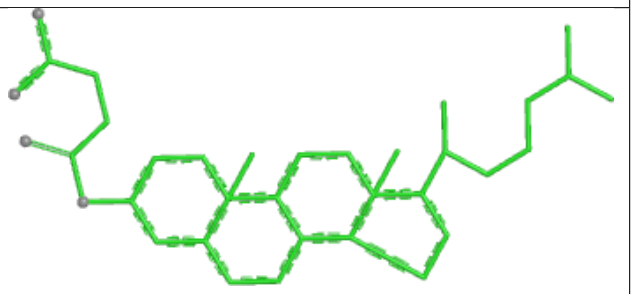
Torsions

Rings

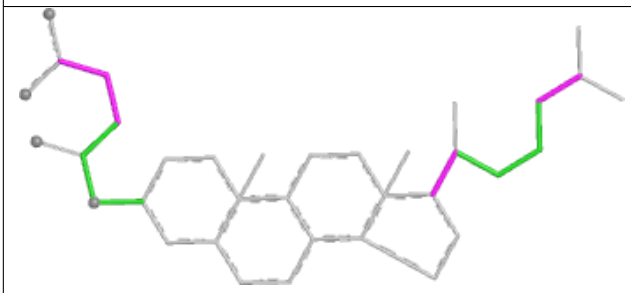
Ligand Y01 B 804



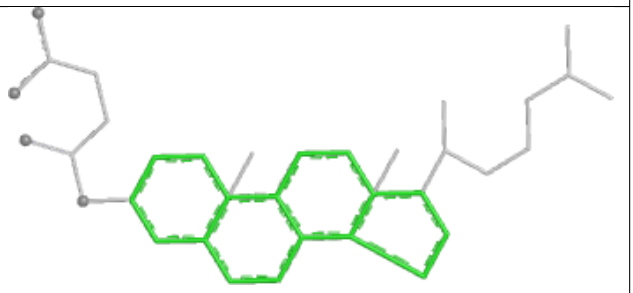
Bond lengths



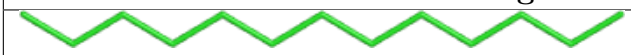
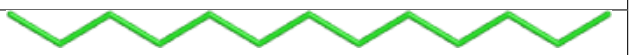
Bond angles

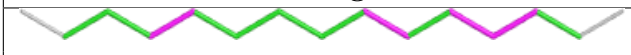


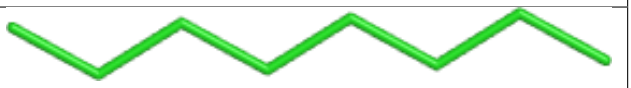
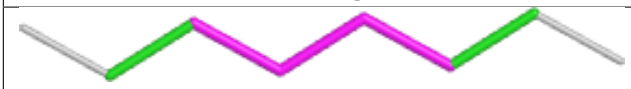
Torsions

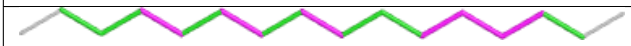


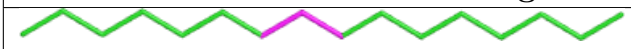
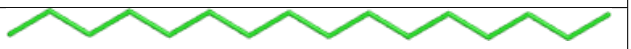
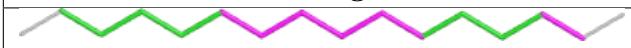
Rings

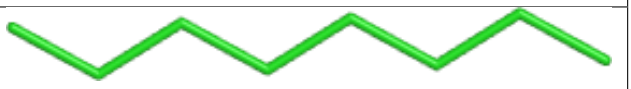
Ligand PCW D 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PCW A 813	
 Bond lengths	 Bond angles
 Torsions	 Rings

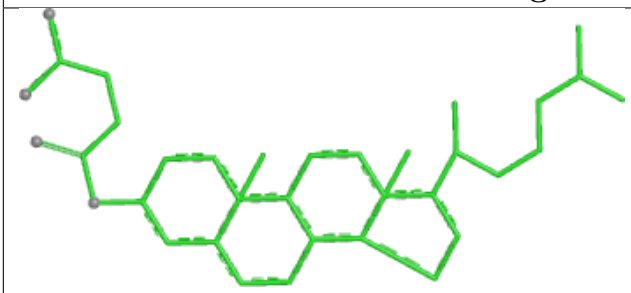
Ligand PCW B 809	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PCW D 805	
 Bond lengths	 Bond angles
 Torsions	 Rings

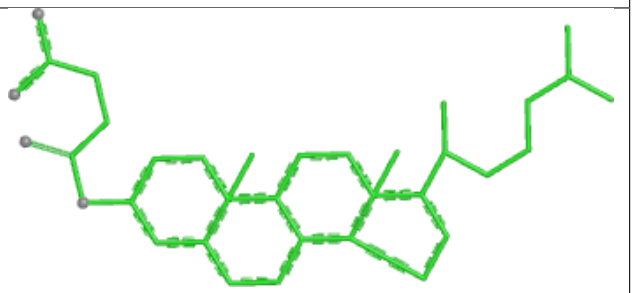
Ligand PCW B 807	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PCW D 812	
 Bond lengths	 Bond angles
 Torsions	 Rings

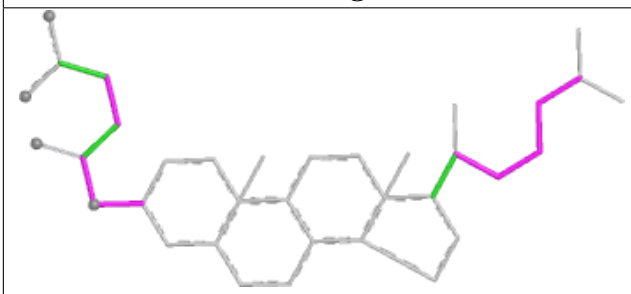
Ligand Y01 C 801



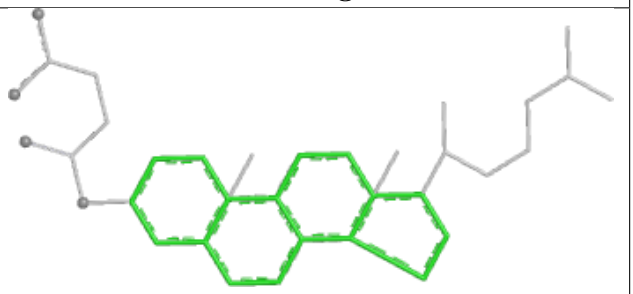
Bond lengths



Bond angles



Torsions



Rings

Ligand PCW B 810

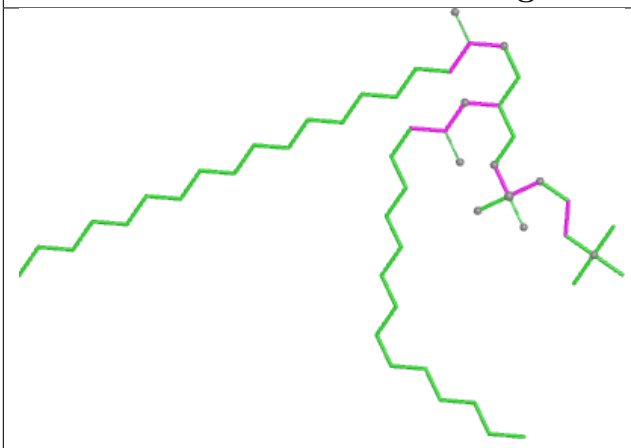
Bond lengths

Bond angles

Torsions

Rings

Ligand PCW A 811



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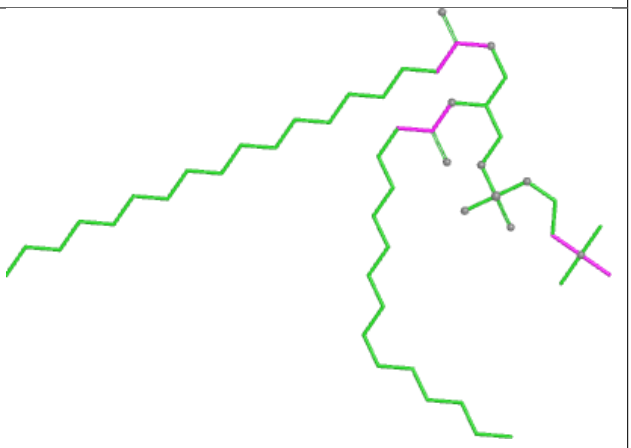

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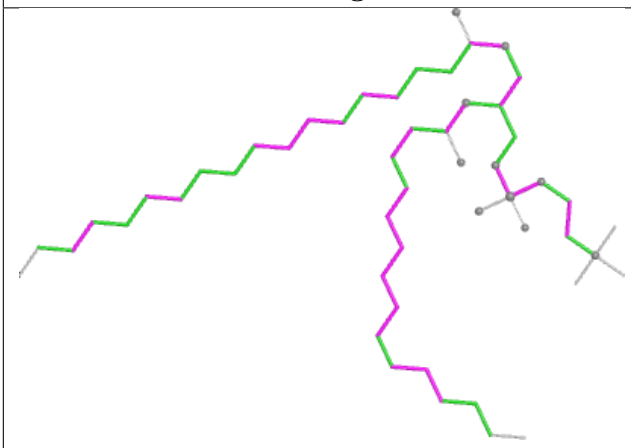

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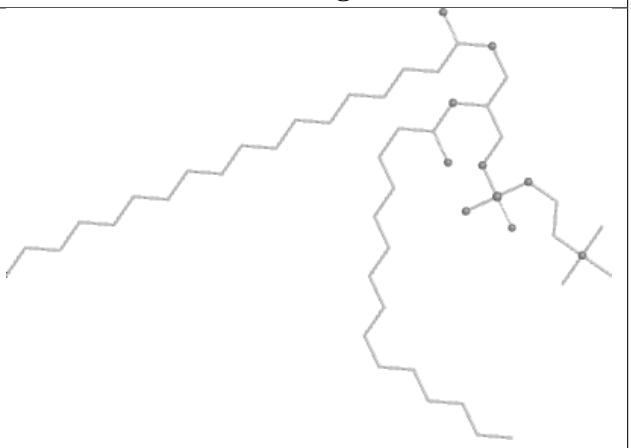
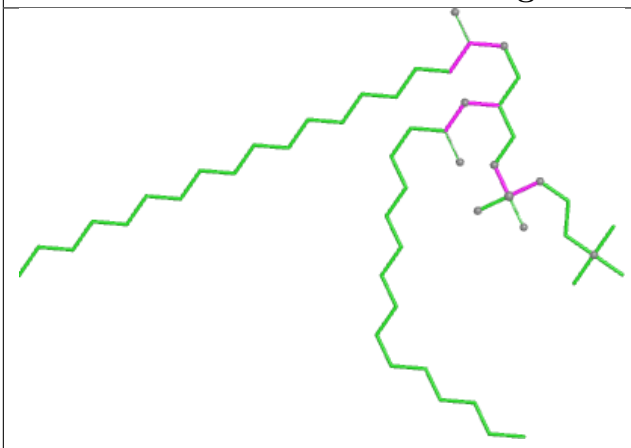


