Full wwPDB EM Validation Report ⓘ

May 26, 2024 – 10:26 AM EDT

PDB ID	:	7S89
EMDB ID	:	EMD-24891
Title	:	Open apo-state cryo-EM structure of human TRPV6 in cNW11 nanodiscs
Authors	:	Neuberger, A.; Nadezhdin, K.D.; Sobolevsky, A.I.
Deposited on	:	2021-09-17
Resolution	:	2.54 Å(reported)
Based on initial model	:	7K4A

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:

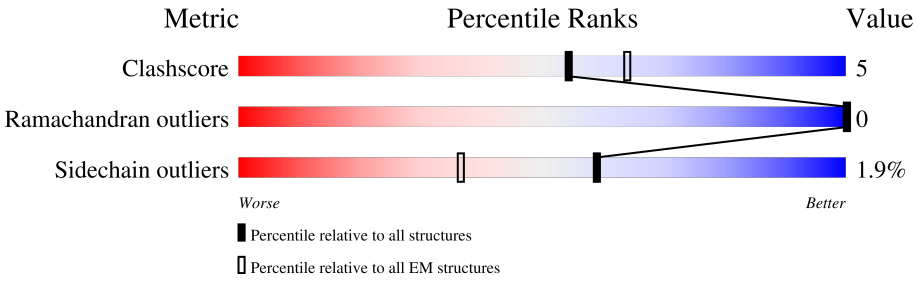
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance

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

The reported resolution of this entry is 2.54 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	683	6% 75% 11% • 13%
1	B	683	6% 75% 11% • 13%
1	C	683	6% 75% 11% • 13%
1	D	683	6% 75% 11% • 13%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 20425 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	594	Total 4766	C 3078	N 806	O 843	S 39	0	0
1	B	594	Total 4766	C 3078	N 806	O 843	S 39	0	0
1	C	594	Total 4766	C 3078	N 806	O 843	S 39	0	0
1	D	594	Total 4766	C 3078	N 806	O 843	S 39	0	0

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	668	VAL	-	expression tag	UNP Q9H1D0
A	669	PRO	-	expression tag	UNP Q9H1D0
A	670	ARG	-	expression tag	UNP Q9H1D0
A	671	GLY	-	expression tag	UNP Q9H1D0
A	672	SER	-	expression tag	UNP Q9H1D0
A	673	ALA	-	expression tag	UNP Q9H1D0
A	674	ALA	-	expression tag	UNP Q9H1D0
A	675	ALA	-	expression tag	UNP Q9H1D0
A	676	TRP	-	expression tag	UNP Q9H1D0
A	677	SER	-	expression tag	UNP Q9H1D0
A	678	HIS	-	expression tag	UNP Q9H1D0
A	679	PRO	-	expression tag	UNP Q9H1D0
A	680	GLN	-	expression tag	UNP Q9H1D0
A	681	PHE	-	expression tag	UNP Q9H1D0
A	682	GLU	-	expression tag	UNP Q9H1D0
A	683	LYS	-	expression tag	UNP Q9H1D0
B	668	VAL	-	expression tag	UNP Q9H1D0
B	669	PRO	-	expression tag	UNP Q9H1D0
B	670	ARG	-	expression tag	UNP Q9H1D0
B	671	GLY	-	expression tag	UNP Q9H1D0
B	672	SER	-	expression tag	UNP Q9H1D0

Continued on next page...

Continued from previous page...

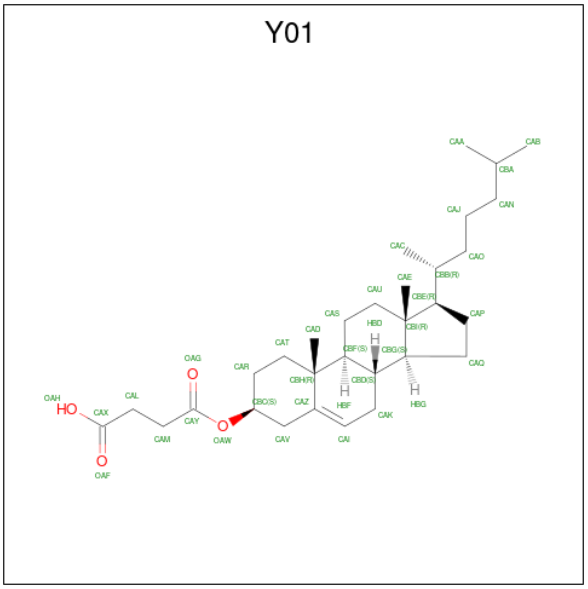
Chain	Residue	Modelled	Actual	Comment	Reference
B	673	ALA	-	expression tag	UNP Q9H1D0
B	674	ALA	-	expression tag	UNP Q9H1D0
B	675	ALA	-	expression tag	UNP Q9H1D0
B	676	TRP	-	expression tag	UNP Q9H1D0
B	677	SER	-	expression tag	UNP Q9H1D0
B	678	HIS	-	expression tag	UNP Q9H1D0
B	679	PRO	-	expression tag	UNP Q9H1D0
B	680	GLN	-	expression tag	UNP Q9H1D0
B	681	PHE	-	expression tag	UNP Q9H1D0
B	682	GLU	-	expression tag	UNP Q9H1D0
B	683	LYS	-	expression tag	UNP Q9H1D0
C	668	VAL	-	expression tag	UNP Q9H1D0
C	669	PRO	-	expression tag	UNP Q9H1D0
C	670	ARG	-	expression tag	UNP Q9H1D0
C	671	GLY	-	expression tag	UNP Q9H1D0
C	672	SER	-	expression tag	UNP Q9H1D0
C	673	ALA	-	expression tag	UNP Q9H1D0
C	674	ALA	-	expression tag	UNP Q9H1D0
C	675	ALA	-	expression tag	UNP Q9H1D0
C	676	TRP	-	expression tag	UNP Q9H1D0
C	677	SER	-	expression tag	UNP Q9H1D0
C	678	HIS	-	expression tag	UNP Q9H1D0
C	679	PRO	-	expression tag	UNP Q9H1D0
C	680	GLN	-	expression tag	UNP Q9H1D0
C	681	PHE	-	expression tag	UNP Q9H1D0
C	682	GLU	-	expression tag	UNP Q9H1D0
C	683	LYS	-	expression tag	UNP Q9H1D0
D	668	VAL	-	expression tag	UNP Q9H1D0
D	669	PRO	-	expression tag	UNP Q9H1D0
D	670	ARG	-	expression tag	UNP Q9H1D0
D	671	GLY	-	expression tag	UNP Q9H1D0
D	672	SER	-	expression tag	UNP Q9H1D0
D	673	ALA	-	expression tag	UNP Q9H1D0
D	674	ALA	-	expression tag	UNP Q9H1D0
D	675	ALA	-	expression tag	UNP Q9H1D0
D	676	TRP	-	expression tag	UNP Q9H1D0
D	677	SER	-	expression tag	UNP Q9H1D0
D	678	HIS	-	expression tag	UNP Q9H1D0
D	679	PRO	-	expression tag	UNP Q9H1D0
D	680	GLN	-	expression tag	UNP Q9H1D0
D	681	PHE	-	expression tag	UNP Q9H1D0
D	682	GLU	-	expression tag	UNP Q9H1D0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	683	LYS	-	expression tag	UNP Q9H1D0

- Molecule 2 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: $C_{31}H_{50}O_4$).



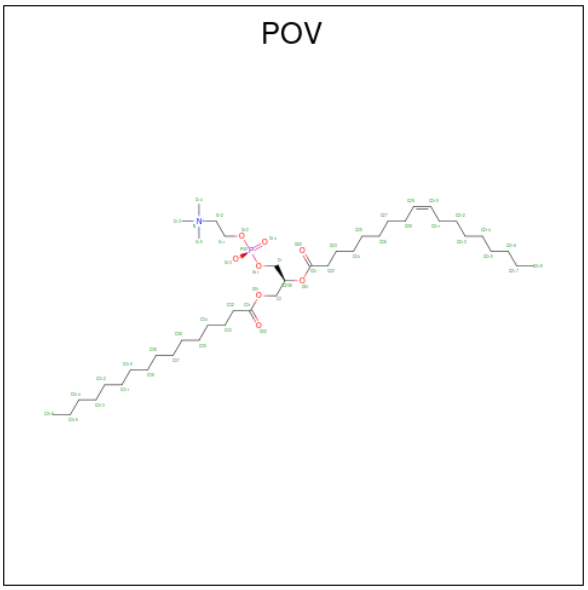
Mol	Chain	Residues	Atoms	AltConf
2	A	1	Total C O 35 31 4	0
2	A	1	Total C O 35 31 4	0
2	A	1	Total C O 35 31 4	0
2	B	1	Total C O 35 31 4	0
2	B	1	Total C O 35 31 4	0
2	B	1	Total C O 35 31 4	0
2	C	1	Total C O 35 31 4	0
2	C	1	Total C O 35 31 4	0
2	C	1	Total C O 35 31 4	0
2	D	1	Total C O 35 31 4	0
2	D	1	Total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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
2	D	1	Total C O 35 31 4	0

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



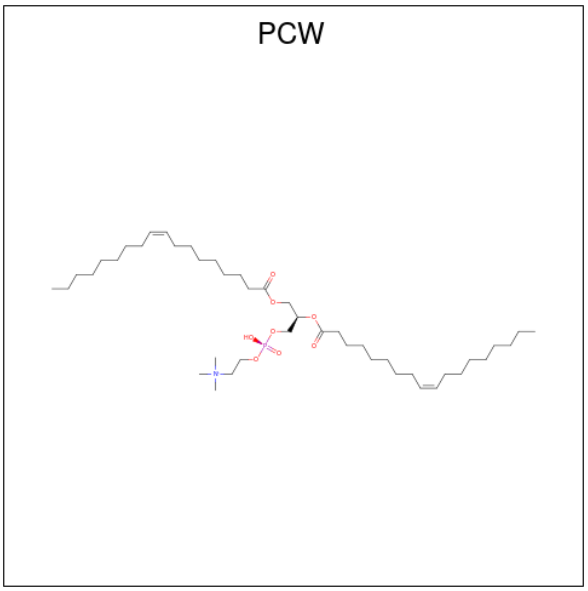
Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total C 13 13	0
3	A	1	Total C N O P 52 42 1 8 1	0
3	A	1	Total C 20 20	0
3	A	1	Total C 14 14	0
3	A	1	Total C O 18 16 2	0
3	A	1	Total C 20 20	0
3	A	1	Total C O 31 28 3	0
3	A	1	Total C N O P 52 42 1 8 1	0
3	B	1	Total C N O P 52 42 1 8 1	0
3	B	1	Total C 13 13	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
3	B	1	Total C N O P 52 42 1 8 1	0
3	B	1	Total C 14 14	0
3	B	1	Total C O 18 16 2	0
3	B	1	Total C 20 20	0
3	B	1	Total C O 31 28 3	0
3	C	1	Total C N O P 52 42 1 8 1	0
3	C	1	Total C 13 13	0
3	C	1	Total C N O P 52 42 1 8 1	0
3	C	1	Total C 14 14	0
3	C	1	Total C O 18 16 2	0
3	C	1	Total C 20 20	0
3	C	1	Total C O 31 28 3	0
3	D	1	Total C O 31 28 3	0
3	D	1	Total C N O P 52 42 1 8 1	0
3	D	1	Total C 13 13	0
3	D	1	Total C N O P 52 42 1 8 1	0
3	D	1	Total C 14 14	0
3	D	1	Total C O 18 16 2	0

- Molecule 4 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: $C_{44}H_{85}NO_8P$).



Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total C 13 13	0
4	B	1	Total C 13 13	0
4	C	1	Total C 13 13	0
4	D	1	Total C 13 13	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 6 is water.