Rings

Ligand PCW A 803



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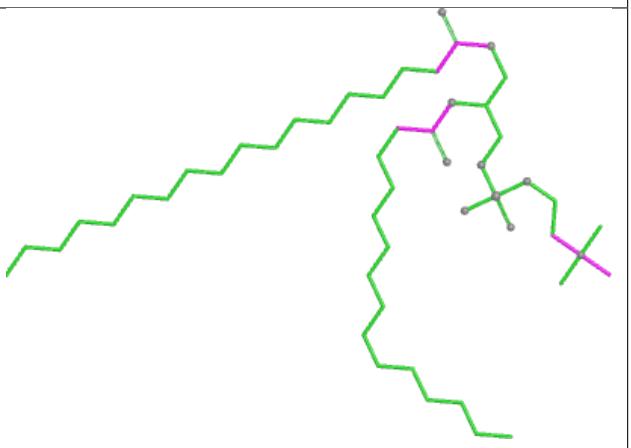
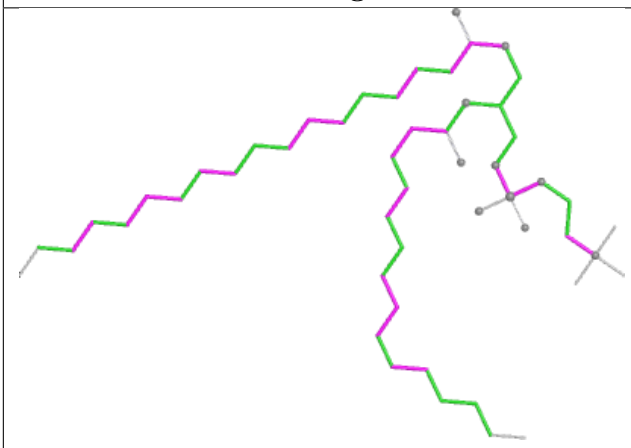
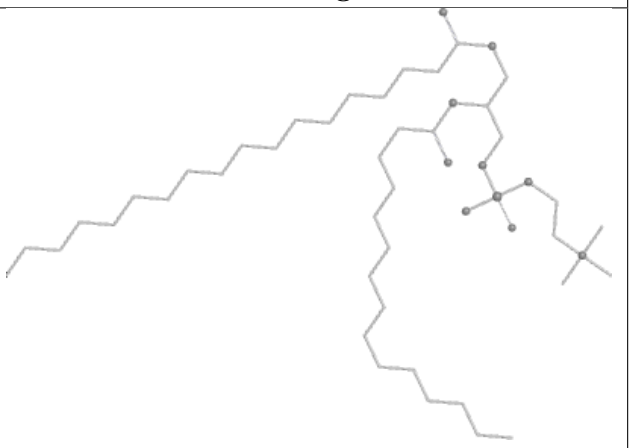


Bond angles

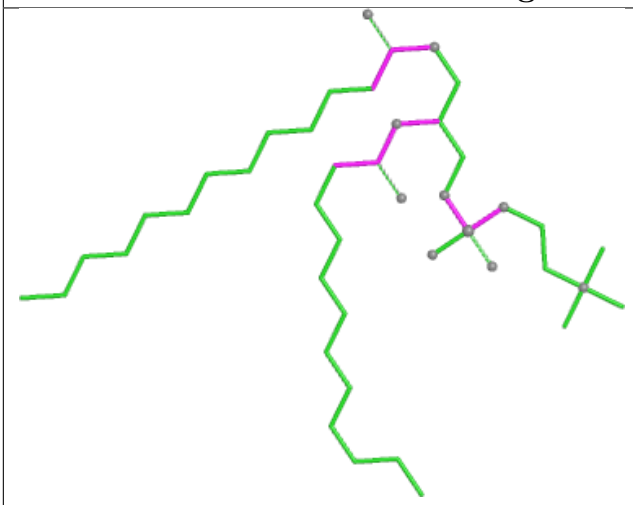


Torsions



Rings

Ligand PCW C 813



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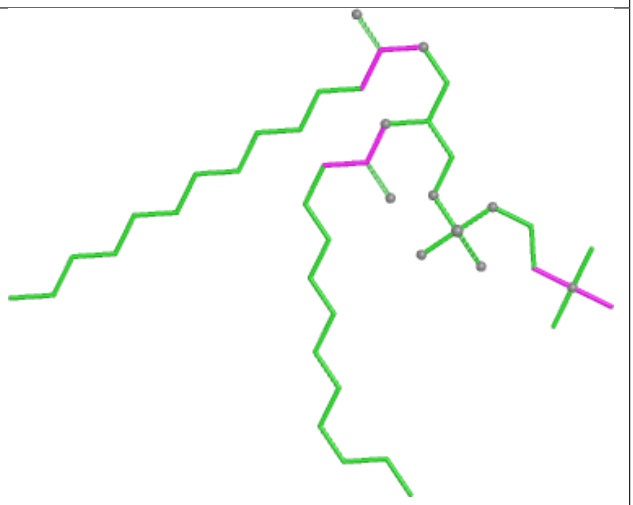
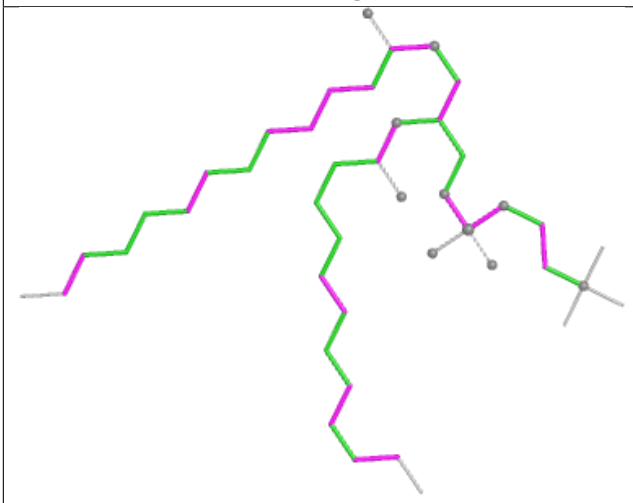
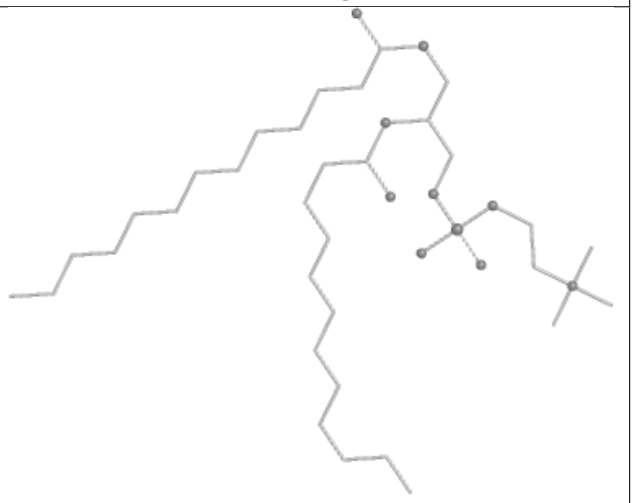


Bond angles



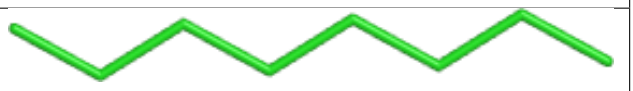
Torsions



Rings

Ligand PCW C 810

Bond lengths

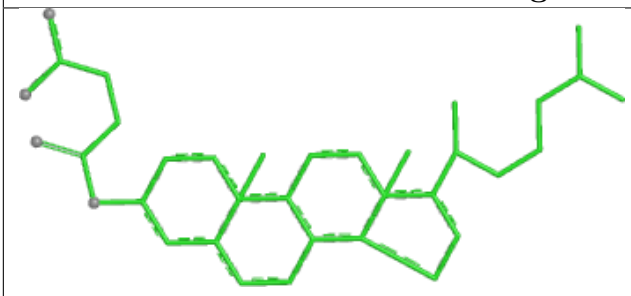


Bond angles

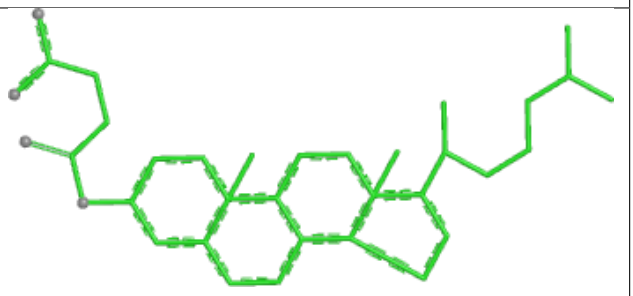
Torsions

Rings

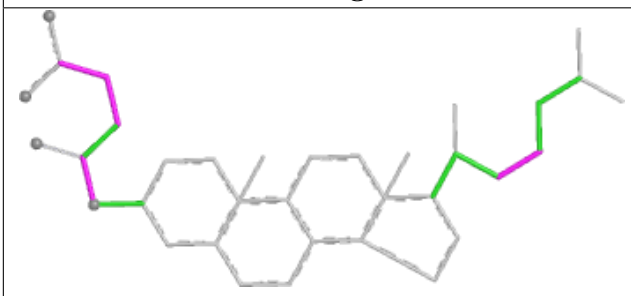
Ligand Y01 C 806



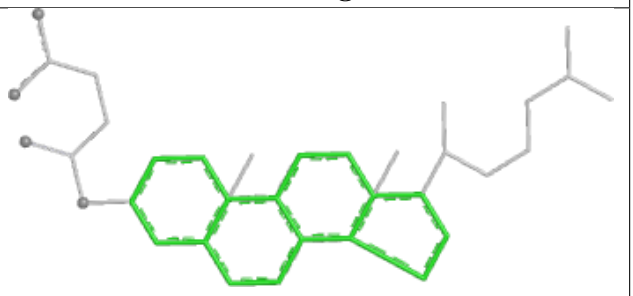
Bond lengths



Bond angles



Torsions

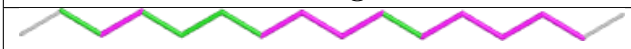


Rings

Ligand PCW C 811

Bond lengths

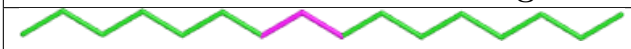
Bond angles



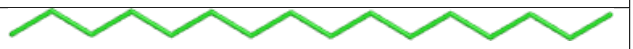
Torsions

Rings

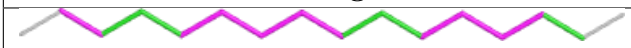
Ligand PCW D 813



Bond lengths



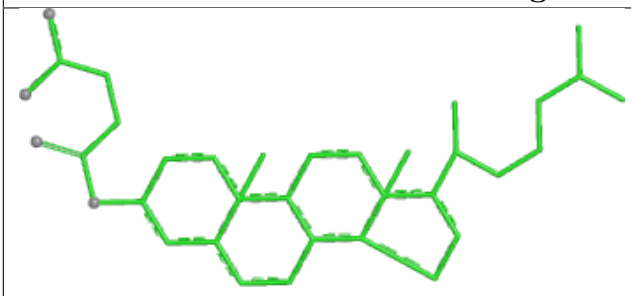
Bond angles



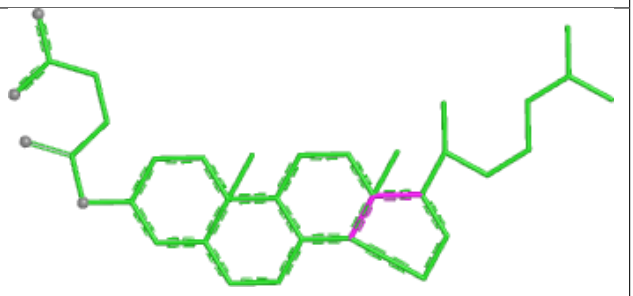
Torsions

Rings

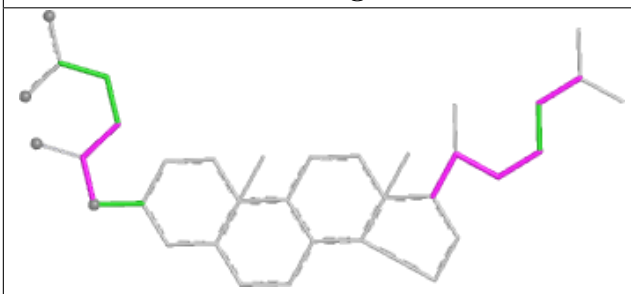
Ligand Y01 A 812



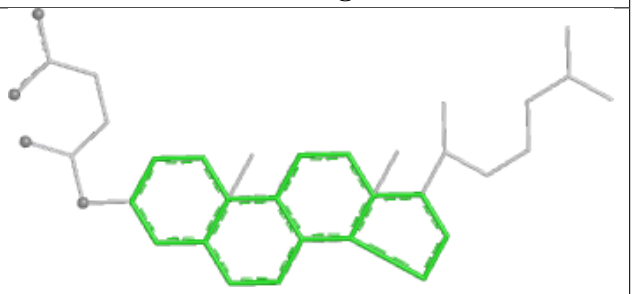
Bond lengths



Bond angles

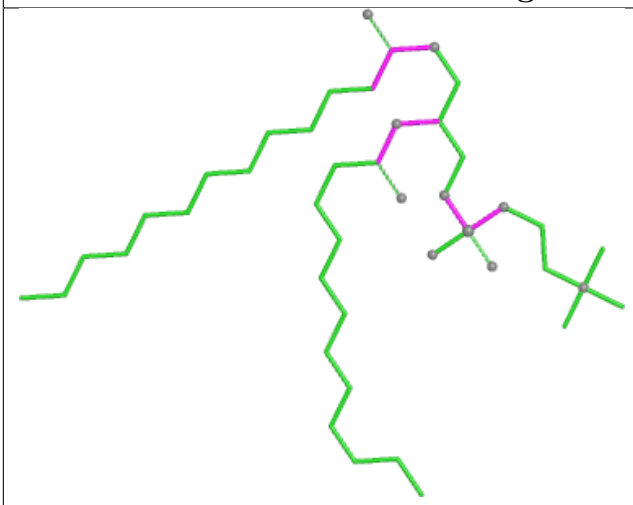


Torsions

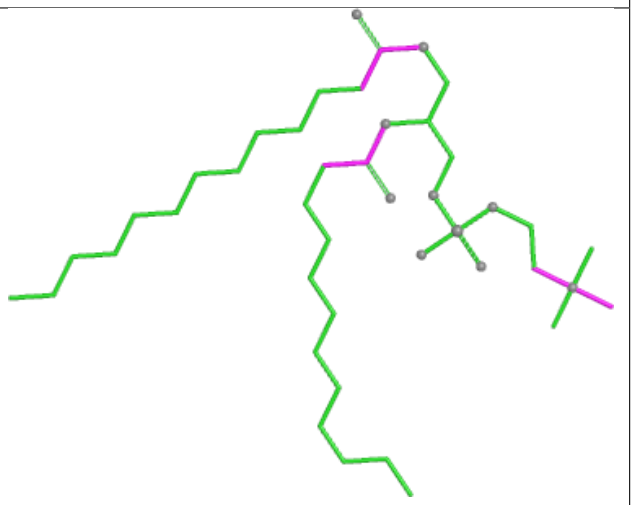


Rings

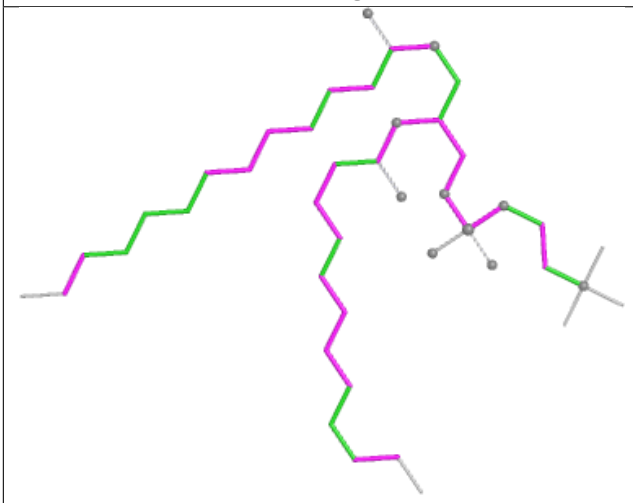
Ligand PCW D 802



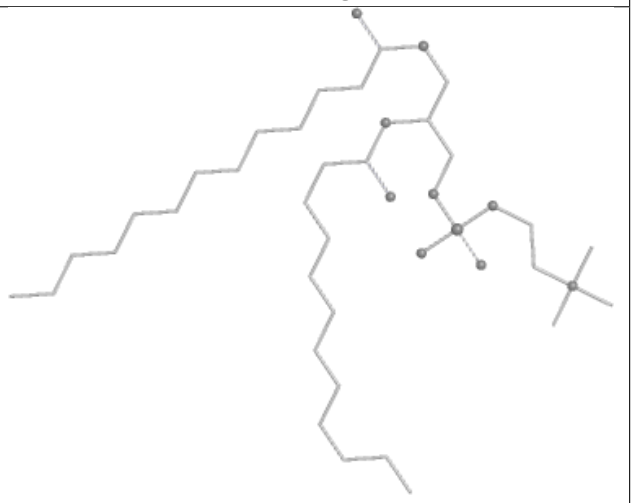
Bond lengths



Bond angles



Torsions



Rings

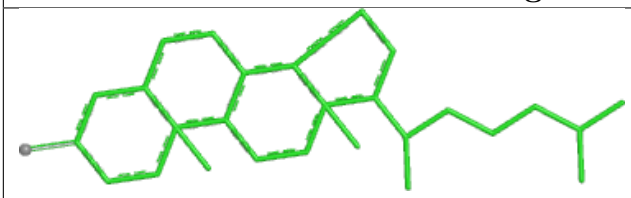
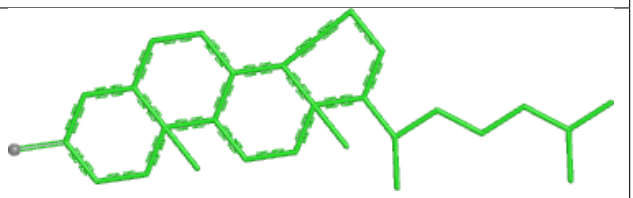
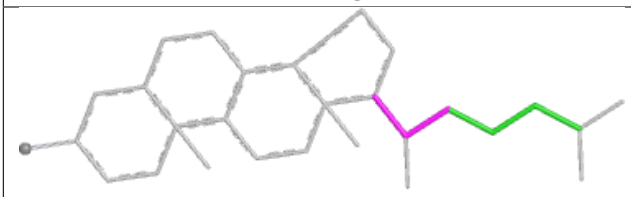
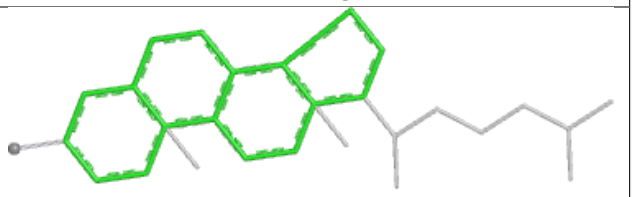
Ligand PCW A 808

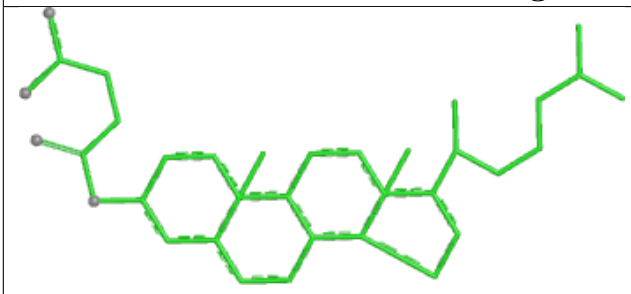
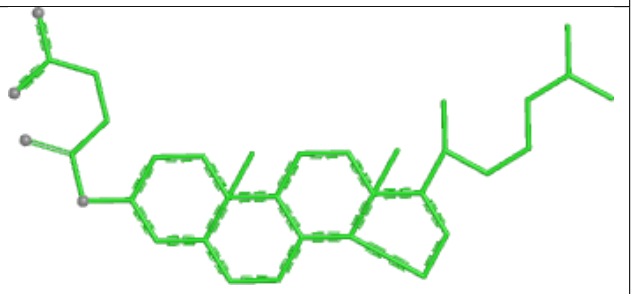
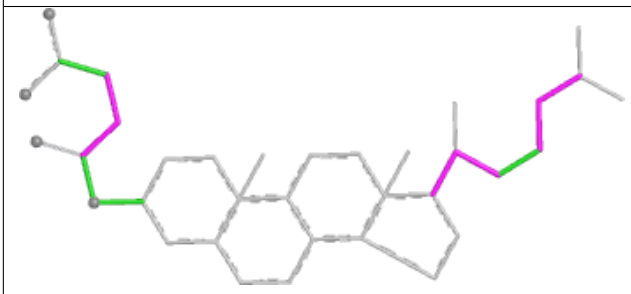
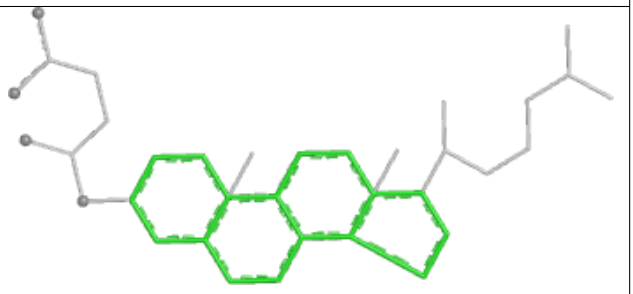
Bond lengths

Bond angles

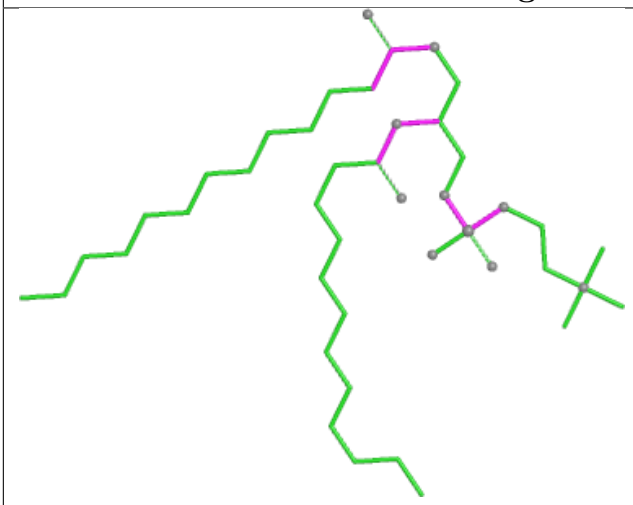
Torsions

Rings

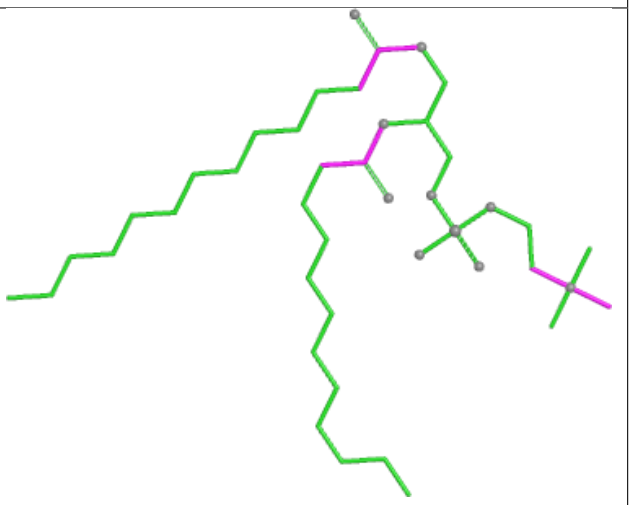
Ligand CLR B 805	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand Y01 A 801	
	