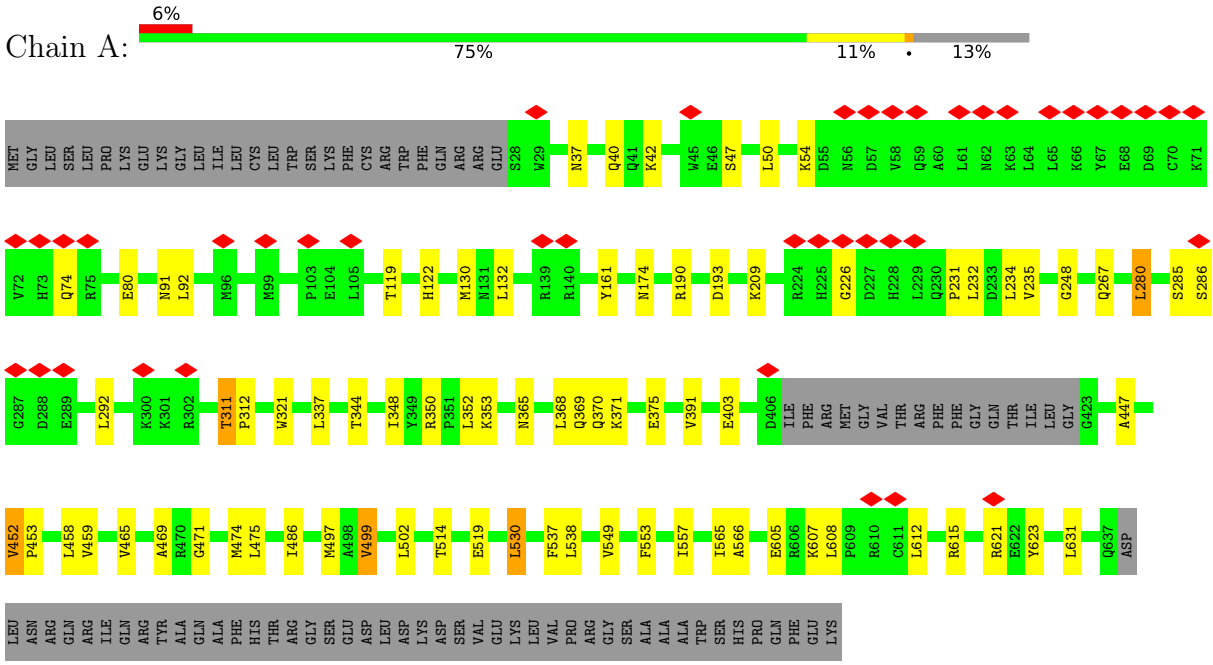
Mol	Chain	Residues	Atoms	AltConf
6	A	22	Total O 22 22	0
6	B	22	Total O 22 22	0
6	C	22	Total O 22 22	0
6	D	22	Total O 22 22	0

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.

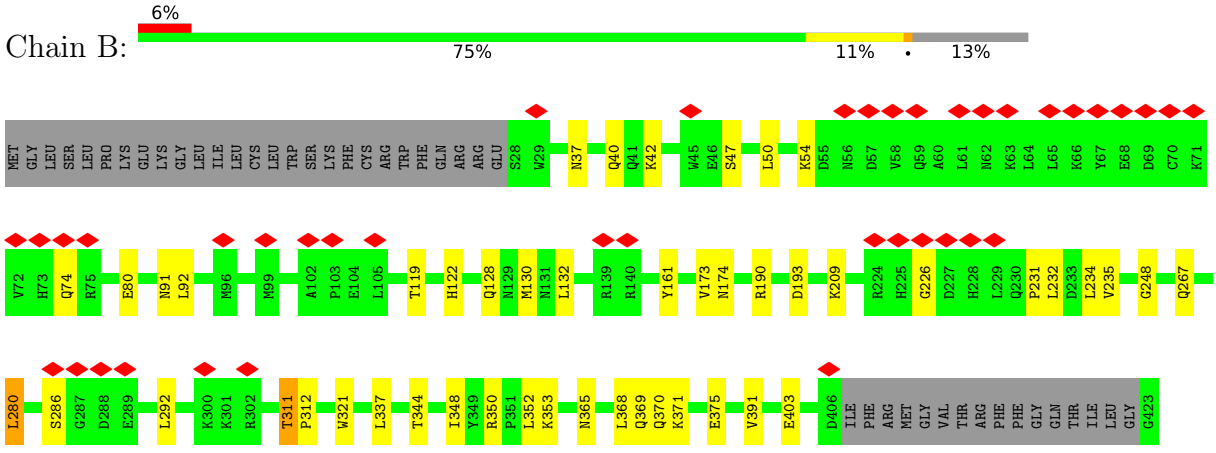
• Molecule 1: Transient receptor potential cation channel subfamily V member 6

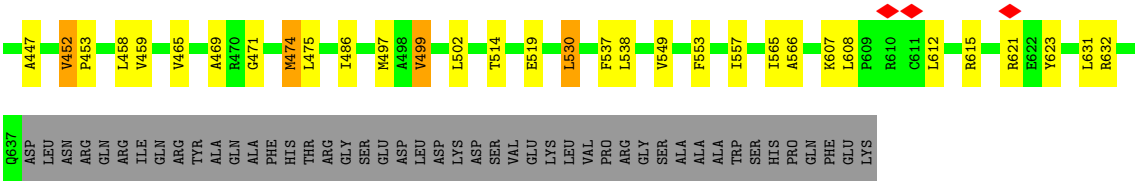
Chain A:



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

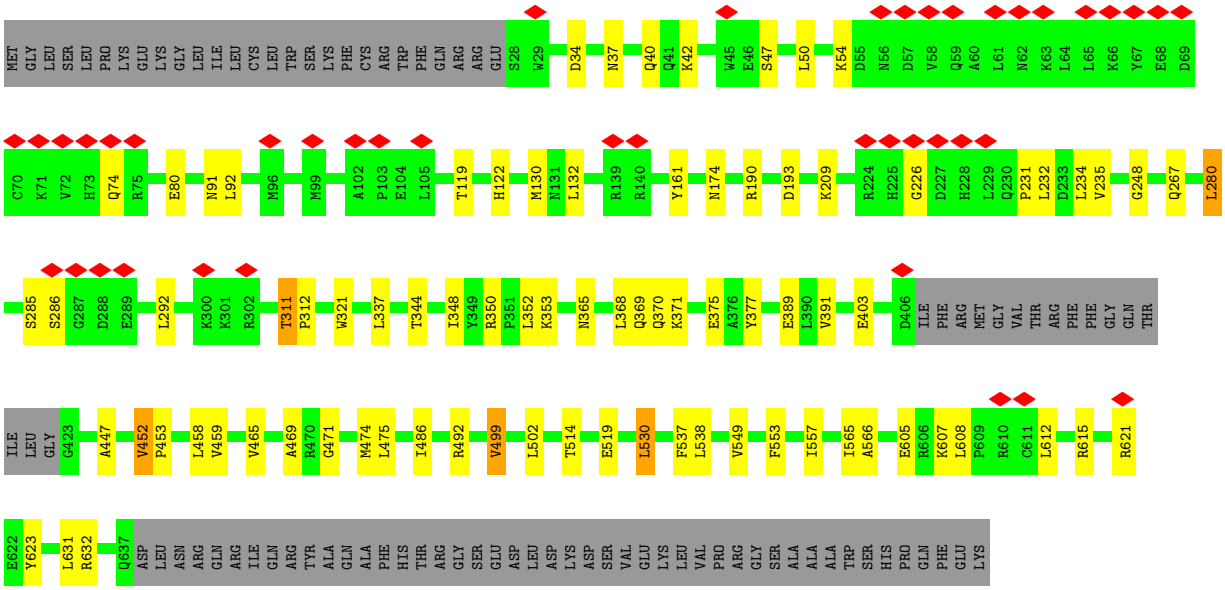
Chain B:





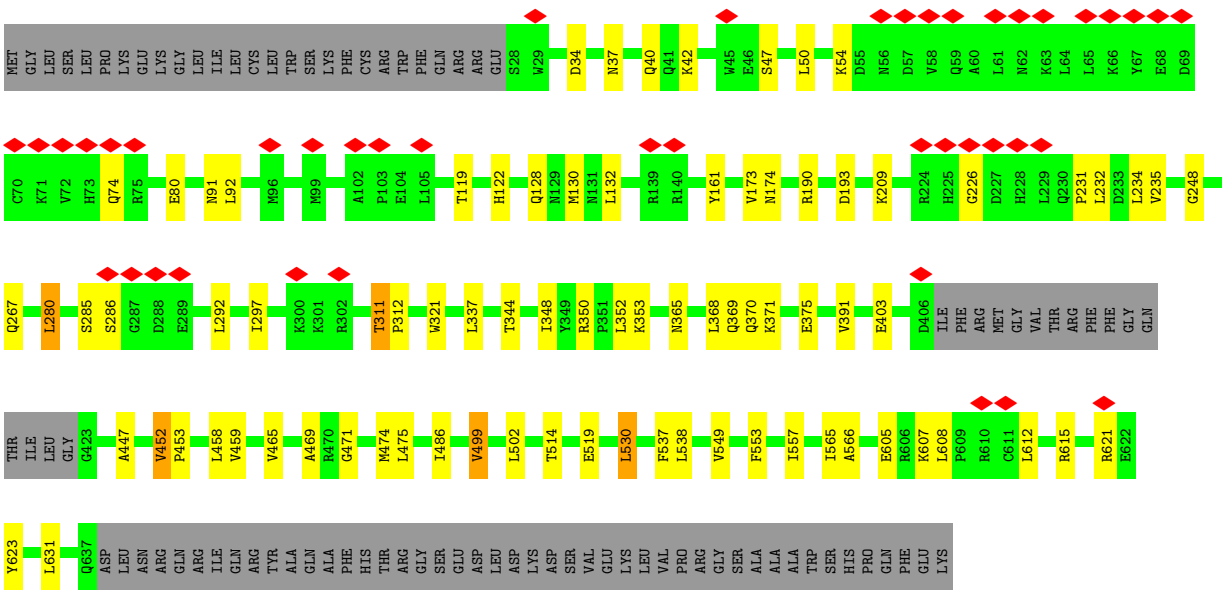
• Molecule 1: Transient receptor potential cation channel subfamily V member 6

Chain C:



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

Chain D:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	153950	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 ($e^-/Å^2$)	60	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	0.185	Depositor
Minimum map value	-0.108	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	212.224, 212.224, 212.224	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.829, 0.829, 0.829	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.46	0/4875	0.61	3/6616 (0.0%)
1	B	0.46	0/4875	0.61	3/6616 (0.0%)
1	C	0.46	0/4875	0.61	3/6616 (0.0%)
1	D	0.46	0/4875	0.61	3/6616 (0.0%)
All	All	0.46	0/19500	0.61	12/26464 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	530	LEU	CA-CB-CG	6.16	129.47	115.30
1	D	530	LEU	CA-CB-CG	6.15	129.44	115.30
1	C	530	LEU	CA-CB-CG	6.13	129.40	115.30
1	B	530	LEU	CA-CB-CG	6.13	129.39	115.30
1	C	337	LEU	CA-CB-CG	5.25	127.37	115.30
1	A	337	LEU	CA-CB-CG	5.24	127.35	115.30
1	B	337	LEU	CA-CB-CG	5.23	127.34	115.30
1	D	337	LEU	CA-CB-CG	5.23	127.33	115.30
1	D	280	LEU	CA-CB-CG	5.12	127.07	115.30
1	B	280	LEU	CA-CB-CG	5.11	127.06	115.30
1	A	280	LEU	CA-CB-CG	5.11	127.05	115.30
1	C	280	LEU	CA-CB-CG	5.10	127.03	115.30

There are no chirality outliers.

There are no planarity outliers.

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	4766	0	4818	50	0
1	B	4766	0	4818	53	0
1	C	4766	0	4818	53	0
1	D	4766	0	4818	52	0
2	A	105	0	147	11	0
2	B	105	0	147	12	0
2	C	105	0	147	13	0
2	D	105	0	147	9	0
3	A	220	0	350	13	0
3	B	200	0	316	11	0
3	C	200	0	316	7	0
3	D	180	0	282	7	0
4	A	13	0	20	0	0
4	B	13	0	20	0	0
4	C	13	0	20	0	0
4	D	13	0	20	0	0
5	A	1	0	0	0	0
6	A	22	0	0	0	0
6	B	22	0	0	0	0
6	C	22	0	0	0	0
6	D	22	0	0	0	0
All	All	20425	0	21204	226	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 5.