Bond lengths	Bond angles
	
Torsions	Rings

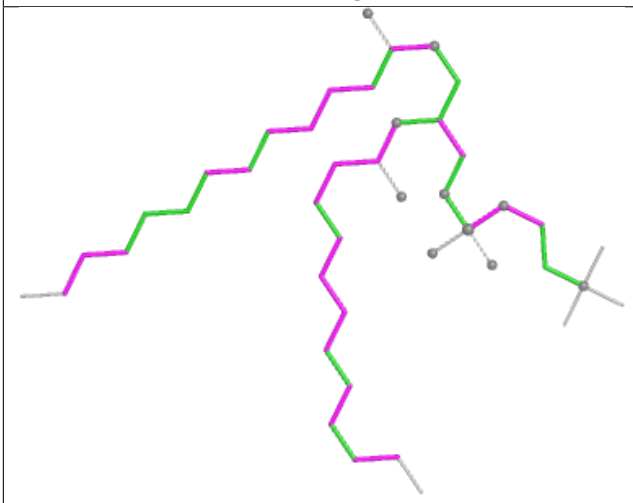
Ligand PCW B 813



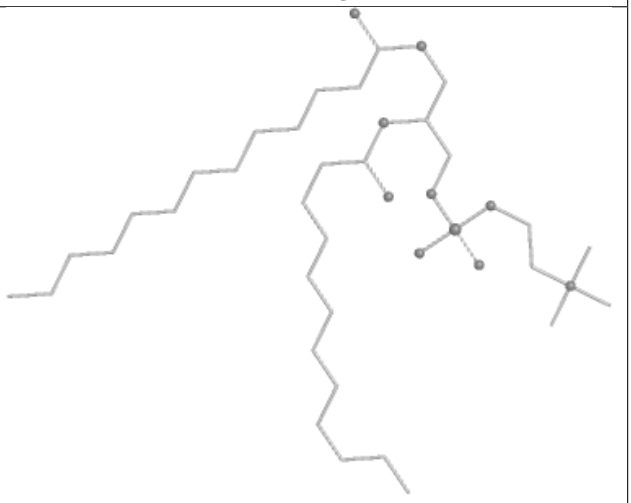
Bond lengths



Bond angles



Torsions



Rings

Ligand PCW C 812

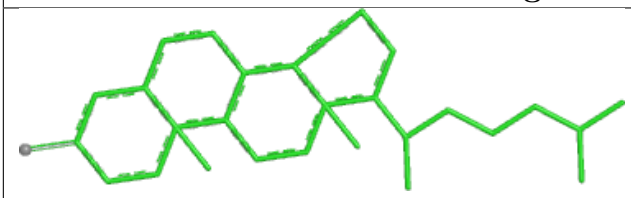
Bond lengths

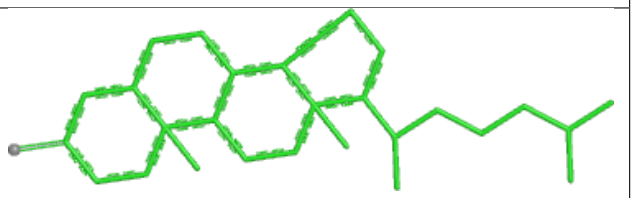
Bond angles

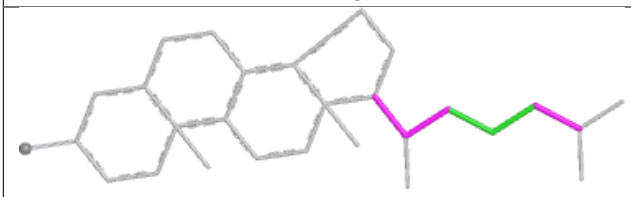
Torsions

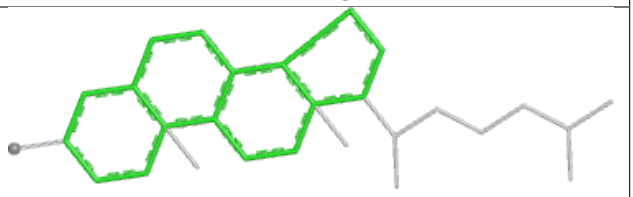
Rings

Ligand CLR A 802

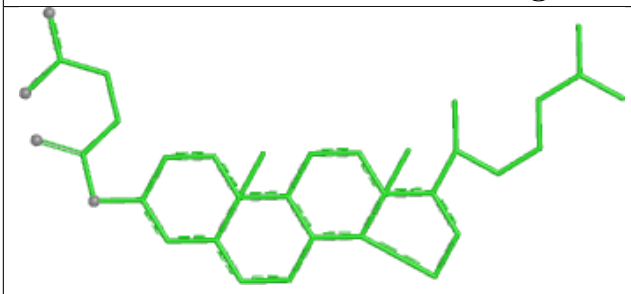

Bond lengths

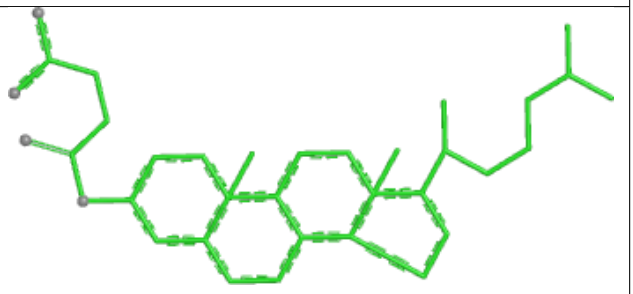

Bond angles

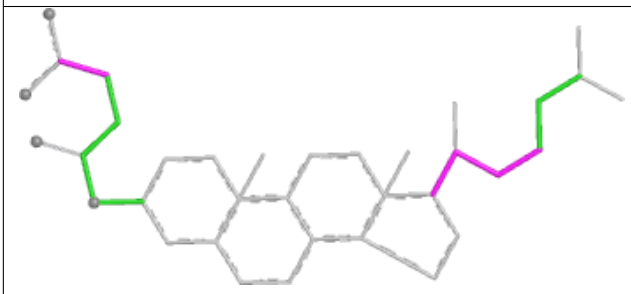

Torsions

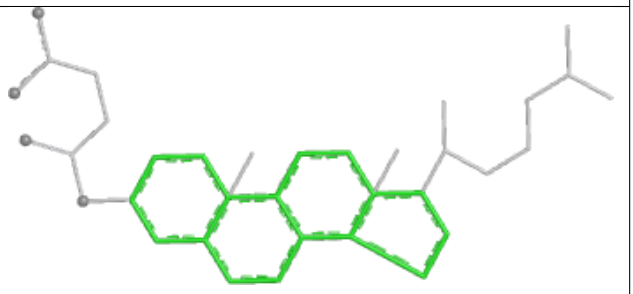

Rings

Ligand Y01 C 804


Bond lengths


Bond angles


Torsions


Rings

Ligand PCW A 814


Bond lengths


Bond angles


Torsions


Rings

Ligand PCW B 802

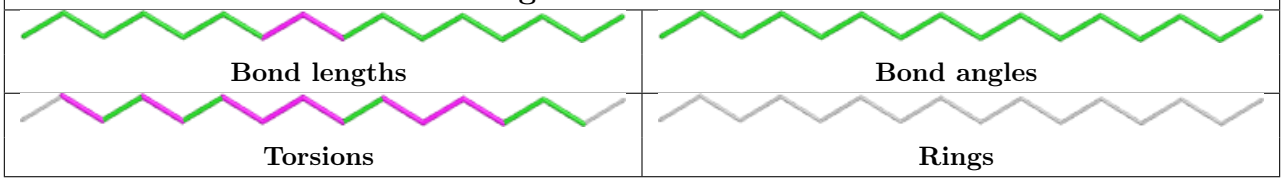

Bond lengths


Bond angles

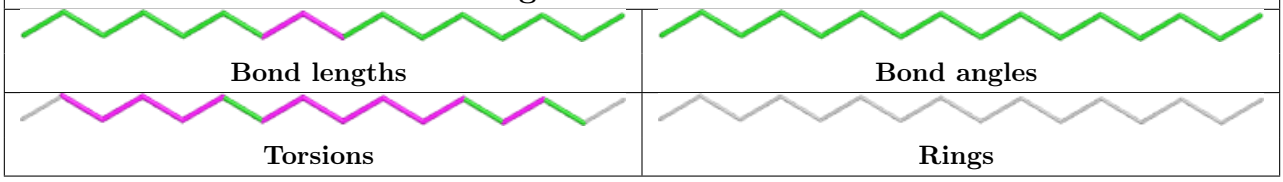

Torsions


Rings

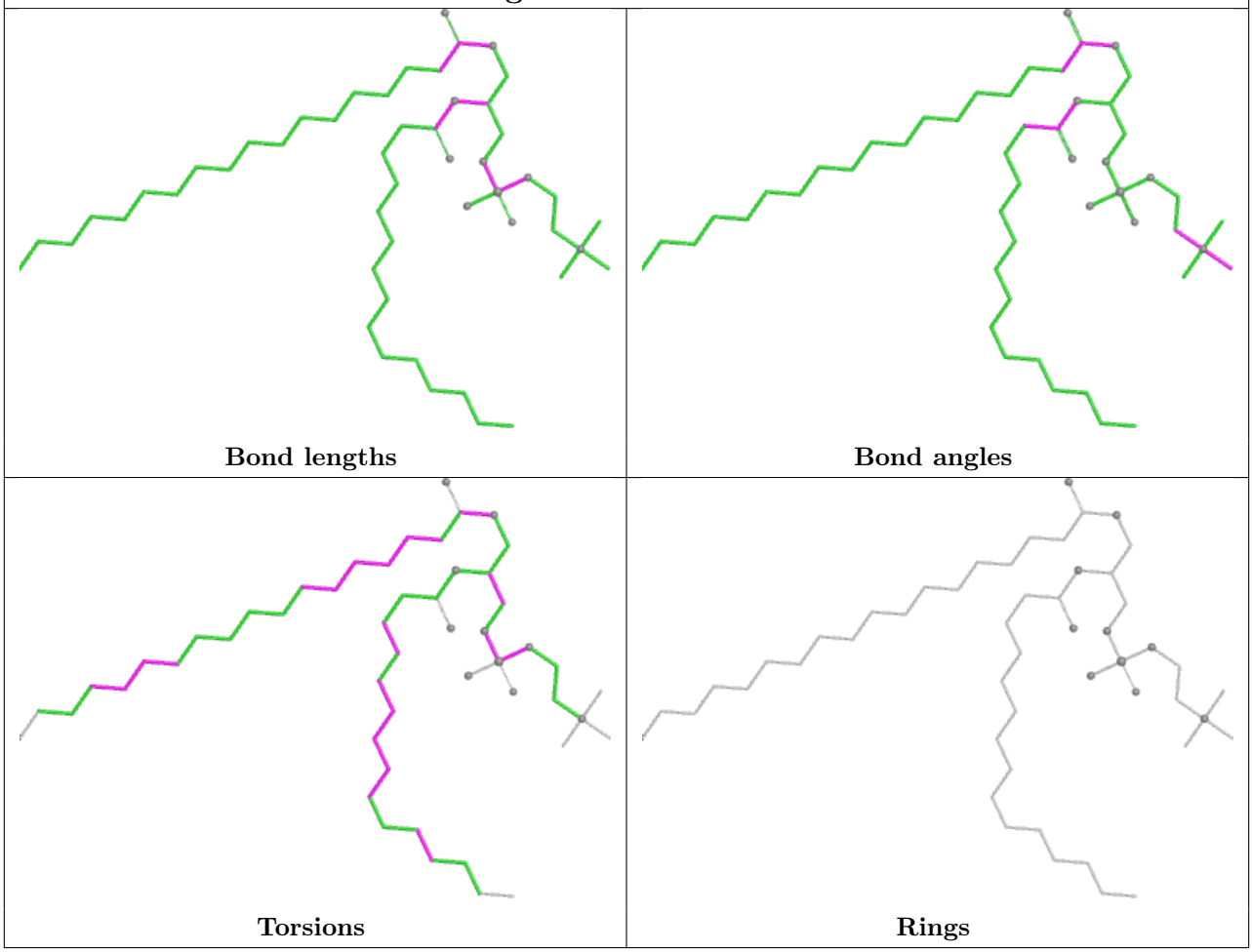
Ligand PCW C 808



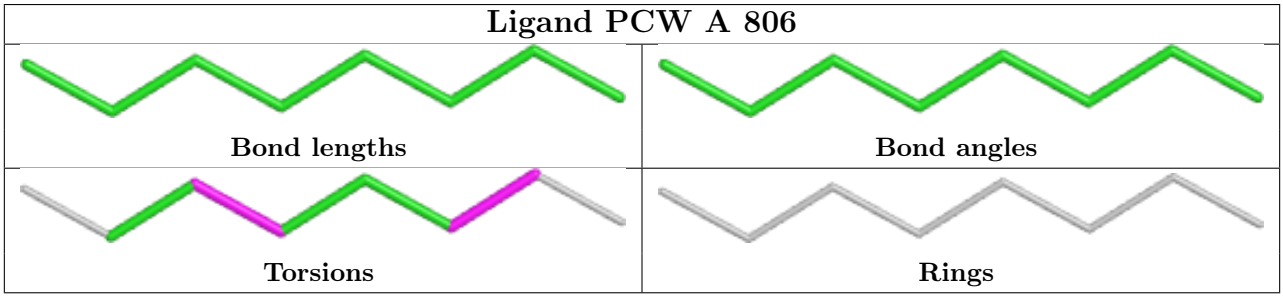
Ligand PCW B 803



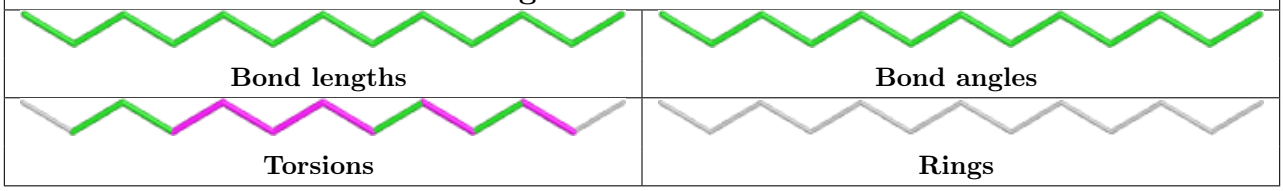
Ligand PCW D 808



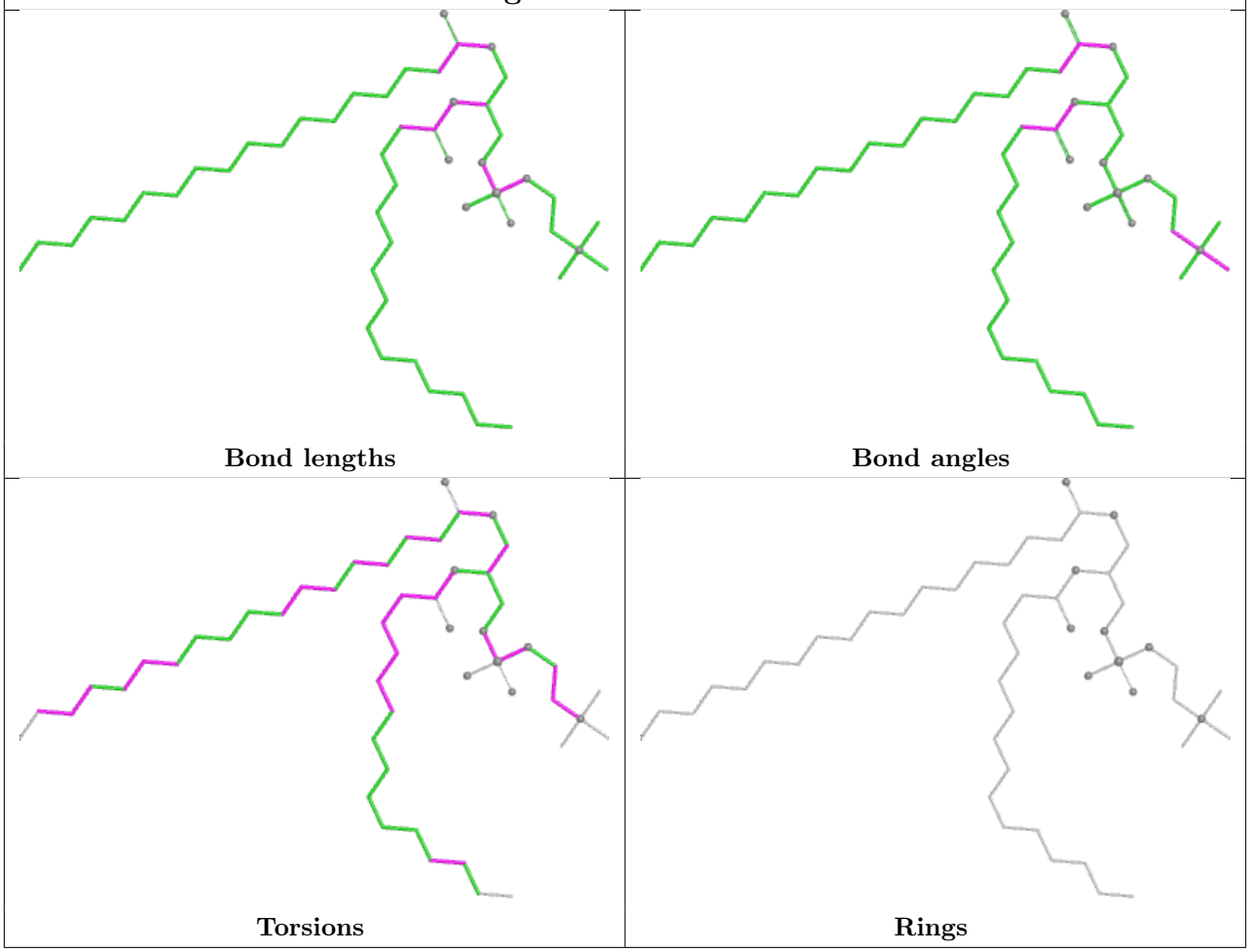
Ligand PCW A 806



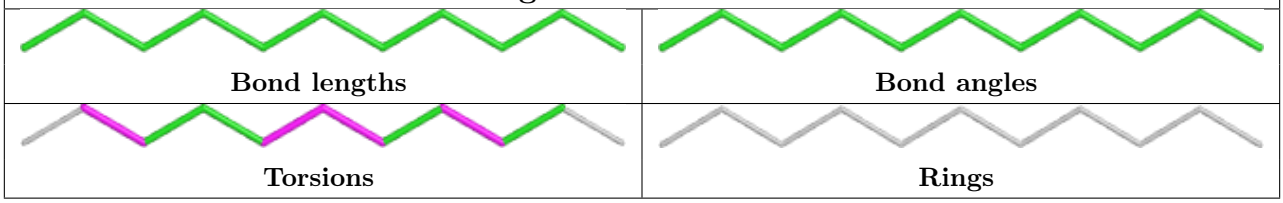
Ligand PCW B 812



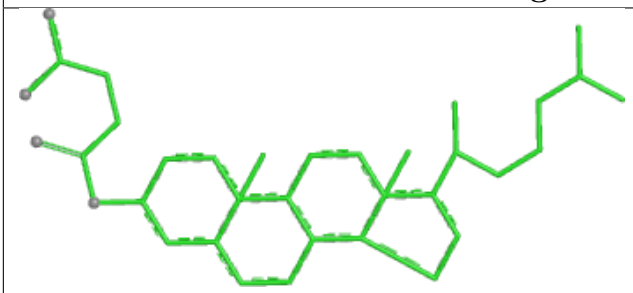
Ligand PCW D 803



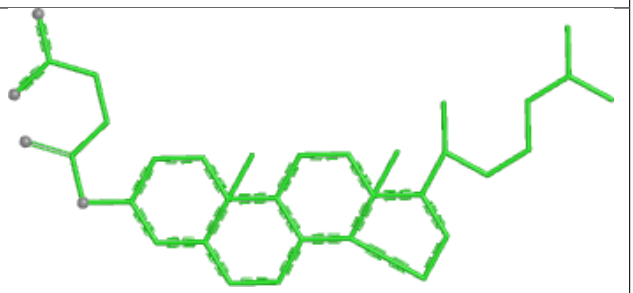
Ligand PCW B 808



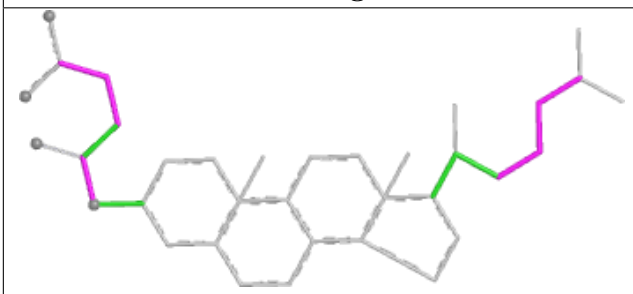
Ligand Y01 B 801



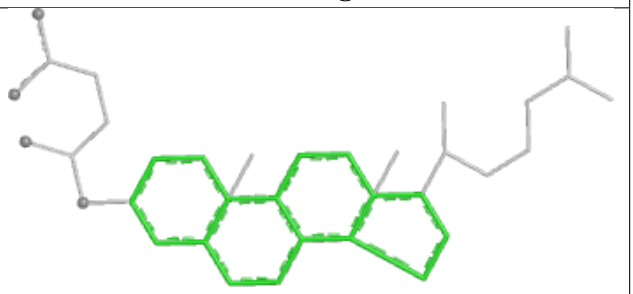
Bond lengths



Bond angles



Torsions



Rings

Ligand PCW A 809

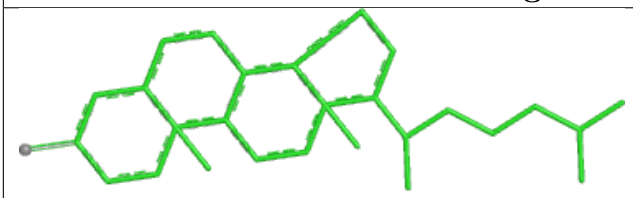
Bond lengths

Bond angles

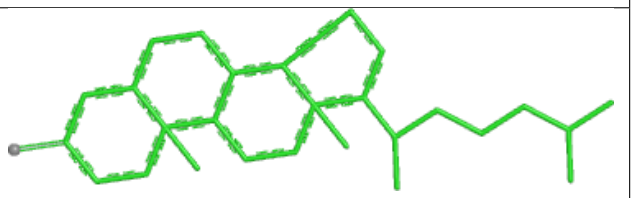
Torsions

Rings

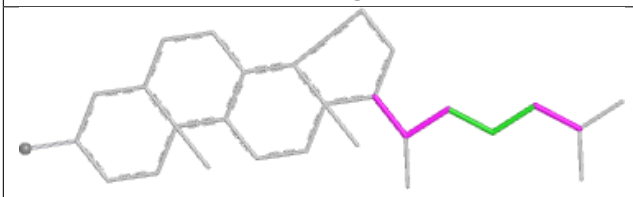
Ligand CLR D 807



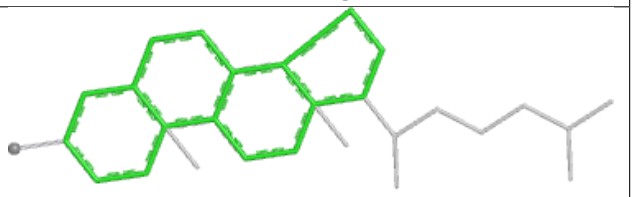
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

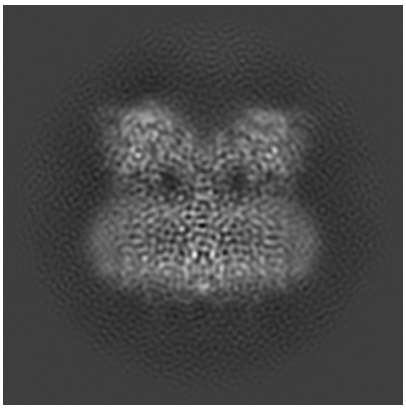
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-45936. These allow visual inspection of the internal detail of the map and identification of artifacts.

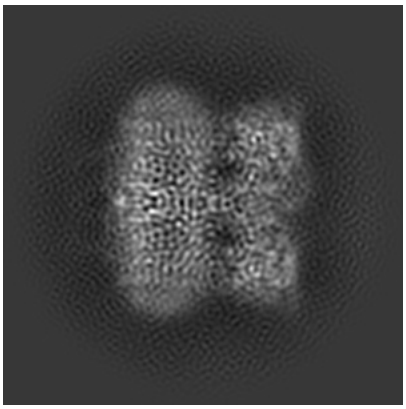
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

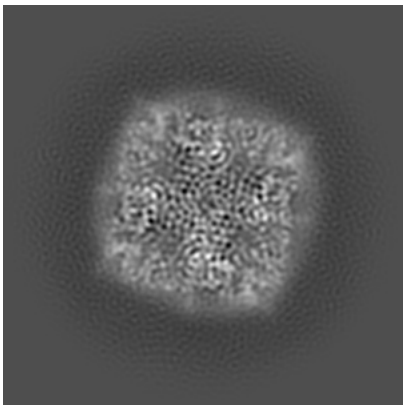
6.1.1 Primary map



X

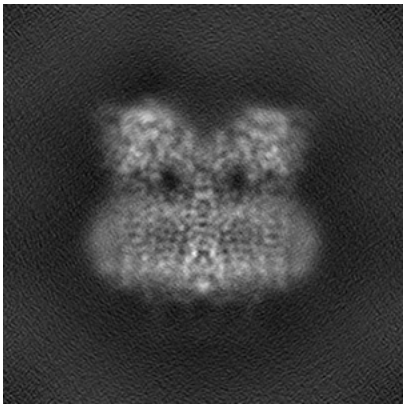


Y

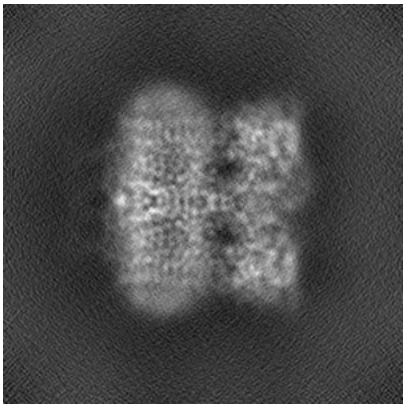


Z

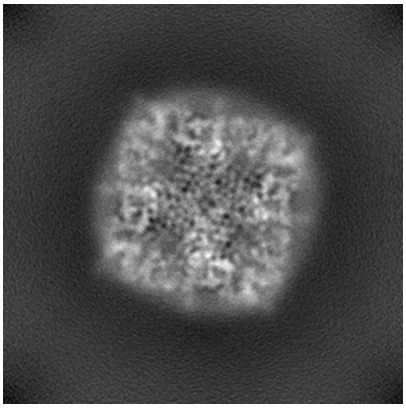
6.1.2 Raw map



X



Y

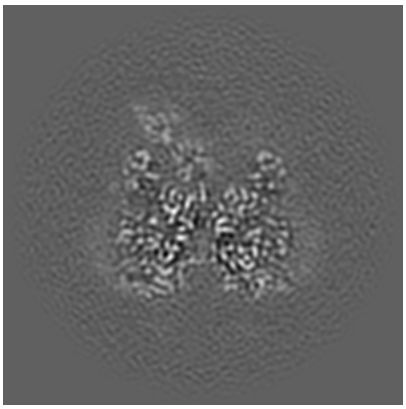


Z

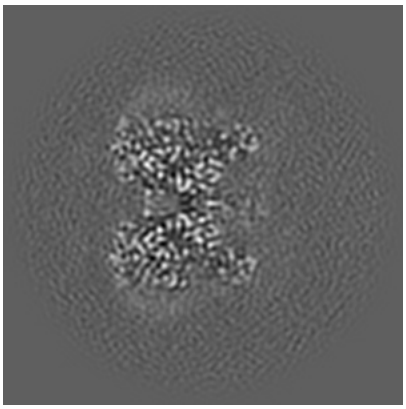
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