All (226) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:VAL:HG21	2:A:802:Y01:HAN1	1.73	0.70
1:C:459:VAL:HG21	2:C:704:Y01:HAN1	1.74	0.70
1:D:459:VAL:HG21	2:D:706:Y01:HAN1	1.74	0.70
1:B:459:VAL:HG21	2:B:704:Y01:HAN1	1.73	0.69
1:C:623:TYR:HA	1:D:42:LYS:HD2	1.83	0.60
1:A:190:ARG:HG2	1:A:232:LEU:HD13	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:ARG:HG2	1:B:232:LEU:HD13	1.84	0.60
1:D:190:ARG:HG2	1:D:232:LEU:HD13	1.84	0.60
1:B:623:TYR:HA	1:C:42:LYS:HD2	1.84	0.59
1:C:190:ARG:HG2	1:C:232:LEU:HD13	1.84	0.59
1:D:391:VAL:HG13	2:D:705:Y01:HAB3	1.85	0.58
1:A:623:TYR:HA	1:B:42:LYS:HD2	1.86	0.58
1:C:391:VAL:HG13	2:C:703:Y01:HAB3	1.85	0.57
1:B:391:VAL:HG13	2:B:703:Y01:HAB3	1.86	0.57
1:D:553:PHE:H	3:D:704:POV:H12A	1.70	0.57
1:C:553:PHE:H	3:C:702:POV:H12A	1.70	0.57
1:A:553:PHE:H	3:A:812:POV:H12A	1.70	0.57
1:B:553:PHE:H	3:B:702:POV:H12A	1.70	0.57
1:C:47:SER:OG	1:C:74:GLN:NE2	2.35	0.56
1:A:486:ILE:HD12	2:A:802:Y01:HAD3	1.87	0.56
1:A:391:VAL:HG13	2:A:801:Y01:HAB3	1.86	0.56
1:D:452:VAL:HG13	1:D:453:PRO:HD3	1.88	0.56
1:A:452:VAL:HG13	1:A:453:PRO:HD3	1.88	0.56
1:A:42:LYS:HD2	1:D:623:TYR:HA	1.87	0.56
1:B:452:VAL:HG13	1:B:453:PRO:HD3	1.88	0.55
1:C:403:GLU:OE2	1:C:607:LYS:NZ	2.40	0.55
1:C:459:VAL:CG2	2:C:704:Y01:HAN1	2.37	0.55
1:A:403:GLU:OE2	1:A:607:LYS:NZ	2.40	0.55
1:C:452:VAL:HG13	1:C:453:PRO:HD3	1.88	0.55
1:D:403:GLU:OE2	1:D:607:LYS:NZ	2.40	0.55
1:B:403:GLU:OE2	1:B:607:LYS:NZ	2.40	0.55
1:B:486:ILE:HD12	2:B:704:Y01:HAD3	1.88	0.54
1:C:486:ILE:HD12	2:C:704:Y01:HAD3	1.89	0.54
1:A:459:VAL:CG2	2:A:802:Y01:HAN1	2.37	0.54
1:D:459:VAL:CG2	2:D:706:Y01:HAN1	2.37	0.54
2:A:802:Y01:HAQ1	1:B:565:ILE:CD1	2.38	0.54
1:D:486:ILE:HD12	2:D:706:Y01:HAD3	1.89	0.54
1:B:47:SER:OG	1:B:74:GLN:NE2	2.35	0.53
1:C:403:GLU:OE2	2:C:703:Y01:HAV2	2.09	0.53
1:B:459:VAL:CG2	2:B:704:Y01:HAN1	2.37	0.53
1:D:403:GLU:OE2	2:D:705:Y01:HAV2	2.09	0.53
2:B:704:Y01:HAQ1	1:C:565:ILE:CD1	2.39	0.53
1:C:54:LYS:O	1:C:91:ASN:ND2	2.39	0.53
1:C:280:LEU:HD22	1:C:631:LEU:HB2	1.91	0.52
1:A:565:ILE:CD1	2:D:706:Y01:HAQ1	2.40	0.52
1:D:280:LEU:HD22	1:D:631:LEU:HB2	1.91	0.52
1:B:403:GLU:OE2	2:B:703:Y01:HAV2	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:LEU:HD22	1:B:631:LEU:HB2	1.91	0.52
1:C:267:GLN:NE2	1:D:37:ASN:O	2.43	0.51
2:C:704:Y01:HAQ1	1:D:565:ILE:CD1	2.40	0.51
1:A:403:GLU:OE2	2:A:801:Y01:HAV2	2.09	0.51
1:A:280:LEU:HD22	1:A:631:LEU:HB2	1.91	0.51
1:C:161:TYR:OH	1:C:193:ASP:OD2	2.22	0.51
1:A:47:SER:OG	1:A:74:GLN:NE2	2.35	0.51
1:D:47:SER:OG	1:D:74:GLN:NE2	2.35	0.51
1:B:190:ARG:NH2	1:B:226:GLY:O	2.45	0.50
1:C:190:ARG:NH2	1:C:226:GLY:O	2.44	0.50
1:B:267:GLN:NE2	1:C:37:ASN:O	2.44	0.50
1:A:371:LYS:HB3	1:A:375:GLU:HG3	1.93	0.50
1:C:370:GLN:NE2	1:C:447:ALA:O	2.45	0.50
1:A:190:ARG:NH2	1:A:226:GLY:O	2.45	0.50
1:D:371:LYS:HB3	1:D:375:GLU:HG3	1.93	0.49
1:D:190:ARG:NH2	1:D:226:GLY:O	2.45	0.49
1:B:161:TYR:OH	1:B:193:ASP:OD2	2.22	0.49
1:B:371:LYS:HB3	1:B:375:GLU:HG3	1.93	0.49
1:D:370:GLN:NE2	1:D:447:ALA:O	2.45	0.49
1:C:232:LEU:HA	1:C:235:VAL:HG23	1.95	0.49
1:C:371:LYS:HB3	1:C:375:GLU:HG3	1.93	0.49
1:A:353:LYS:HE3	1:A:369:GLN:HE21	1.77	0.49
1:A:370:GLN:NE2	1:A:447:ALA:O	2.45	0.49
1:D:469:ALA:HB1	1:D:475:LEU:HB3	1.95	0.49
1:A:403:GLU:OE2	2:A:801:Y01:HAI	2.12	0.49
1:C:469:ALA:HB1	1:C:475:LEU:HB3	1.95	0.49
1:A:161:TYR:OH	1:A:193:ASP:OD2	2.22	0.48
1:B:370:GLN:NE2	1:B:447:ALA:O	2.45	0.48
3:B:702:POV:H21E	3:B:702:POV:H212	1.55	0.48
1:A:565:ILE:HD12	2:D:706:Y01:HAQ1	1.95	0.48
1:B:54:LYS:O	1:B:91:ASN:ND2	2.39	0.48
1:C:403:GLU:OE2	2:C:703:Y01:HAI	2.14	0.48
1:C:286:SER:HA	1:C:615:ARG:HH12	1.78	0.48
1:D:403:GLU:OE2	2:D:705:Y01:HAI	2.13	0.48
1:A:54:LYS:O	1:A:91:ASN:ND2	2.39	0.48
1:B:232:LEU:HA	1:B:235:VAL:HG23	1.95	0.48
1:A:248:GLY:HA3	1:A:292:LEU:HD11	1.96	0.48
1:B:286:SER:HA	1:B:615:ARG:HH12	1.78	0.48
1:D:232:LEU:HA	1:D:235:VAL:HG23	1.95	0.48
1:B:403:GLU:OE2	2:B:703:Y01:HAI	2.13	0.48
1:C:557:ILE:HG23	3:C:702:POV:H21C	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:353:LYS:HE3	1:D:369:GLN:HE21	1.77	0.48
1:D:248:GLY:HA3	1:D:292:LEU:HD11	1.96	0.48
1:B:353:LYS:HE3	1:B:369:GLN:HE21	1.77	0.48
2:B:704:Y01:HAQ1	1:C:565:ILE:HD12	1.96	0.48
2:A:802:Y01:HAQ1	1:B:565:ILE:HD12	1.95	0.48
1:C:353:LYS:HE3	1:C:369:GLN:HE21	1.78	0.48
3:A:812:POV:H35	3:A:812:POV:H32	1.69	0.47
1:D:286:SER:HA	1:D:615:ARG:HH12	1.78	0.47
1:A:232:LEU:HA	1:A:235:VAL:HG23	1.95	0.47
1:A:286:SER:HA	1:A:615:ARG:HH12	1.78	0.47
1:D:54:LYS:O	1:D:91:ASN:ND2	2.39	0.47
1:A:267:GLN:NE2	1:B:37:ASN:O	2.47	0.47
2:C:704:Y01:HAQ1	1:D:565:ILE:HD12	1.97	0.47
1:A:469:ALA:HB1	1:A:475:LEU:HB3	1.95	0.47
1:B:469:ALA:HB1	1:B:475:LEU:HB3	1.95	0.47
3:A:807:POV:H29	3:A:807:POV:H212	1.79	0.47
1:D:47:SER:HB2	1:D:50:LEU:HB2	1.97	0.47
3:C:702:POV:H32	3:C:702:POV:H35	1.70	0.47
2:C:703:Y01:HAA1	2:C:703:Y01:HAJ2	1.77	0.47
3:D:704:POV:H35	3:D:704:POV:H32	1.71	0.47
1:B:248:GLY:HA3	1:B:292:LEU:HD11	1.96	0.46
3:B:702:POV:H35	3:B:702:POV:H32	1.70	0.46
1:C:47:SER:HB2	1:C:50:LEU:HB2	1.97	0.46
1:A:47:SER:HB2	1:A:50:LEU:HB2	1.97	0.46
1:C:231:PRO:HD2	1:C:234:LEU:HB2	1.97	0.46
1:A:368:LEU:HB2	1:B:514:THR:HA	1.96	0.46
1:A:514:THR:HA	1:D:368:LEU:HB2	1.97	0.46
3:A:804:POV:H215	3:A:804:POV:H212	1.78	0.46
1:C:248:GLY:HA3	1:C:292:LEU:HD11	1.96	0.46
1:D:231:PRO:HD2	1:D:234:LEU:HB2	1.97	0.46
1:A:119:THR:H	1:A:122:HIS:HD2	1.64	0.46
1:B:231:PRO:HD2	1:B:234:LEU:HB2	1.97	0.46
3:B:706:POV:H36A	3:B:706:POV:H33A	1.66	0.46
1:C:368:LEU:HB2	1:D:514:THR:HA	1.98	0.46
1:B:368:LEU:HB2	1:C:514:THR:HA	1.97	0.46
1:C:119:THR:H	1:C:122:HIS:HD2	1.64	0.46
2:C:704:Y01:HAC3	2:C:704:Y01:HAJ1	1.79	0.46
1:B:119:THR:H	1:B:122:HIS:HD2	1.64	0.46
1:C:40:GLN:NE2	1:C:80:GLU:OE1	2.49	0.46
1:D:119:THR:H	1:D:122:HIS:HD2	1.64	0.46
1:B:557:ILE:HG23	3:B:702:POV:H21C	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:GLN:NE2	1:A:80:GLU:OE1	2.49	0.45
1:A:231:PRO:HD2	1:A:234:LEU:HB2	1.97	0.45
1:A:519:GLU:HG2	1:A:549:VAL:HG11	1.98	0.45
1:B:47:SER:HB2	1:B:50:LEU:HB2	1.97	0.45
3:C:706:POV:H36A	3:C:706:POV:H33A	1.66	0.45
1:D:519:GLU:HG2	1:D:549:VAL:HG11	1.98	0.45
3:D:704:POV:H21E	3:D:704:POV:H212	1.55	0.45
1:A:37:ASN:O	1:D:267:GLN:NE2	2.50	0.45
1:C:311:THR:HG23	1:C:312:PRO:HD3	1.99	0.45
1:D:40:GLN:NE2	1:D:80:GLU:OE1	2.49	0.45
3:D:704:POV:H213	3:D:704:POV:H31A	1.98	0.45
2:A:802:Y01:HAC3	2:A:802:Y01:HAJ1	1.78	0.45
3:A:804:POV:H33A	3:A:804:POV:H36A	1.66	0.45
1:B:632:ARG:NE	1:C:34:ASP:OD1	2.46	0.45
1:D:311:THR:HG23	1:D:312:PRO:HD3	1.99	0.45
1:B:40:GLN:NE2	1:B:80:GLU:OE1	2.49	0.45
1:C:519:GLU:HG2	1:C:549:VAL:HG11	1.98	0.44
3:A:812:POV:H13B	3:A:812:POV:H11	1.83	0.44
3:A:809:POV:H213	3:A:809:POV:H210	1.67	0.44
1:B:311:THR:HG23	1:B:312:PRO:HD3	1.99	0.44
1:A:557:ILE:HG23	3:A:812:POV:H21C	1.98	0.44
2:A:801:Y01:HAA1	2:A:801:Y01:HAJ2	1.77	0.44
1:B:519:GLU:HG2	1:B:549:VAL:HG11	1.98	0.44
1:D:161:TYR:OH	1:D:193:ASP:OD2	2.22	0.44
1:D:537:PHE:CD1	1:D:566:ALA:HB1	2.53	0.44
3:C:702:POV:H21E	3:C:702:POV:H212	1.55	0.44
3:A:805:POV:H210	3:A:805:POV:H213	1.67	0.44
2:B:704:Y01:HAC3	2:B:704:Y01:HAJ1	1.79	0.44
1:A:311:THR:HG23	1:A:312:PRO:HD3	1.99	0.44
1:A:350:ARG:HG3	1:A:352:LEU:HD13	2.00	0.44
1:B:537:PHE:CD1	1:B:566:ALA:HB1	2.53	0.44
3:C:702:POV:H31A	3:C:702:POV:H213	2.00	0.44
3:B:702:POV:H31A	3:B:702:POV:H213	2.00	0.43
1:D:502:LEU:HD23	1:D:530:LEU:HD11	2.00	0.43
1:D:557:ILE:HG23	3:D:704:POV:H21C	1.99	0.43
1:B:92:LEU:HD12	1:B:132:LEU:HD23	2.00	0.43
2:B:703:Y01:HAJ2	2:B:703:Y01:HAA1	1.77	0.43
1:C:502:LEU:HD23	1:C:530:LEU:HD11	2.00	0.43
3:D:708:POV:H31G	3:D:708:POV:H31D	1.89	0.43
1:A:537:PHE:CD1	1:A:566:ALA:HB1	2.53	0.43
3:A:812:POV:H31A	3:A:812:POV:H213	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:LEU:HD23	1:A:530:LEU:HD11	2.00	0.43
1:C:537:PHE:CD1	1:C:566:ALA:HB1	2.53	0.43
3:B:702:POV:H13B	3:B:702:POV:H11	1.83	0.43
1:C:350:ARG:HG3	1:C:352:LEU:HD13	2.00	0.43
1:D:92:LEU:HD12	1:D:132:LEU:HD23	2.00	0.43
3:D:708:POV:H215	3:D:708:POV:H212	1.77	0.43
1:B:465:VAL:HB	1:C:499:VAL:HG21	2.01	0.43
3:A:803:POV:H35	3:A:803:POV:H32	1.82	0.43
3:A:804:POV:H31G	3:A:804:POV:H31D	1.87	0.43
1:B:350:ARG:HG3	1:B:352:LEU:HD13	2.00	0.43
1:D:608:LEU:HD22	1:D:612:LEU:HD12	2.01	0.43
1:A:608:LEU:HD22	1:A:612:LEU:HD12	2.01	0.42
1:B:608:LEU:HD22	1:B:612:LEU:HD12	2.01	0.42
1:C:92:LEU:HD12	1:C:132:LEU:HD23	2.01	0.42
1:B:502:LEU:HD23	1:B:530:LEU:HD11	2.00	0.42
1:D:350:ARG:HG3	1:D:352:LEU:HD13	2.00	0.42
1:C:285:SER:OG	1:C:605:GLU:OE2	2.37	0.42
1:C:465:VAL:HB	1:D:499:VAL:HG21	2.01	0.42
1:D:344:THR:O	1:D:348:ILE:HG12	2.20	0.42
1:D:553:PHE:HD1	2:D:703:Y01:OAF	2.02	0.42
1:A:92:LEU:HD12	1:A:132:LEU:HD23	2.00	0.42
1:C:344:THR:O	1:C:348:ILE:HG12	2.20	0.42
3:B:706:POV:H215	3:B:706:POV:H212	1.78	0.42
3:B:708:POV:H29	3:B:708:POV:H212	1.79	0.42
1:A:285:SER:OG	1:A:605:GLU:OE2	2.37	0.42
1:A:344:THR:O	1:A:348:ILE:HG12	2.20	0.41
1:C:537:PHE:HD2	1:C:538:LEU:HD12	1.85	0.41
1:B:344:THR:O	1:B:348:ILE:HG12	2.20	0.41
1:C:377:TYR:OH	1:C:389:GLU:OE1	2.31	0.41
2:C:701:Y01:HAE2	2:C:701:Y01:HBB	1.94	0.41
1:D:537:PHE:HD2	1:D:538:LEU:HD12	1.85	0.41
3:A:812:POV:H212	3:A:812:POV:H21E	1.55	0.41
1:C:553:PHE:HD1	2:C:701:Y01:OAF	2.02	0.41
1:C:608:LEU:HD22	1:C:612:LEU:HD12	2.01	0.41
3:C:708:POV:H29	3:C:708:POV:H212	1.78	0.41
1:D:285:SER:OG	1:D:605:GLU:OE2	2.37	0.41
1:D:321:TRP:HZ2	1:D:471:GLY:HA2	1.86	0.41
1:A:465:VAL:HB	1:B:499:VAL:HG21	2.03	0.41
1:B:321:TRP:HZ2	1:B:471:GLY:HA2	1.86	0.41
1:B:553:PHE:HD1	2:B:701:Y01:OAF	2.02	0.41
1:C:632:ARG:NE	1:D:34:ASP:OD1	2.46	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:706:POV:H31G	3:B:706:POV:H31D	1.88	0.41
1:A:537:PHE:HD2	1:A:538:LEU:HD12	1.85	0.41
1:A:553:PHE:HD1	2:A:811:Y01:OAF	2.03	0.41
1:C:321:TRP:HZ2	1:C:471:GLY:HA2	1.86	0.41
1:D:128:GLN:NE2	1:D:173:VAL:O	2.54	0.41
1:A:497:MET:SD	2:B:701:Y01:HAB3	2.61	0.40
1:B:128:GLN:NE2	1:B:173:VAL:O	2.54	0.40
3:B:711:POV:H35A	3:B:711:POV:H32A	1.86	0.40
1:B:497:MET:SD	2:C:701:Y01:HAB3	2.61	0.40
1:A:321:TRP:HZ2	1:A:471:GLY:HA2	1.86	0.40
1:B:557:ILE:HD13	1:B:557:ILE:HG21	1.90	0.40
1:A:499:VAL:HG21	1:D:465:VAL:HB	2.04	0.40
1:B:474:MET:HB3	1:C:492:ARG:HD2	2.04	0.40
1:B:537:PHE:HD2	1:B:538:LEU:HD12	1.85	0.40
1:D:297:ILE:HD13	1:D:297:ILE:HA	1.96	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	590/683 (86%)	575 (98%)	15 (2%)	0	100	100
1	B	590/683 (86%)	575 (98%)	15 (2%)	0	100	100
1	C	590/683 (86%)	575 (98%)	15 (2%)	0	100	100
1	D	590/683 (86%)	575 (98%)	15 (2%)	0	100	100
All	All	2360/2732 (86%)	2300 (98%)	60 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	516/593 (87%)	506 (98%)	10 (2%)	57 72
1	B	516/593 (87%)	506 (98%)	10 (2%)	57 72
1	C	516/593 (87%)	506 (98%)	10 (2%)	57 72
1	D	516/593 (87%)	506 (98%)	10 (2%)	57 72
All	All	2064/2372 (87%)	2024 (98%)	40 (2%)	59 72