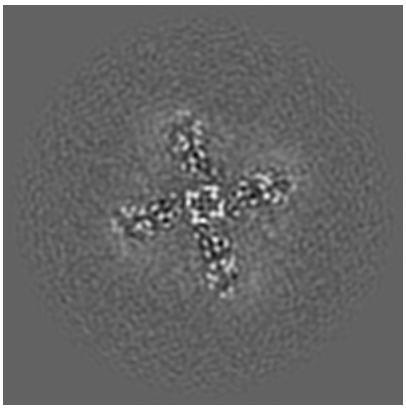
6.2.1 Primary map



X Index: 128

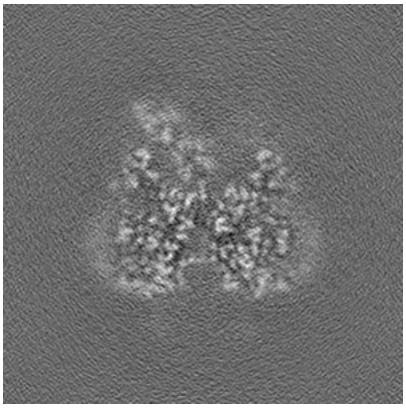


Y Index: 128

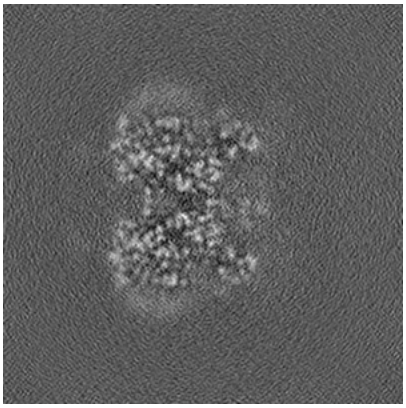


Z Index: 128

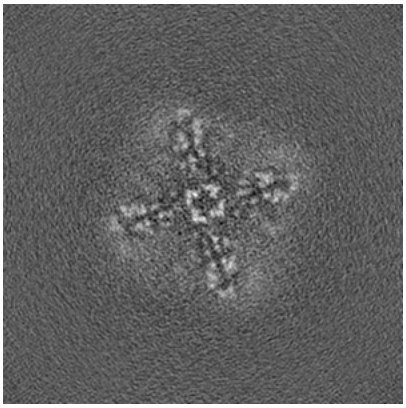
6.2.2 Raw map



X Index: 128



Y Index: 128

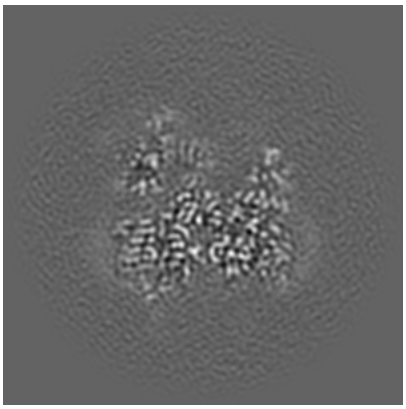


Z Index: 128

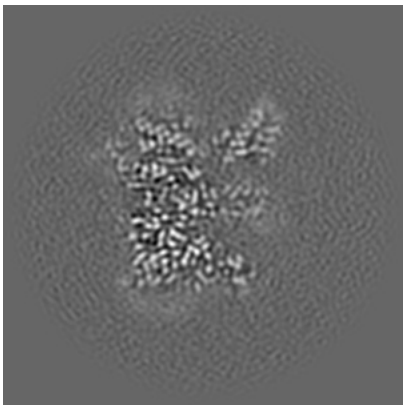
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

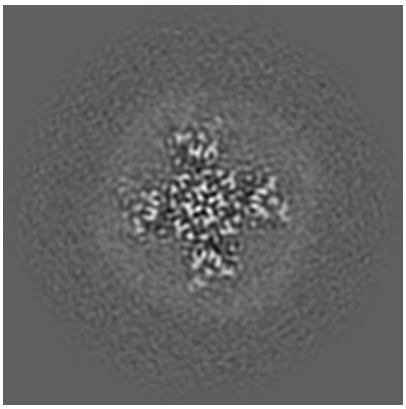
6.3.1 Primary map



X Index: 124

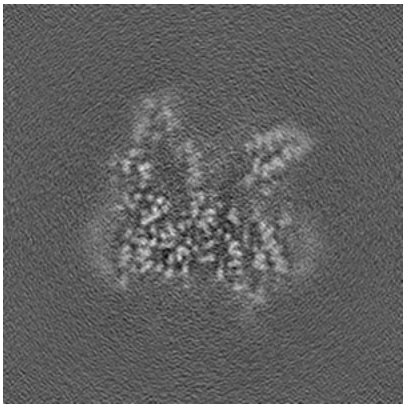


Y Index: 120

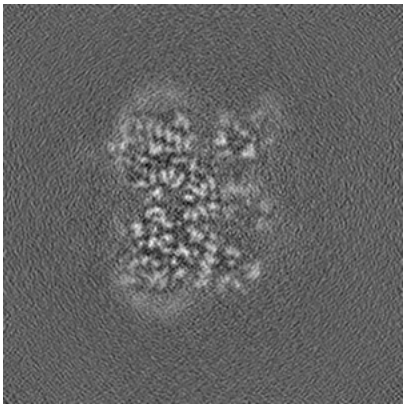


Z Index: 117

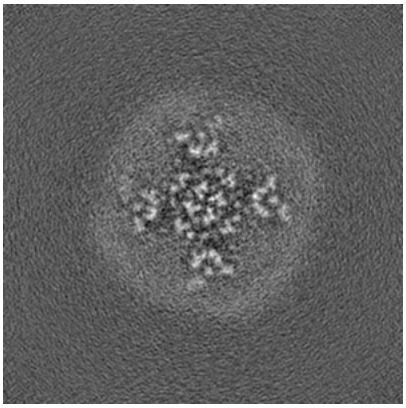
6.3.2 Raw map



X Index: 137



Y Index: 123

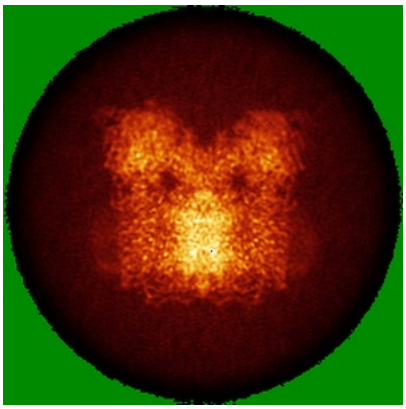


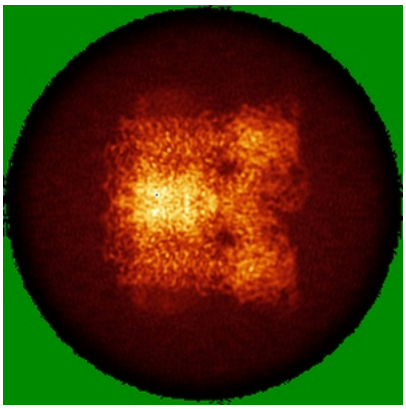
Z Index: 117

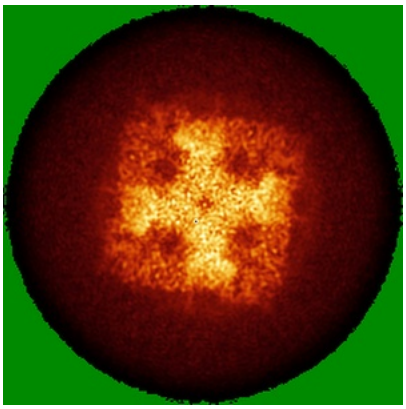
The images above show the largest variance slices of the map in three orthogonal directions.

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

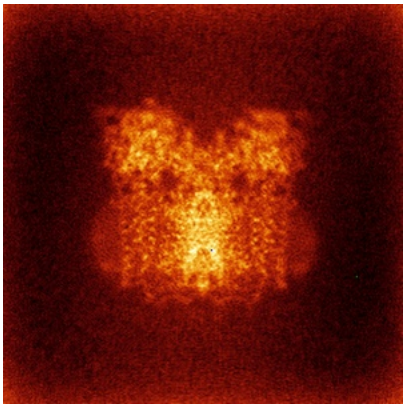
6.4.1 Primary map

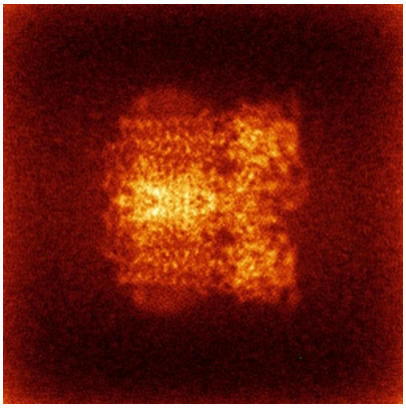

X

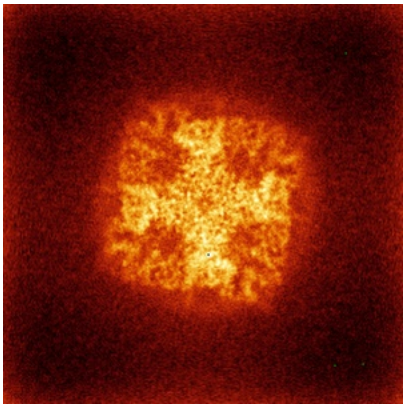

Y


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.

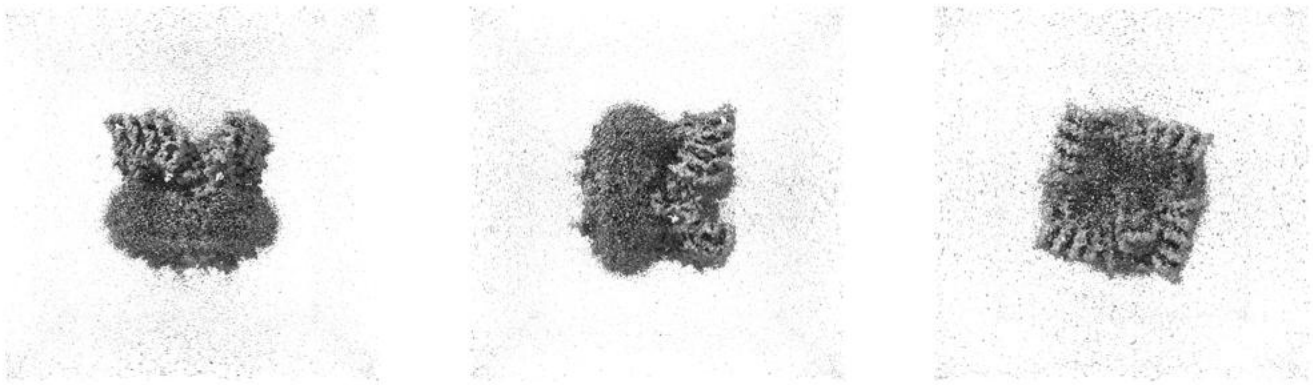
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.109. 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.

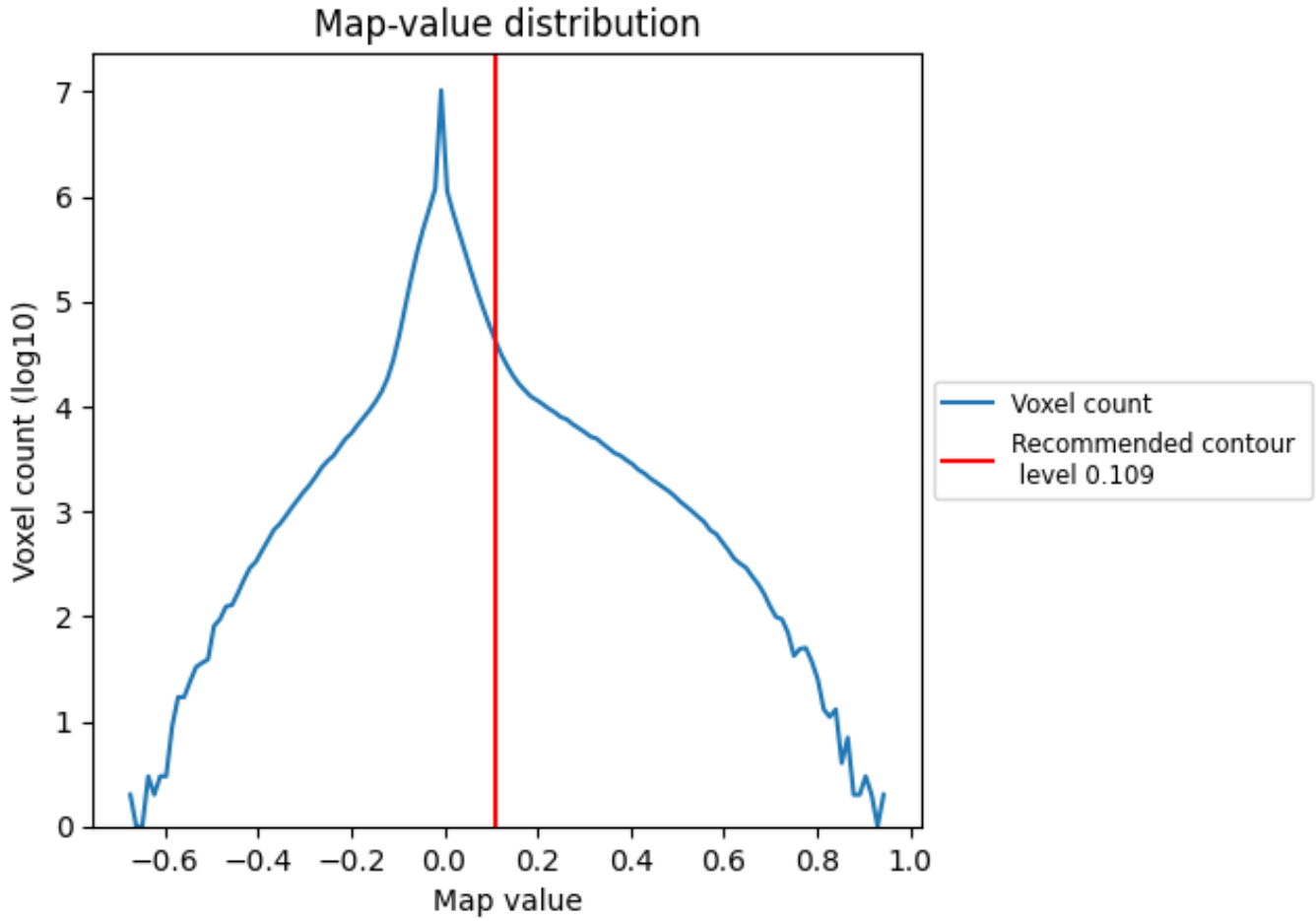
6.6 Mask visualisation (i)

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

7 Map analysis

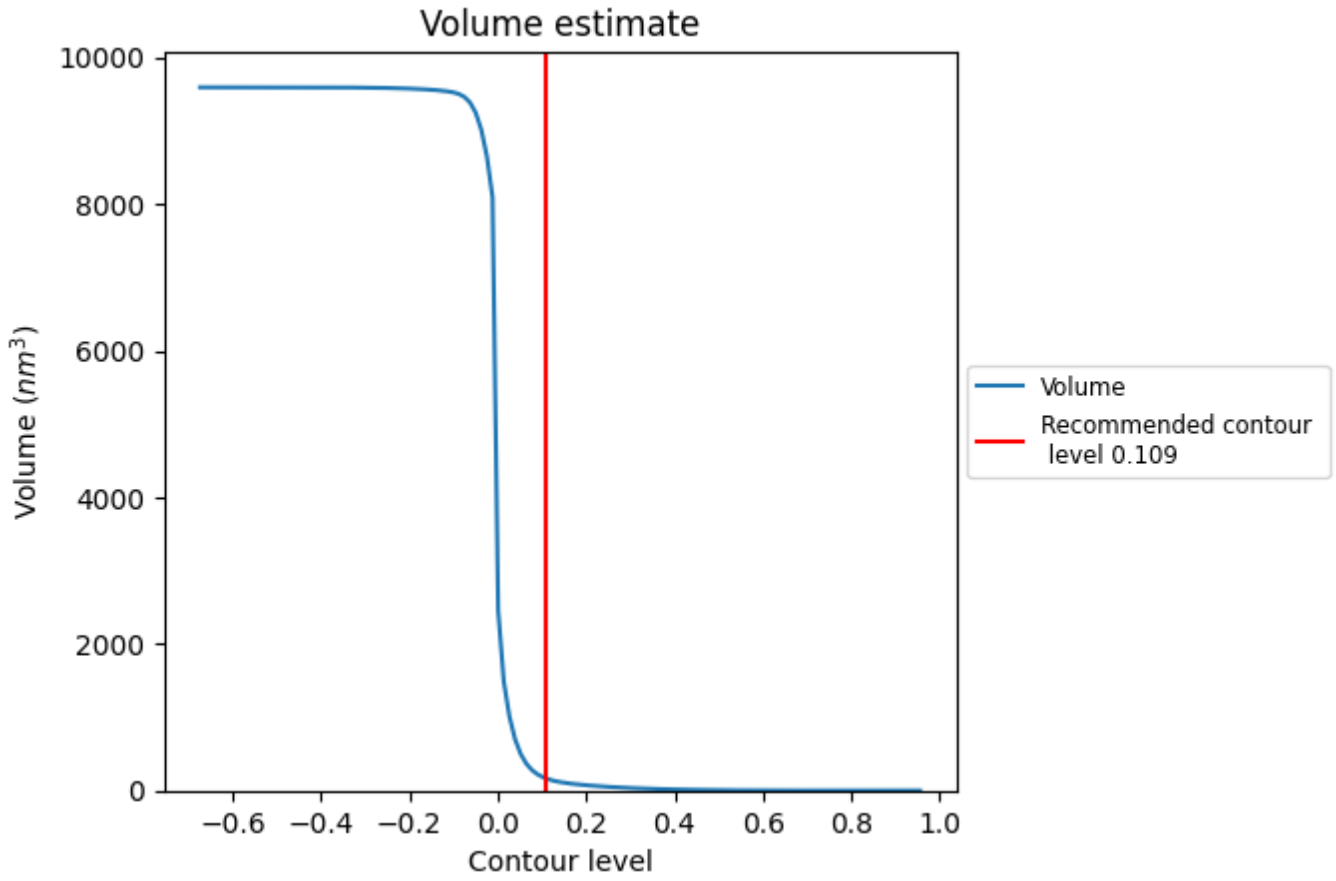
This section contains the results of statistical analysis of the map.

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.

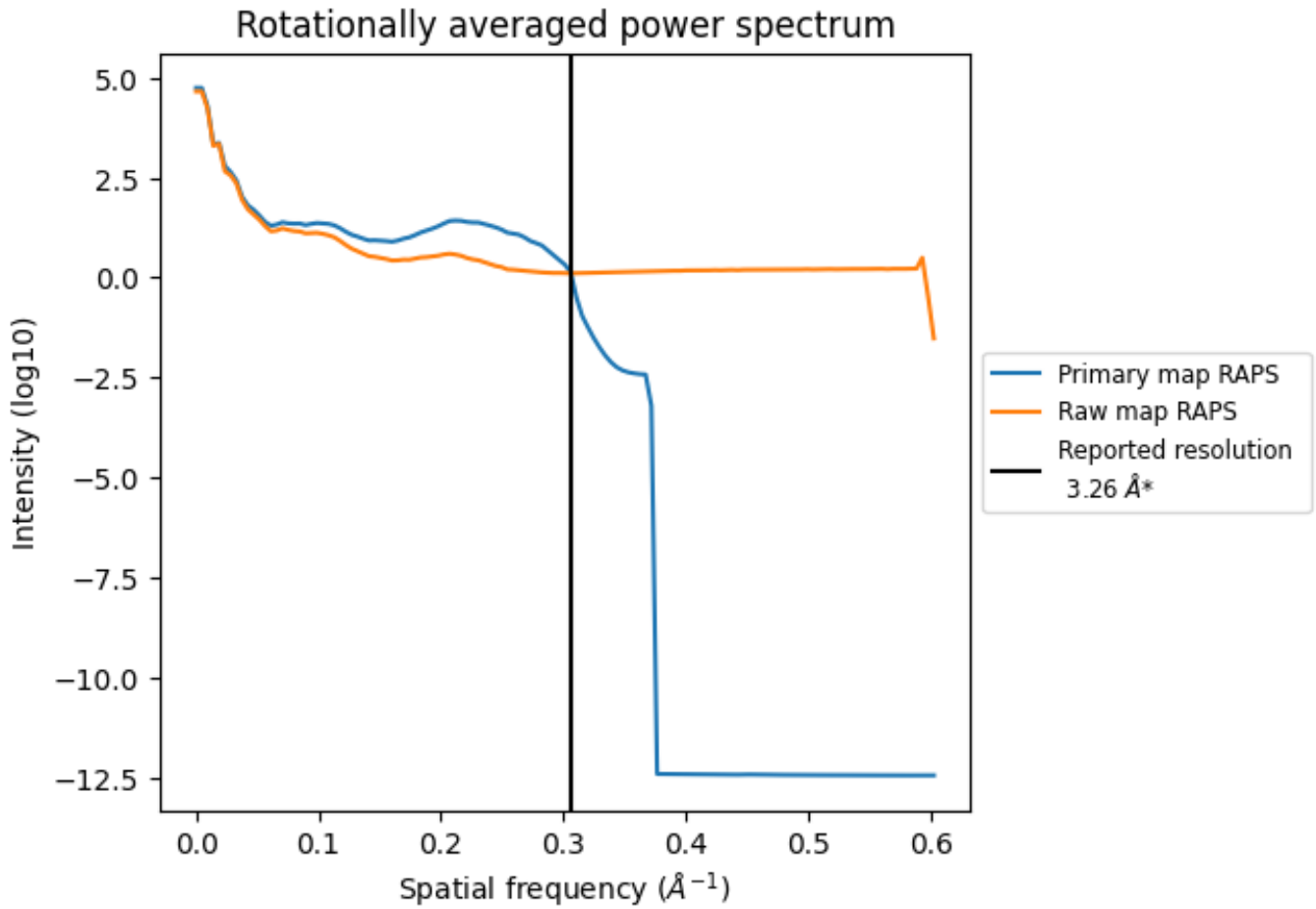
7.2 Volume estimate (i)



The volume at the recommended contour level is 167 nm^3; this corresponds to an approximate mass of 151 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)