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	130	MET
1	A	174	ASN
1	A	209	LYS
1	A	311	THR
1	A	365	ASN
1	A	452	VAL
1	A	458	LEU
1	A	474	MET
1	A	499	VAL
1	A	621	ARG
1	B	130	MET
1	B	174	ASN
1	B	209	LYS
1	B	311	THR
1	B	365	ASN
1	B	452	VAL
1	B	458	LEU
1	B	474	MET
1	B	499	VAL
1	B	621	ARG
1	C	130	MET
1	C	174	ASN
1	C	209	LYS
1	C	311	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	365	ASN
1	C	452	VAL
1	C	458	LEU
1	C	474	MET
1	C	499	VAL
1	C	621	ARG
1	D	130	MET
1	D	174	ASN
1	D	209	LYS
1	D	311	THR
1	D	365	ASN
1	D	452	VAL
1	D	458	LEU
1	D	474	MET
1	D	499	VAL
1	D	621	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	174	ASN
1	A	217	ASN
1	A	365	ASN
1	A	369	GLN
1	B	174	ASN
1	B	217	ASN
1	B	267	GLN
1	B	365	ASN
1	B	369	GLN
1	C	174	ASN
1	C	217	ASN
1	C	267	GLN
1	C	365	ASN
1	C	369	GLN
1	D	174	ASN
1	D	217	ASN
1	D	267	GLN
1	D	365	ASN
1	D	369	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 45 ligands modelled in this entry, 1 is monoatomic - leaving 44 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	$\#\|Z\| > 2$
2	Y01	D	706	-	38,38,38	0.46	0	57,57,57	0.49	0
3	POV	B	706	-	51,51,51	1.05	3 (5%)	57,59,59	0.97	3 (5%)
3	POV	D	710	-	17,17,51	1.45	2 (11%)	17,17,59	0.87	0
3	POV	A	810	-	29,29,51	0.85	1 (3%)	28,28,59	0.71	1 (3%)
3	POV	D	702	-	29,29,51	0.85	1 (3%)	28,28,59	0.71	1 (3%)
3	POV	B	711	-	29,29,51	0.85	1 (3%)	28,28,59	0.71	1 (3%)
2	Y01	B	703	-	38,38,38	0.45	0	57,57,57	0.47	0
3	POV	B	710	-	18,18,51	0.68	0	16,16,59	0.45	0
3	POV	D	708	-	51,51,51	1.04	3 (5%)	57,59,59	0.97	3 (5%)
3	POV	C	708	-	17,17,51	1.45	2 (11%)	17,17,59	0.88	0
2	Y01	B	704	-	38,38,38	0.46	0	57,57,57	0.50	0
3	POV	B	702	-	51,51,51	1.08	3 (5%)	57,59,59	0.92	3 (5%)
3	POV	B	705	-	12,12,51	0.62	0	11,11,59	0.30	0
4	PCW	D	701	-	12,12,53	0.75	0	11,11,61	0.58	0
3	POV	A	807	-	17,17,51	1.45	2 (11%)	17,17,59	0.88	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	POV	A	803	-	12,12,51	0.62	0	11,11,59	0.30	0
3	POV	A	809	-	18,18,51	0.68	0	16,16,59	0.45	0
2	Y01	D	703	-	38,38,38	0.44	0	57,57,57	0.51	0
3	POV	A	805	-	18,18,51	0.68	0	16,16,59	0.45	0
3	POV	D	707	-	12,12,51	0.61	0	11,11,59	0.28	0
4	PCW	C	709	-	12,12,53	0.75	0	11,11,61	0.61	0
2	Y01	C	704	-	38,38,38	0.46	0	57,57,57	0.49	0
3	POV	C	711	-	29,29,51	0.85	1 (3%)	28,28,59	0.72	1 (3%)
4	PCW	B	709	-	12,12,53	0.75	0	11,11,61	0.60	0
3	POV	C	702	-	51,51,51	1.08	3 (5%)	57,59,59	0.92	3 (5%)
3	POV	A	812	-	51,51,51	1.08	3 (5%)	57,59,59	0.92	3 (5%)
2	Y01	A	802	-	38,38,38	0.46	0	57,57,57	0.49	0
3	POV	D	704	-	51,51,51	1.08	3 (5%)	57,59,59	0.92	3 (5%)
2	Y01	A	811	-	38,38,38	0.44	0	57,57,57	0.50	0
2	Y01	C	701	-	38,38,38	0.44	0	57,57,57	0.51	0
2	Y01	A	801	-	38,38,38	0.45	0	57,57,57	0.47	0
2	Y01	C	703	-	38,38,38	0.45	0	57,57,57	0.47	0
3	POV	C	707	-	13,13,51	0.71	0	12,12,59	0.39	0
3	POV	B	707	-	13,13,51	0.71	0	12,12,59	0.39	0
2	Y01	D	705	-	38,38,38	0.44	0	57,57,57	0.46	0
4	PCW	A	808	-	12,12,53	0.75	0	11,11,61	0.60	0
2	Y01	B	701	-	38,38,38	0.44	0	57,57,57	0.51	0
3	POV	B	708	-	17,17,51	1.45	2 (11%)	17,17,59	0.87	0
3	POV	C	710	-	18,18,51	0.68	0	16,16,59	0.45	0
3	POV	A	804	-	51,51,51	1.04	3 (5%)	57,59,59	0.97	3 (5%)
3	POV	D	709	-	13,13,51	0.71	0	12,12,59	0.39	0
3	POV	C	706	-	51,51,51	1.05	3 (5%)	57,59,59	0.97	3 (5%)
3	POV	A	806	-	13,13,51	0.71	0	12,12,59	0.39	0
3	POV	C	705	-	12,12,51	0.62	0	11,11,59	0.29	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
2	Y01	D	706	-	-	9/19/77/77	0/4/4/4
3	POV	B	706	-	-	36/55/55/55	-
3	POV	D	710	-	-	7/15/15/55	-
3	POV	A	810	-	-	17/26/26/55	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	POV	D	702	-	-	17/26/26/55	-
3	POV	B	711	-	-	17/26/26/55	-
2	Y01	B	703	-	-	11/19/77/77	0/4/4/4
3	POV	B	710	-	-	14/14/14/55	-
3	POV	D	708	-	-	36/55/55/55	-
3	POV	C	708	-	-	7/15/15/55	-
2	Y01	B	704	-	-	9/19/77/77	0/4/4/4
3	POV	B	702	-	-	26/55/55/55	-
3	POV	B	705	-	-	7/10/10/55	-
4	PCW	D	701	-	-	6/10/10/57	-
3	POV	A	807	-	-	7/15/15/55	-
3	POV	A	803	-	-	6/10/10/55	-
3	POV	A	809	-	-	14/14/14/55	-
2	Y01	D	703	-	-	15/19/77/77	0/4/4/4
3	POV	A	805	-	-	14/14/14/55	-
3	POV	D	707	-	-	8/10/10/55	-
4	PCW	C	709	-	-	6/10/10/57	-
2	Y01	C	704	-	-	9/19/77/77	0/4/4/4
3	POV	C	711	-	-	17/26/26/55	-
4	PCW	B	709	-	-	6/10/10/57	-
3	POV	C	702	-	-	26/55/55/55	-
3	POV	A	812	-	-	26/55/55/55	-
2	Y01	A	802	-	-	9/19/77/77	0/4/4/4
3	POV	D	704	-	-	26/55/55/55	-
2	Y01	A	811	-	-	15/19/77/77	0/4/4/4
2	Y01	C	701	-	-	15/19/77/77	0/4/4/4
2	Y01	A	801	-	-	11/19/77/77	0/4/4/4
2	Y01	C	703	-	-	11/19/77/77	0/4/4/4
3	POV	C	707	-	-	5/11/11/55	-
3	POV	B	707	-	-	5/11/11/55	-
2	Y01	D	705	-	-	11/19/77/77	0/4/4/4
4	PCW	A	808	-	-	6/10/10/57	-
2	Y01	B	701	-	-	15/19/77/77	0/4/4/4
3	POV	B	708	-	-	7/15/15/55	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	POV	C	710	-	-	14/14/14/55	-
3	POV	A	804	-	-	36/55/55/55	-
3	POV	D	709	-	-	5/11/11/55	-
3	POV	C	706	-	-	36/55/55/55	-
3	POV	A	806	-	-	5/11/11/55	-
3	POV	C	705	-	-	7/10/10/55	-