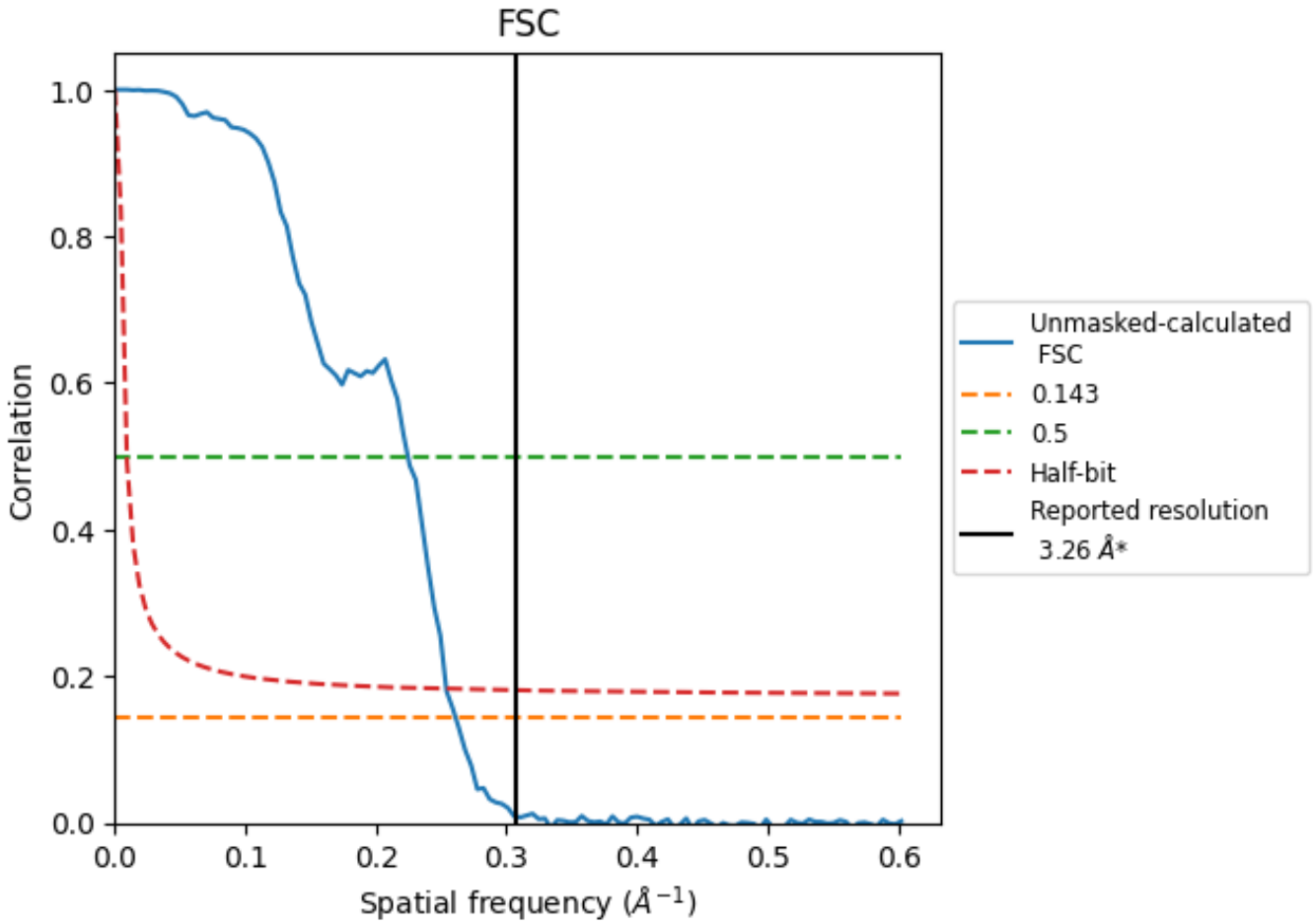


*Reported resolution corresponds to spatial frequency of 0.307 $Å^{-1}$

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 0.307 Å^{-1}

8.2 Resolution estimates (i)

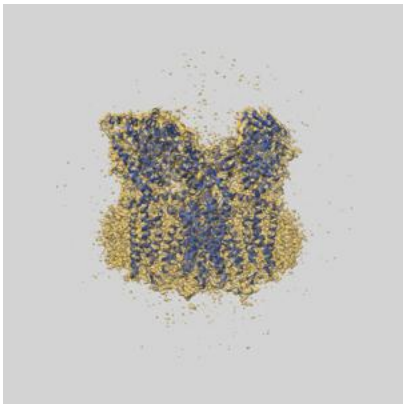
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.26	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.83	4.45	3.94

*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 3.83 differs from the reported value 3.26 by more than 10 %

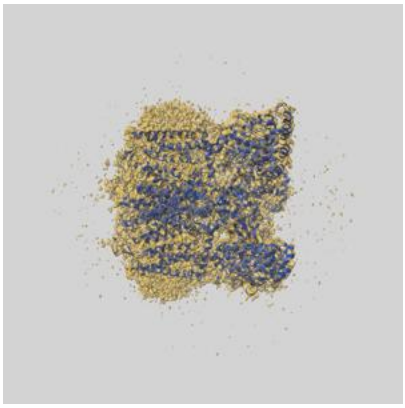
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-45936 and PDB model 9CUK. Per-residue inclusion information can be found in section 3 on page 8.

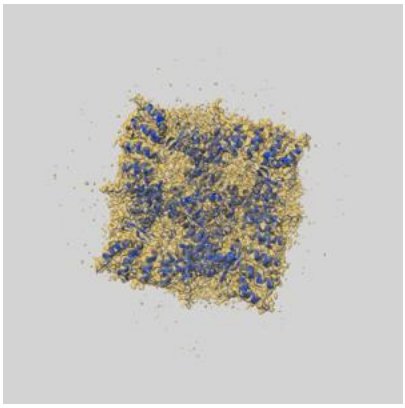
9.1 Map-model overlay



X



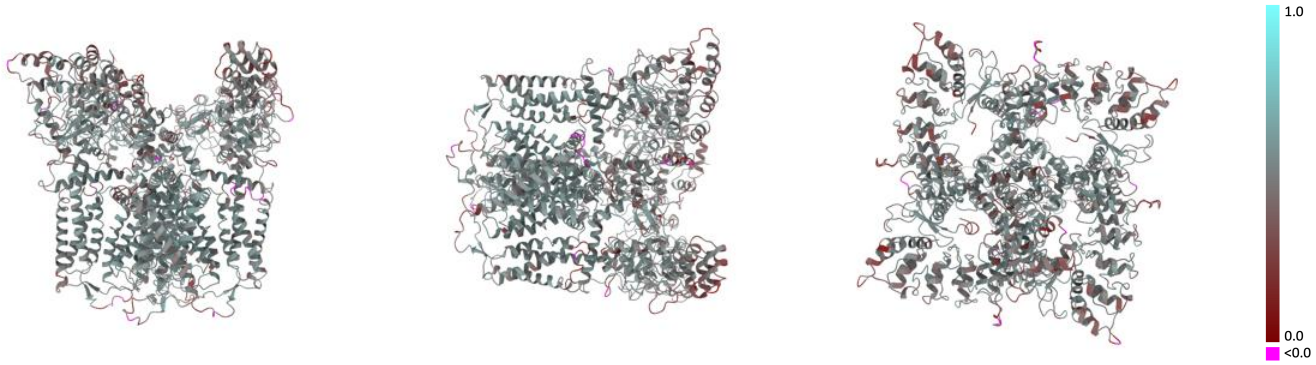
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.109 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.

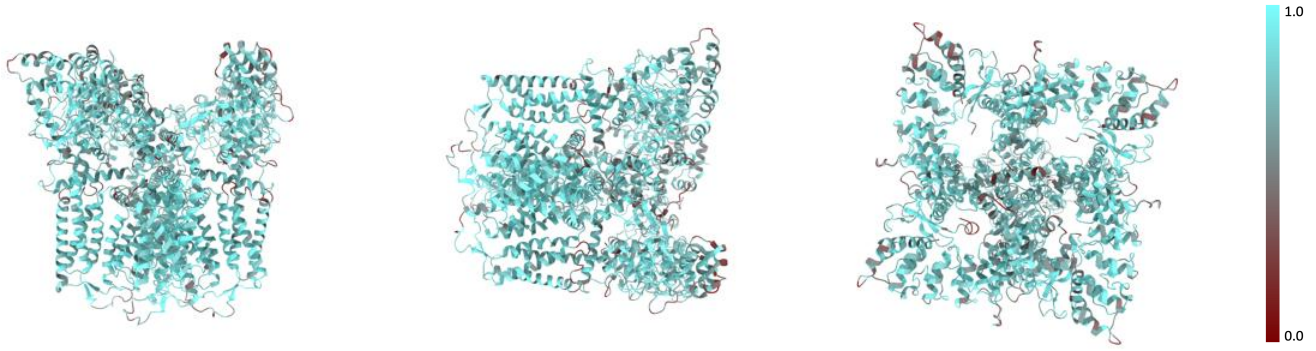
9.2 Q-score mapped to coordinate model (i)



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.

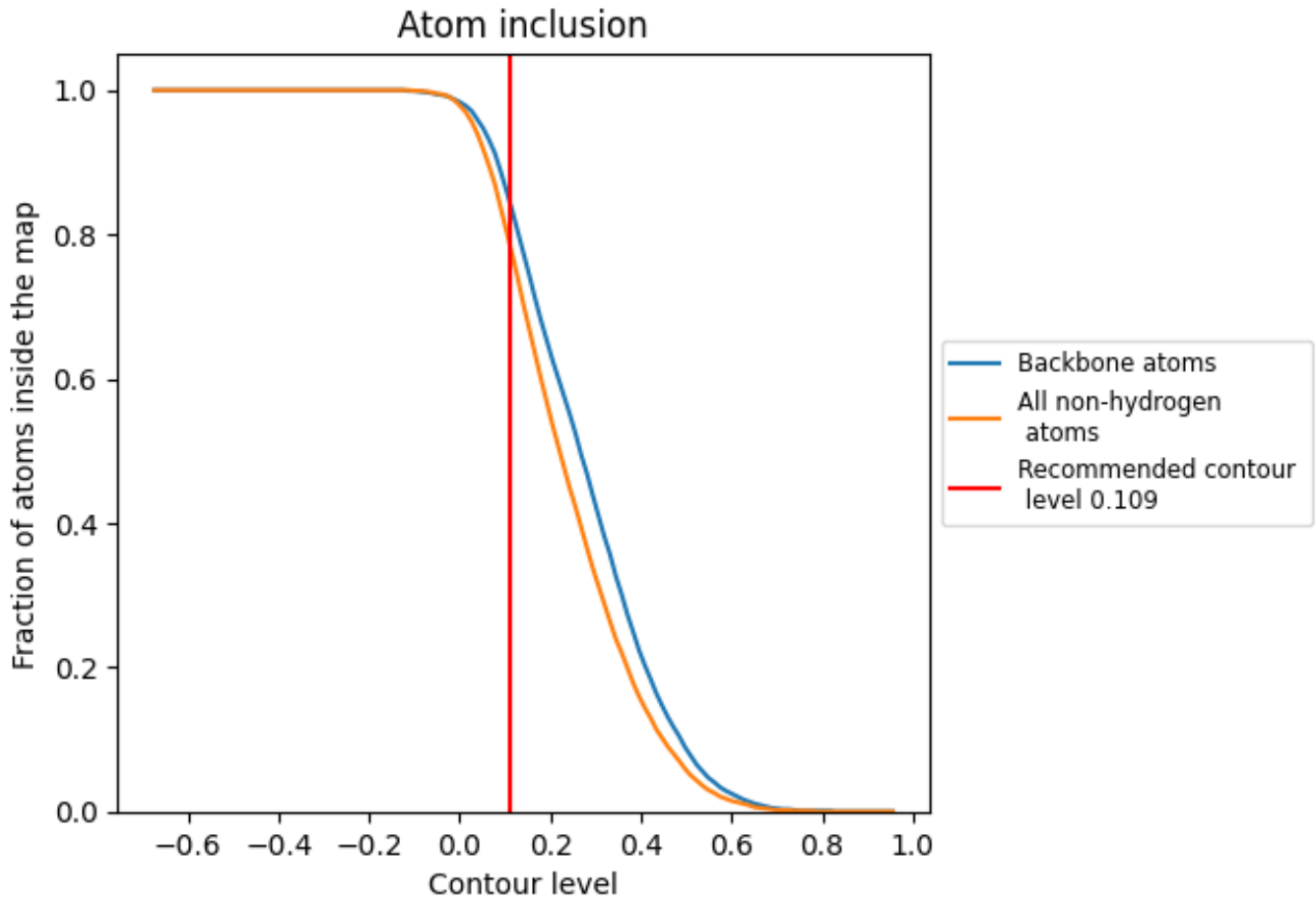
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.109).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 79% 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 (0.109) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7890	0.4820
A	0.7940	0.4820
B	0.7810	0.4780
C	0.8000	0.4860
D	0.8160	0.4940
E	0.6710	0.4340