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	710	POV	C29-C210	4.09	1.55	1.31
3	C	708	POV	C29-C210	4.08	1.55	1.31
3	A	807	POV	C29-C210	4.08	1.55	1.31
3	B	708	POV	C29-C210	4.07	1.55	1.31
3	A	807	POV	O21-C21	3.10	1.41	1.30
3	B	708	POV	O21-C21	3.09	1.41	1.30
3	C	708	POV	O21-C21	3.08	1.41	1.30
3	D	710	POV	O21-C21	3.08	1.41	1.30
3	D	704	POV	O21-C21	2.91	1.42	1.34
3	C	702	POV	O21-C21	2.91	1.42	1.34
3	B	702	POV	O21-C21	2.90	1.42	1.34
3	A	812	POV	O21-C21	2.90	1.42	1.34
3	C	706	POV	O21-C21	2.76	1.42	1.34
3	A	804	POV	O21-C21	2.75	1.42	1.34
3	D	708	POV	O21-C21	2.74	1.42	1.34
3	A	812	POV	O31-C31	2.74	1.41	1.33
3	B	706	POV	O21-C21	2.72	1.42	1.34
3	B	702	POV	O31-C31	2.71	1.41	1.33
3	C	702	POV	O31-C31	2.70	1.41	1.33
3	D	704	POV	O31-C31	2.70	1.41	1.33
3	B	706	POV	O31-C31	2.56	1.40	1.33
3	C	706	POV	O31-C31	2.55	1.40	1.33
3	A	804	POV	O31-C31	2.54	1.40	1.33
3	D	708	POV	O31-C31	2.53	1.40	1.33
3	C	706	POV	O21-C2	-2.51	1.40	1.46
3	B	706	POV	O21-C2	-2.50	1.40	1.46
3	D	708	POV	O21-C2	-2.49	1.40	1.46
3	A	804	POV	O21-C2	-2.49	1.40	1.46
3	A	810	POV	O31-C31	2.40	1.40	1.33
3	C	711	POV	O31-C31	2.37	1.40	1.33
3	D	702	POV	O31-C31	2.37	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	711	POV	O31-C31	2.36	1.40	1.33
3	D	704	POV	O21-C2	-2.25	1.41	1.46
3	B	702	POV	O21-C2	-2.24	1.41	1.46
3	C	702	POV	O21-C2	-2.23	1.41	1.46
3	A	812	POV	O21-C2	-2.20	1.41	1.46

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	704	POV	O21-C21-C22	4.17	120.49	111.50
3	C	702	POV	O21-C21-C22	4.15	120.45	111.50
3	A	812	POV	O21-C21-C22	4.14	120.43	111.50
3	B	702	POV	O21-C21-C22	4.14	120.42	111.50
3	A	804	POV	O21-C21-C22	3.94	119.98	111.50
3	C	706	POV	O21-C21-C22	3.92	119.95	111.50
3	B	706	POV	O21-C21-C22	3.91	119.93	111.50
3	D	708	POV	O21-C21-C22	3.89	119.89	111.50
3	D	708	POV	C14-N-C12	2.69	120.91	109.92
3	A	804	POV	C14-N-C12	2.68	120.88	109.92
3	B	706	POV	C14-N-C12	2.67	120.85	109.92
3	C	706	POV	C14-N-C12	2.67	120.85	109.92
3	A	804	POV	O31-C31-C32	2.59	120.04	111.91
3	D	708	POV	O31-C31-C32	2.58	120.01	111.91
3	B	706	POV	O31-C31-C32	2.58	119.99	111.91
3	C	706	POV	O31-C31-C32	2.57	119.98	111.91
3	B	702	POV	O31-C31-C32	2.40	119.43	111.91
3	C	702	POV	O31-C31-C32	2.39	119.40	111.91
3	D	704	POV	O31-C31-C32	2.37	119.35	111.91
3	A	812	POV	O31-C31-C32	2.37	119.34	111.91
3	A	812	POV	C14-N-C12	2.17	118.79	109.92
3	B	702	POV	C14-N-C12	2.17	118.79	109.92
3	C	702	POV	C14-N-C12	2.16	118.76	109.92
3	D	704	POV	C14-N-C12	2.13	118.65	109.92
3	C	711	POV	O31-C31-C32	2.07	118.40	111.91
3	D	702	POV	O31-C31-C32	2.06	118.36	111.91
3	B	711	POV	O31-C31-C32	2.05	118.35	111.91
3	A	810	POV	O31-C31-C32	2.04	118.33	111.91

There are no chirality outliers.

All (612) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	811	Y01	CAM-CAY-OAW-CBC
2	B	701	Y01	CAM-CAY-OAW-CBC
2	C	701	Y01	CAM-CAY-OAW-CBC
2	D	703	Y01	CAM-CAY-OAW-CBC
3	A	804	POV	C11-O12-P-O11
3	A	804	POV	C11-O12-P-O13
3	A	804	POV	O12-C11-C12-N
3	A	804	POV	O22-C21-O21-C2
3	A	812	POV	C1-O11-P-O12
3	A	812	POV	C1-O11-P-O13
3	A	812	POV	C1-O11-P-O14
3	A	812	POV	O12-C11-C12-N
3	B	702	POV	C1-O11-P-O12
3	B	702	POV	C1-O11-P-O13
3	B	702	POV	C1-O11-P-O14
3	B	702	POV	O12-C11-C12-N
3	B	706	POV	C11-O12-P-O13
3	B	706	POV	O12-C11-C12-N
3	B	706	POV	O22-C21-O21-C2
3	C	702	POV	C1-O11-P-O12
3	C	702	POV	C1-O11-P-O13
3	C	702	POV	C1-O11-P-O14
3	C	702	POV	O12-C11-C12-N
3	C	706	POV	C11-O12-P-O13
3	C	706	POV	O12-C11-C12-N
3	C	706	POV	O22-C21-O21-C2
3	D	704	POV	C1-O11-P-O12
3	D	704	POV	C1-O11-P-O13
3	D	704	POV	C1-O11-P-O14
3	D	704	POV	O12-C11-C12-N
3	D	708	POV	C11-O12-P-O13
3	D	708	POV	O12-C11-C12-N
3	D	708	POV	O22-C21-O21-C2
2	A	811	Y01	OAG-CAY-OAW-CBC
2	B	701	Y01	OAG-CAY-OAW-CBC
2	C	701	Y01	OAG-CAY-OAW-CBC
2	D	703	Y01	OAG-CAY-OAW-CBC
3	A	804	POV	C22-C21-O21-C2
3	B	706	POV	C22-C21-O21-C2
3	C	706	POV	C22-C21-O21-C2
3	D	708	POV	C22-C21-O21-C2
2	A	811	Y01	CAJ-CAO-CBB-CAC
2	B	701	Y01	CAJ-CAO-CBB-CAC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	701	Y01	CAJ-CAO-CBB-CAC
2	D	703	Y01	CAJ-CAO-CBB-CAC
2	A	811	Y01	CAC-CBB-CBE-CAP
2	B	701	Y01	CAC-CBB-CBE-CAP
2	C	701	Y01	CAC-CBB-CBE-CAP
2	D	703	Y01	CAC-CBB-CBE-CAP
2	A	811	Y01	CAO-CBB-CBE-CBI
2	B	701	Y01	CAO-CBB-CBE-CBI
2	C	701	Y01	CAO-CBB-CBE-CBI
2	D	703	Y01	CAO-CBB-CBE-CBI
3	C	706	POV	C33-C34-C35-C36
3	D	704	POV	C212-C213-C214-C215
2	A	811	Y01	CAC-CBB-CBE-CBI
2	B	701	Y01	CAC-CBB-CBE-CBI
2	C	701	Y01	CAC-CBB-CBE-CBI
2	D	703	Y01	CAC-CBB-CBE-CBI
3	A	812	POV	C212-C213-C214-C215
3	B	706	POV	C33-C34-C35-C36
3	A	804	POV	C33-C34-C35-C36
3	B	702	POV	C212-C213-C214-C215
3	C	702	POV	C212-C213-C214-C215
3	D	708	POV	C212-C213-C214-C215
3	A	804	POV	C212-C213-C214-C215
3	B	706	POV	C212-C213-C214-C215
3	D	708	POV	C33-C34-C35-C36
3	C	706	POV	C212-C213-C214-C215
2	B	704	Y01	CAJ-CAO-CBB-CAC
2	D	706	Y01	CAJ-CAO-CBB-CAC
3	A	812	POV	C32-C31-O31-C3
3	B	702	POV	C32-C31-O31-C3
3	C	702	POV	C32-C31-O31-C3
2	A	811	Y01	CAO-CBB-CBE-CAP
2	B	701	Y01	CAO-CBB-CBE-CAP
2	C	701	Y01	CAO-CBB-CBE-CAP
2	D	703	Y01	CAO-CBB-CBE-CAP
2	A	811	Y01	CAJ-CAO-CBB-CBE
2	B	701	Y01	CAJ-CAO-CBB-CBE
2	C	701	Y01	CAJ-CAO-CBB-CBE
2	D	703	Y01	CAJ-CAO-CBB-CBE
2	A	801	Y01	CAJ-CAO-CBB-CAC
2	A	802	Y01	CAJ-CAO-CBB-CAC
2	B	703	Y01	CAJ-CAO-CBB-CAC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	703	Y01	CAJ-CAO-CBB-CAC
2	C	704	Y01	CAJ-CAO-CBB-CAC
2	D	705	Y01	CAJ-CAO-CBB-CAC
3	A	812	POV	C11-C12-N-C13
3	B	702	POV	C11-C12-N-C13
3	C	702	POV	C11-C12-N-C13
3	D	704	POV	C11-C12-N-C13
3	D	708	POV	C11-C12-N-C14
3	D	704	POV	C32-C31-O31-C3
3	D	702	POV	C32-C33-C34-C35
3	B	711	POV	C32-C33-C34-C35
3	C	711	POV	C32-C33-C34-C35
3	A	810	POV	C32-C33-C34-C35
2	A	802	Y01	CAO-CAJ-CAN-CBA
2	B	704	Y01	CAO-CAJ-CAN-CBA
2	C	704	Y01	CAO-CAJ-CAN-CBA
2	D	706	Y01	CAO-CAJ-CAN-CBA
2	A	801	Y01	CAO-CAJ-CAN-CBA
2	B	701	Y01	CAN-CAJ-CAO-CBB
2	B	703	Y01	CAO-CAJ-CAN-CBA
2	C	703	Y01	CAO-CAJ-CAN-CBA
2	D	705	Y01	CAO-CAJ-CAN-CBA
2	A	811	Y01	CAN-CAJ-CAO-CBB
2	C	701	Y01	CAN-CAJ-CAO-CBB
2	D	703	Y01	CAN-CAJ-CAO-CBB
3	A	812	POV	C11-C12-N-C14
3	B	702	POV	C11-C12-N-C14
3	C	702	POV	C11-C12-N-C14
3	D	704	POV	C11-C12-N-C14
3	A	810	POV	C31-C32-C33-C34
3	D	704	POV	O32-C31-O31-C3
3	A	805	POV	C212-C213-C214-C215
3	A	812	POV	O32-C31-O31-C3
3	B	702	POV	O32-C31-O31-C3
3	C	702	POV	O32-C31-O31-C3
3	A	809	POV	C210-C211-C212-C213
3	C	710	POV	C210-C211-C212-C213
3	B	710	POV	C212-C213-C214-C215
3	C	710	POV	C212-C213-C214-C215
3	A	809	POV	C212-C213-C214-C215
3	B	706	POV	C11-O12-P-O11
3	C	706	POV	C11-O12-P-O11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	D	708	POV	C11-O12-P-O11
3	B	711	POV	C31-C32-C33-C34
3	C	711	POV	C31-C32-C33-C34
3	D	702	POV	C31-C32-C33-C34
3	A	804	POV	C11-C12-N-C13
3	A	804	POV	C11-C12-N-C14
3	A	804	POV	C11-C12-N-C15
3	B	706	POV	C11-C12-N-C13
3	B	706	POV	C11-C12-N-C14
3	C	706	POV	C11-C12-N-C13
3	C	706	POV	C11-C12-N-C14
3	D	708	POV	C11-C12-N-C13
3	D	708	POV	C11-C12-N-C15
3	A	805	POV	C210-C211-C212-C213
3	A	807	POV	C210-C211-C212-C213
3	B	708	POV	C210-C211-C212-C213
3	B	710	POV	C210-C211-C212-C213
2	A	811	Y01	CAX-CAL-CAM-CAY
3	B	711	POV	C34-C35-C36-C37
3	C	711	POV	C34-C35-C36-C37
3	D	702	POV	C34-C35-C36-C37
3	D	708	POV	C312-C313-C314-C315
3	A	810	POV	C32-C31-O31-C3
3	A	810	POV	C34-C35-C36-C37
3	B	702	POV	C24-C25-C26-C27
3	C	702	POV	C24-C25-C26-C27
3	C	710	POV	C211-C212-C213-C214
3	D	704	POV	C24-C25-C26-C27
3	A	812	POV	C21-C22-C23-C24
3	A	804	POV	C312-C313-C314-C315
3	A	805	POV	C211-C212-C213-C214
3	A	809	POV	C211-C212-C213-C214
3	A	812	POV	C24-C25-C26-C27
3	B	702	POV	C35-C36-C37-C38
3	B	706	POV	C312-C313-C314-C315
3	B	710	POV	C211-C212-C213-C214
3	C	706	POV	C312-C313-C314-C315
3	A	812	POV	C35-C36-C37-C38
3	A	804	POV	C25-C26-C27-C28
3	C	706	POV	C25-C26-C27-C28
3	D	708	POV	C25-C26-C27-C28
3	B	702	POV	C21-C22-C23-C24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	702	POV	C21-C22-C23-C24
3	D	704	POV	C21-C22-C23-C24
3	B	711	POV	C32-C31-O31-C3
3	C	711	POV	C32-C31-O31-C3
3	D	702	POV	C32-C31-O31-C3
3	B	706	POV	C25-C26-C27-C28
3	C	702	POV	C35-C36-C37-C38
3	D	704	POV	C35-C36-C37-C38
3	A	810	POV	C36-C37-C38-C39
3	B	711	POV	C36-C37-C38-C39
3	C	711	POV	C36-C37-C38-C39
3	D	702	POV	C36-C37-C38-C39
3	C	708	POV	C210-C211-C212-C213
3	A	804	POV	C35-C36-C37-C38
3	C	706	POV	C35-C36-C37-C38
3	D	708	POV	C35-C36-C37-C38
3	D	710	POV	C25-C26-C27-C28
2	A	802	Y01	CAX-CAL-CAM-CAY
2	B	701	Y01	CAX-CAL-CAM-CAY
2	B	704	Y01	CAX-CAL-CAM-CAY
2	C	704	Y01	CAX-CAL-CAM-CAY
2	D	706	Y01	CAX-CAL-CAM-CAY
3	A	812	POV	C11-C12-N-C15
3	B	706	POV	C11-C12-N-C15
3	C	706	POV	C11-C12-N-C15
3	D	704	POV	C11-C12-N-C15
2	A	811	Y01	CAJ-CAN-CBA-CAA
2	A	811	Y01	CAJ-CAN-CBA-CAB
2	B	701	Y01	CAJ-CAN-CBA-CAA
2	B	701	Y01	CAJ-CAN-CBA-CAB
2	C	701	Y01	CAJ-CAN-CBA-CAA
2	C	701	Y01	CAJ-CAN-CBA-CAB
2	D	703	Y01	CAJ-CAN-CBA-CAA
2	D	703	Y01	CAJ-CAN-CBA-CAB
3	B	706	POV	C35-C36-C37-C38
3	C	707	POV	C213-C214-C215-C216
3	C	708	POV	C25-C26-C27-C28
3	D	709	POV	C213-C214-C215-C216
3	A	805	POV	C214-C215-C216-C217
3	A	806	POV	C213-C214-C215-C216
3	B	707	POV	C213-C214-C215-C216
3	B	708	POV	C25-C26-C27-C28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	710	POV	C213-C214-C215-C216
3	A	804	POV	C21-C22-C23-C24
3	B	706	POV	C21-C22-C23-C24
3	C	706	POV	C21-C22-C23-C24
3	D	708	POV	C21-C22-C23-C24
3	A	805	POV	C213-C214-C215-C216
3	A	809	POV	C213-C214-C215-C216
3	A	809	POV	C214-C215-C216-C217
3	B	710	POV	C214-C215-C216-C217
3	B	711	POV	O21-C2-C3-O31
3	C	710	POV	C213-C214-C215-C216
3	C	710	POV	C214-C215-C216-C217
3	C	711	POV	O21-C2-C3-O31
3	D	702	POV	O21-C2-C3-O31
3	D	704	POV	C211-C212-C213-C214
3	A	807	POV	C25-C26-C27-C28
3	A	810	POV	O21-C2-C3-O31
3	A	812	POV	C211-C212-C213-C214
3	B	702	POV	C211-C212-C213-C214
3	C	702	POV	C211-C212-C213-C214
3	D	708	POV	C24-C25-C26-C27
3	A	804	POV	C24-C25-C26-C27
3	B	706	POV	C24-C25-C26-C27
3	C	706	POV	C24-C25-C26-C27
4	D	701	PCW	C23-C24-C25-C26
2	C	701	Y01	CAX-CAL-CAM-CAY
2	D	703	Y01	CAX-CAL-CAM-CAY
4	C	709	PCW	C23-C24-C25-C26
3	D	708	POV	C31-C32-C33-C34
4	A	808	PCW	C23-C24-C25-C26
3	A	810	POV	O32-C31-O31-C3
3	C	711	POV	O32-C31-O31-C3
3	D	702	POV	O32-C31-O31-C3
3	B	702	POV	C11-C12-N-C15
3	C	702	POV	C11-C12-N-C15
3	A	804	POV	C211-C212-C213-C214
3	B	706	POV	C211-C212-C213-C214
4	B	709	PCW	C23-C24-C25-C26
3	C	708	POV	C23-C24-C25-C26
3	D	710	POV	C23-C24-C25-C26
3	B	711	POV	O32-C31-O31-C3
3	A	804	POV	C31-C32-C33-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	706	POV	C31-C32-C33-C34
3	A	803	POV	C311-C310-C39-C38
3	B	705	POV	C311-C310-C39-C38
3	C	706	POV	C211-C212-C213-C214
3	D	708	POV	C313-C314-C315-C316
3	B	708	POV	C23-C24-C25-C26
2	B	703	Y01	CAO-CBB-CBE-CBI
2	C	703	Y01	CAO-CBB-CBE-CBI
2	D	705	Y01	CAO-CBB-CBE-CBI
3	D	710	POV	C210-C211-C212-C213
3	C	706	POV	C31-C32-C33-C34
3	A	807	POV	C23-C24-C25-C26
3	A	804	POV	C313-C314-C315-C316
3	B	706	POV	C313-C314-C315-C316
3	C	705	POV	C311-C310-C39-C38
3	D	704	POV	C31-C32-C33-C34
3	C	706	POV	C313-C314-C315-C316
4	D	701	PCW	C21-C22-C23-C24
3	B	706	POV	C36-C37-C38-C39
3	C	706	POV	C36-C37-C38-C39
2	A	801	Y01	CAO-CBB-CBE-CBI
3	A	804	POV	C36-C37-C38-C39
3	A	810	POV	C37-C38-C39-C310
3	D	707	POV	C311-C310-C39-C38
3	D	708	POV	C36-C37-C38-C39
3	B	711	POV	C37-C38-C39-C310
3	C	711	POV	C37-C38-C39-C310
3	D	702	POV	C37-C38-C39-C310
3	D	704	POV	C213-C214-C215-C216
4	A	808	PCW	C21-C22-C23-C24
4	B	709	PCW	C21-C22-C23-C24
3	A	812	POV	C31-C32-C33-C34
4	C	709	PCW	C21-C22-C23-C24
3	B	702	POV	C31-C32-C33-C34
3	C	702	POV	C31-C32-C33-C34
3	C	706	POV	C22-C23-C24-C25
2	A	811	Y01	CAR-CBC-OAW-CAY
3	A	804	POV	C22-C23-C24-C25
3	B	706	POV	C22-C23-C24-C25
3	D	708	POV	C22-C23-C24-C25
3	A	812	POV	C213-C214-C215-C216
3	B	702	POV	C213-C214-C215-C216

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	702	POV	C213-C214-C215-C216
3	A	804	POV	C1-O11-P-O12
3	B	706	POV	C1-O11-P-O12
3	C	706	POV	C1-O11-P-O12
3	D	708	POV	C1-O11-P-O12
3	B	711	POV	C311-C312-C313-C314
3	A	810	POV	C311-C312-C313-C314
3	C	711	POV	C311-C312-C313-C314
3	A	809	POV	C36-C37-C38-C39
3	B	710	POV	C36-C37-C38-C39
3	D	702	POV	C311-C312-C313-C314
3	A	805	POV	C36-C37-C38-C39
3	C	710	POV	C36-C37-C38-C39
3	D	708	POV	C211-C212-C213-C214
3	B	702	POV	C210-C211-C212-C213
4	C	709	PCW	C22-C23-C24-C25
4	D	701	PCW	C22-C23-C24-C25
4	B	709	PCW	C22-C23-C24-C25
3	B	702	POV	C215-C216-C217-C218
4	A	808	PCW	C22-C23-C24-C25
3	A	812	POV	C215-C216-C217-C218
3	C	702	POV	C215-C216-C217-C218
4	A	808	PCW	C24-C25-C26-C27
4	D	701	PCW	C24-C25-C26-C27
3	D	704	POV	C215-C216-C217-C218
4	A	808	PCW	C15-C16-C17-C18
4	B	709	PCW	C24-C25-C26-C27
4	C	709	PCW	C15-C16-C17-C18
4	C	709	PCW	C24-C25-C26-C27
3	A	805	POV	C39-C310-C311-C312
3	A	809	POV	C39-C310-C311-C312
3	B	708	POV	C212-C213-C214-C215
3	B	710	POV	C39-C310-C311-C312
3	C	708	POV	C212-C213-C214-C215
3	C	710	POV	C39-C310-C311-C312
3	D	709	POV	C25-C26-C27-C28
3	D	710	POV	C212-C213-C214-C215
3	A	806	POV	C25-C26-C27-C28
4	D	701	PCW	C15-C16-C17-C18
3	B	707	POV	C25-C26-C27-C28
3	C	707	POV	C25-C26-C27-C28
4	B	709	PCW	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	701	Y01	CAR-CBC-OAW-CAY
2	C	701	Y01	CAR-CBC-OAW-CAY
3	A	812	POV	C210-C211-C212-C213
3	C	702	POV	C210-C211-C212-C213
3	D	704	POV	C210-C211-C212-C213
2	C	701	Y01	CAO-CAJ-CAN-CBA
2	D	703	Y01	CAO-CAJ-CAN-CBA
3	D	707	POV	C34-C35-C36-C37
3	A	805	POV	C215-C216-C217-C218
3	A	805	POV	C34-C35-C36-C37
3	A	807	POV	C212-C213-C214-C215
3	A	809	POV	C34-C35-C36-C37
3	B	710	POV	C34-C35-C36-C37
2	B	701	Y01	CAO-CAJ-CAN-CBA
3	A	809	POV	C215-C216-C217-C218
3	C	710	POV	C34-C35-C36-C37
2	D	705	Y01	CAC-CBB-CBE-CAP
3	A	806	POV	C214-C215-C216-C217
2	A	801	Y01	CAC-CBB-CBE-CBI
2	D	703	Y01	CAR-CBC-OAW-CAY
3	B	710	POV	C215-C216-C217-C218
3	C	710	POV	C215-C216-C217-C218
3	D	709	POV	C214-C215-C216-C217
2	A	811	Y01	CAO-CAJ-CAN-CBA
3	A	810	POV	C213-C214-C215-C216
3	B	711	POV	C213-C214-C215-C216
3	D	702	POV	C213-C214-C215-C216
3	B	707	POV	C214-C215-C216-C217
3	C	711	POV	C213-C214-C215-C216
2	A	801	Y01	CAC-CBB-CBE-CAP
2	B	703	Y01	CAC-CBB-CBE-CAP
2	C	703	Y01	CAC-CBB-CBE-CAP
2	B	703	Y01	CAC-CBB-CBE-CBI
2	C	703	Y01	CAC-CBB-CBE-CBI
2	D	705	Y01	CAC-CBB-CBE-CBI
3	C	707	POV	C214-C215-C216-C217
2	A	802	Y01	CAN-CAJ-CAO-CBB
2	C	704	Y01	CAN-CAJ-CAO-CBB
2	D	706	Y01	CAN-CAJ-CAO-CBB
2	B	704	Y01	CAN-CAJ-CAO-CBB
3	A	803	POV	C34-C35-C36-C37
3	C	705	POV	C34-C35-C36-C37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	705	POV	C34-C35-C36-C37
3	C	705	POV	C310-C311-C312-C313
3	A	803	POV	C310-C311-C312-C313
3	B	705	POV	C310-C311-C312-C313
3	D	707	POV	C310-C311-C312-C313
2	A	801	Y01	CAO-CBB-CBE-CAP
2	B	703	Y01	CAO-CBB-CBE-CAP
2	C	703	Y01	CAO-CBB-CBE-CAP
2	D	705	Y01	CAO-CBB-CBE-CAP
3	A	805	POV	C37-C38-C39-C310
3	B	710	POV	C37-C38-C39-C310
3	A	809	POV	C37-C38-C39-C310
3	C	710	POV	C37-C38-C39-C310
3	C	702	POV	C25-C26-C27-C28
3	C	706	POV	C32-C33-C34-C35
3	D	704	POV	C25-C26-C27-C28
3	A	812	POV	C25-C26-C27-C28
3	B	705	POV	C39-C310-C311-C312
3	A	803	POV	C39-C310-C311-C312
3	A	804	POV	C32-C33-C34-C35
3	C	705	POV	C39-C310-C311-C312
3	B	706	POV	C32-C33-C34-C35
3	B	702	POV	C25-C26-C27-C28
3	C	708	POV	C24-C25-C26-C27
3	A	804	POV	O11-C1-C2-O21
3	B	706	POV	O11-C1-C2-O21
3	C	706	POV	O11-C1-C2-O21
3	D	708	POV	O11-C1-C2-O21
3	D	710	POV	C24-C25-C26-C27
3	D	707	POV	C39-C310-C311-C312
3	B	708	POV	C24-C25-C26-C27
3	A	807	POV	C29-C210-C211-C212
3	B	705	POV	C32-C33-C34-C35
3	D	708	POV	C32-C33-C34-C35
3	C	711	POV	C211-C212-C213-C214
3	C	706	POV	C311-C312-C313-C314
3	D	708	POV	C311-C312-C313-C314
3	A	803	POV	C32-C33-C34-C35
3	A	810	POV	C211-C212-C213-C214
3	B	706	POV	C311-C312-C313-C314
3	D	702	POV	C211-C212-C213-C214
3	B	711	POV	C211-C212-C213-C214

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	D	707	POV	C32-C33-C34-C35
3	A	804	POV	C311-C312-C313-C314
3	C	705	POV	C32-C33-C34-C35
3	A	807	POV	C24-C25-C26-C27
3	A	805	POV	C35-C36-C37-C38
3	A	809	POV	C35-C36-C37-C38
3	B	710	POV	C35-C36-C37-C38
3	C	710	POV	C35-C36-C37-C38
3	C	711	POV	C311-C310-C39-C38
3	A	810	POV	C310-C311-C312-C313
3	C	711	POV	C310-C311-C312-C313
3	D	702	POV	C311-C310-C39-C38
3	D	702	POV	C310-C311-C312-C313
3	B	711	POV	C311-C310-C39-C38
3	B	711	POV	C310-C311-C312-C313
3	A	810	POV	C311-C310-C39-C38
3	A	806	POV	C215-C216-C217-C218
3	B	707	POV	C215-C216-C217-C218
3	C	707	POV	C215-C216-C217-C218
3	B	708	POV	C29-C210-C211-C212
3	D	707	POV	C31-C32-C33-C34
2	A	811	Y01	CAV-CBC-OAW-CAY
3	C	705	POV	C31-C32-C33-C34
3	D	709	POV	C215-C216-C217-C218
3	B	705	POV	C31-C32-C33-C34
3	A	803	POV	C31-C32-C33-C34
3	C	702	POV	C1-C2-C3-O31
3	D	704	POV	C1-C2-C3-O31
3	C	711	POV	C212-C213-C214-C215
3	A	810	POV	C212-C213-C214-C215
3	D	702	POV	C212-C213-C214-C215
3	A	812	POV	C32-C33-C34-C35
3	B	711	POV	C212-C213-C214-C215
3	B	702	POV	C32-C33-C34-C35
3	C	702	POV	C32-C33-C34-C35
3	D	708	POV	C210-C211-C212-C213
3	D	708	POV	O32-C31-O31-C3
2	B	701	Y01	CAV-CBC-OAW-CAY
2	C	701	Y01	CAV-CBC-OAW-CAY
3	A	809	POV	C311-C310-C39-C38
3	B	710	POV	C311-C310-C39-C38
3	D	708	POV	C32-C31-O31-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	805	POV	C311-C310-C39-C38
3	C	710	POV	C311-C310-C39-C38
3	C	710	POV	C33-C34-C35-C36
3	A	805	POV	C33-C34-C35-C36
3	A	809	POV	C33-C34-C35-C36
3	B	710	POV	C33-C34-C35-C36
3	A	804	POV	C1-O11-P-O13
3	A	804	POV	C1-O11-P-O14
3	A	804	POV	C11-O12-P-O14
3	B	706	POV	C1-O11-P-O13
3	B	706	POV	C1-O11-P-O14
3	B	706	POV	C11-O12-P-O14
3	C	706	POV	C1-O11-P-O13
3	C	706	POV	C1-O11-P-O14
3	C	706	POV	C11-O12-P-O14
3	D	708	POV	C1-O11-P-O13
3	D	708	POV	C1-O11-P-O14
3	D	708	POV	C11-O12-P-O14
3	A	804	POV	C32-C31-O31-C3
3	C	708	POV	C29-C210-C211-C212
3	B	711	POV	C3-C2-O21-C21
3	C	711	POV	C3-C2-O21-C21
3	D	702	POV	C3-C2-O21-C21
3	A	804	POV	O32-C31-O31-C3
3	A	810	POV	C3-C2-O21-C21
3	A	804	POV	C210-C211-C212-C213
3	B	706	POV	C210-C211-C212-C213
3	C	706	POV	C210-C211-C212-C213
3	B	706	POV	C32-C31-O31-C3
3	C	706	POV	C32-C31-O31-C3
3	B	706	POV	O32-C31-O31-C3
2	D	703	Y01	CAV-CBC-OAW-CAY
3	D	708	POV	C34-C35-C36-C37
3	C	706	POV	O32-C31-O31-C3
3	D	704	POV	C32-C33-C34-C35
3	D	710	POV	C22-C23-C24-C25
3	A	804	POV	C34-C35-C36-C37
3	C	708	POV	C22-C23-C24-C25
3	B	706	POV	C34-C35-C36-C37
3	D	708	POV	C39-C310-C311-C312
3	A	812	POV	C1-C2-C3-O31
3	B	702	POV	C1-C2-C3-O31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	708	POV	C22-C23-C24-C25
3	A	804	POV	C39-C310-C311-C312
3	A	812	POV	C33-C34-C35-C36
3	B	702	POV	C33-C34-C35-C36
3	B	711	POV	C35-C36-C37-C38
3	C	706	POV	C34-C35-C36-C37
3	C	711	POV	C35-C36-C37-C38
3	D	702	POV	C35-C36-C37-C38
3	A	810	POV	C35-C36-C37-C38
3	A	807	POV	C22-C23-C24-C25
3	C	706	POV	C39-C310-C311-C312
3	D	710	POV	C29-C210-C211-C212
3	B	706	POV	C39-C310-C311-C312
3	D	702	POV	C312-C313-C314-C315
3	C	711	POV	C312-C313-C314-C315
3	A	810	POV	C312-C313-C314-C315
3	B	711	POV	C312-C313-C314-C315
3	D	704	POV	C33-C34-C35-C36
3	A	809	POV	C29-C210-C211-C212
3	C	710	POV	C29-C210-C211-C212
3	D	704	POV	C39-C310-C311-C312
3	C	702	POV	C33-C34-C35-C36
3	A	812	POV	C39-C310-C311-C312
3	B	702	POV	C39-C310-C311-C312
2	B	704	Y01	CAO-CBB-CBE-CAP
2	D	706	Y01	CAO-CBB-CBE-CAP
3	C	702	POV	C39-C310-C311-C312
3	A	805	POV	C29-C210-C211-C212
3	B	710	POV	C29-C210-C211-C212
2	C	704	Y01	CAO-CBB-CBE-CAP
3	B	702	POV	C27-C28-C29-C210
2	B	704	Y01	CAC-CBB-CBE-CBI
2	A	802	Y01	CAO-CBB-CBE-CAP
2	D	705	Y01	CAJ-CAN-CBA-CAA
3	B	706	POV	C23-C24-C25-C26
3	B	707	POV	C211-C212-C213-C214
3	D	709	POV	C211-C212-C213-C214
2	B	703	Y01	CAJ-CAN-CBA-CAA
2	C	703	Y01	CAJ-CAN-CBA-CAA
3	A	806	POV	C211-C212-C213-C214
3	C	706	POV	C23-C24-C25-C26
3	A	804	POV	O11-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	D	708	POV	O11-C1-C2-C3
3	A	804	POV	C23-C24-C25-C26
2	D	706	Y01	CAC-CBB-CBE-CBI
3	D	708	POV	C23-C24-C25-C26
3	C	707	POV	C211-C212-C213-C214
3	D	707	POV	C37-C38-C39-C310
2	A	802	Y01	CAC-CBB-CBE-CBI
3	A	812	POV	C27-C28-C29-C210
3	C	702	POV	C27-C28-C29-C210
3	D	704	POV	C27-C28-C29-C210
2	A	801	Y01	CAX-CAL-CAM-CAY
2	B	703	Y01	CAX-CAL-CAM-CAY
2	D	705	Y01	CAX-CAL-CAM-CAY
2	A	801	Y01	OAG-CAY-OAW-CBC
2	C	704	Y01	CAC-CBB-CBE-CBI
3	D	704	POV	C312-C313-C314-C315
4	A	808	PCW	C19-C20-C21-C22
4	C	709	PCW	C19-C20-C21-C22
2	C	703	Y01	CAX-CAL-CAM-CAY
4	B	709	PCW	C19-C20-C21-C22
4	D	701	PCW	C19-C20-C21-C22
2	B	703	Y01	OAG-CAY-OAW-CBC
2	C	703	Y01	OAG-CAY-OAW-CBC
3	D	704	POV	C22-C23-C24-C25
3	A	804	POV	O21-C21-C22-C23
3	C	706	POV	O21-C21-C22-C23
3	C	705	POV	C37-C38-C39-C310
3	B	706	POV	O11-C1-C2-C3
3	C	706	POV	O11-C1-C2-C3
3	B	706	POV	O21-C21-C22-C23
3	D	708	POV	O21-C21-C22-C23
2	A	801	Y01	CAJ-CAN-CBA-CAA
3	C	702	POV	C22-C23-C24-C25
3	B	702	POV	C312-C313-C314-C315
3	A	812	POV	C22-C23-C24-C25
2	D	705	Y01	OAG-CAY-OAW-CBC
2	A	802	Y01	CAM-CAL-CAX-OAF
3	C	702	POV	C312-C313-C314-C315
3	A	812	POV	C312-C313-C314-C315
3	B	702	POV	C22-C23-C24-C25
3	B	705	POV	C37-C38-C39-C310
3	D	707	POV	C35-C36-C37-C38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	804	POV	O22-C21-C22-C23
3	C	706	POV	O22-C21-C22-C23
3	B	706	POV	O22-C21-C22-C23
3	D	708	POV	O22-C21-C22-C23
2	B	704	Y01	CAO-CBB-CBE-CBI
2	A	802	Y01	CAL-CAM-CAY-OAW
2	D	706	Y01	CAO-CBB-CBE-CBI
2	A	801	Y01	CAL-CAM-CAY-OAW
2	B	703	Y01	CAL-CAM-CAY-OAW
2	C	703	Y01	CAL-CAM-CAY-OAW
2	D	705	Y01	CAL-CAM-CAY-OAW
2	D	706	Y01	CAL-CAM-CAY-OAW
2	A	802	Y01	CAM-CAL-CAX-OAH
2	B	704	Y01	CAL-CAM-CAY-OAW
2	A	801	Y01	CAL-CAM-CAY-OAG
2	C	704	Y01	CAL-CAM-CAY-OAW
2	B	703	Y01	CAL-CAM-CAY-OAG
2	C	703	Y01	CAL-CAM-CAY-OAG
2	B	704	Y01	CAM-CAL-CAX-OAF
2	C	704	Y01	CAM-CAL-CAX-OAF
2	C	704	Y01	CAO-CBB-CBE-CBI
2	D	705	Y01	CAL-CAM-CAY-OAG
2	D	706	Y01	CAM-CAL-CAX-OAF

There are no ring outliers.

27 monomers are involved in 83 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	706	Y01	5	0
3	B	706	POV	3	0
3	B	711	POV	1	0
2	B	703	Y01	4	0
3	D	708	POV	2	0
3	C	708	POV	1	0
2	B	704	Y01	6	0
3	B	702	POV	6	0
3	A	807	POV	1	0
3	A	803	POV	1	0
3	A	809	POV	1	0
2	D	703	Y01	1	0
3	A	805	POV	1	0
2	C	704	Y01	6	0

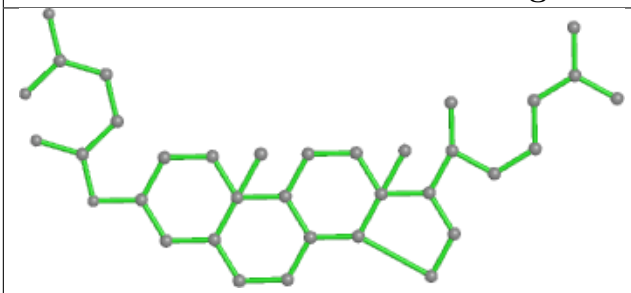
Continued on next page...

Continued from previous page...

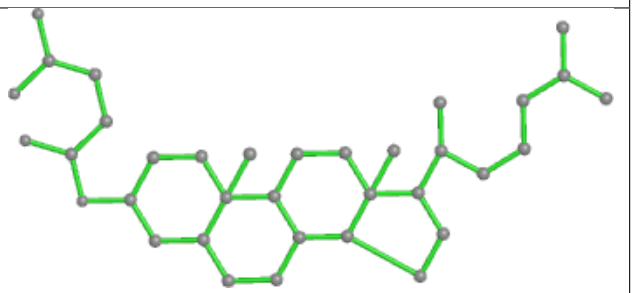
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	702	POV	5	0
3	A	812	POV	6	0
2	A	802	Y01	6	0
3	D	704	POV	5	0
2	A	811	Y01	1	0
2	C	701	Y01	3	0
2	A	801	Y01	4	0
2	C	703	Y01	4	0
2	D	705	Y01	3	0
2	B	701	Y01	2	0
3	B	708	POV	1	0
3	A	804	POV	3	0
3	C	706	POV	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

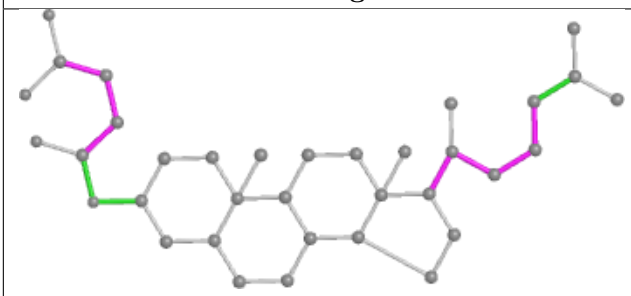
Ligand Y01 D 706



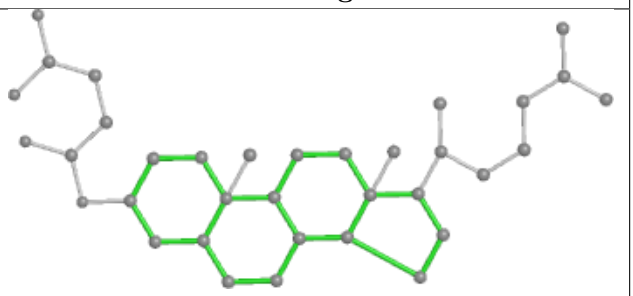
Bond lengths



Bond angles

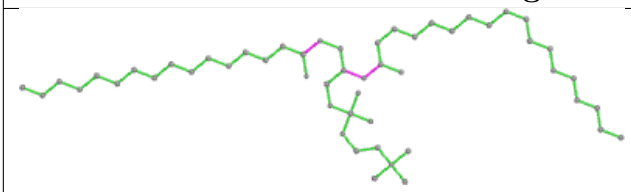


Torsions

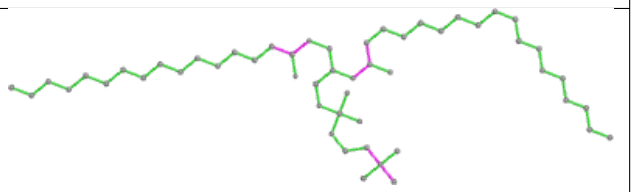


Rings

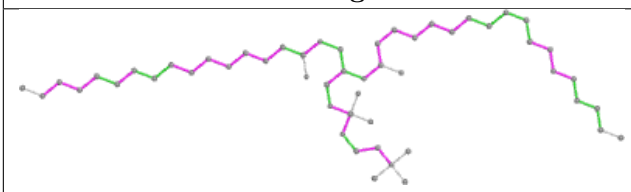
Ligand POV B 706



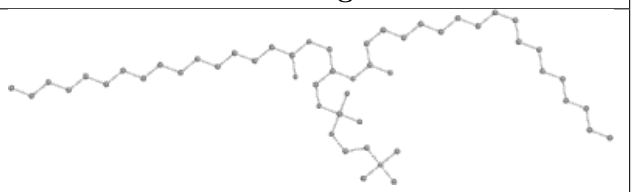
Bond lengths



Bond angles

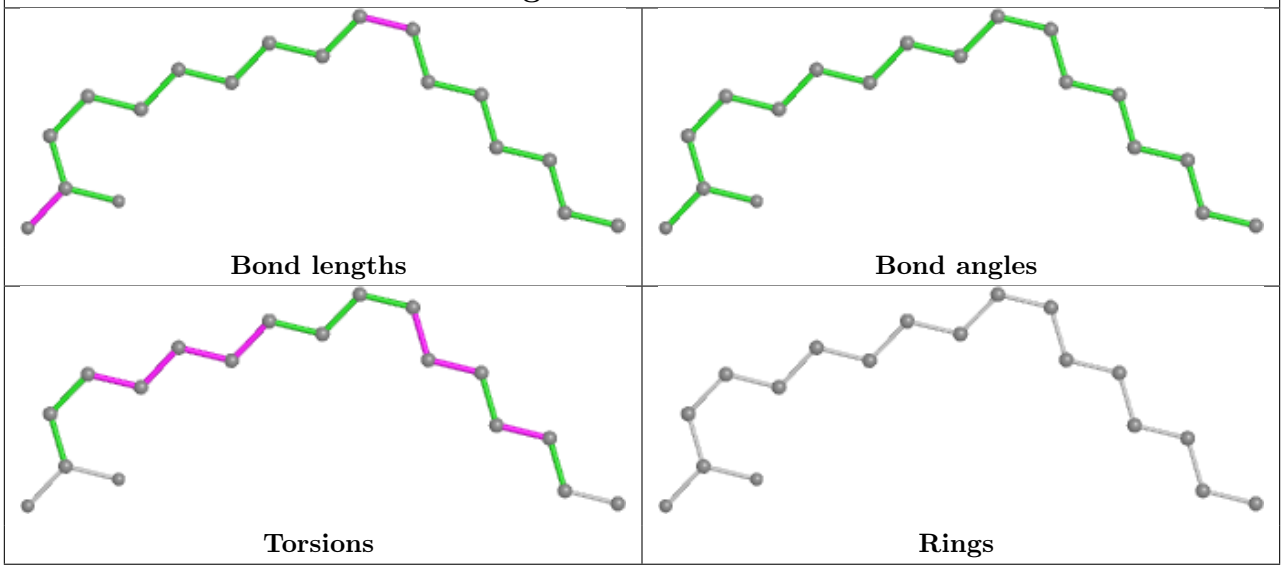


Torsions

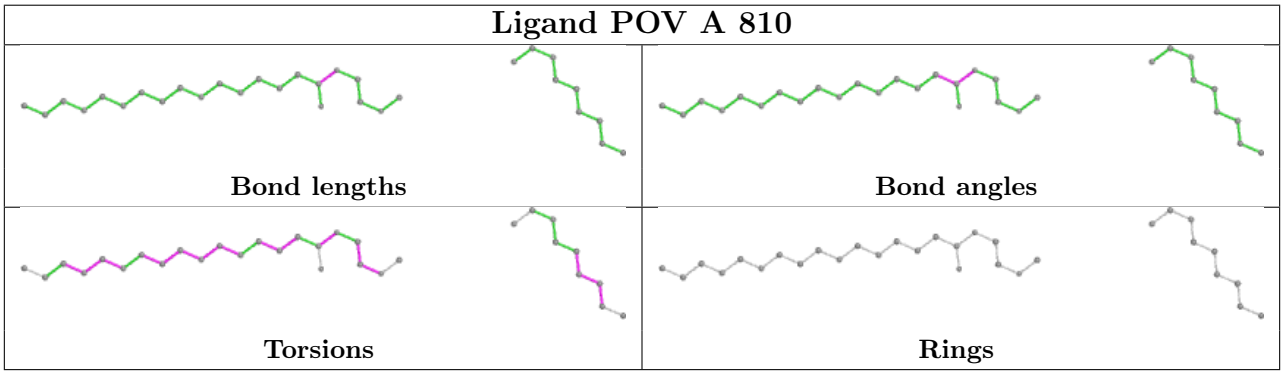


Rings

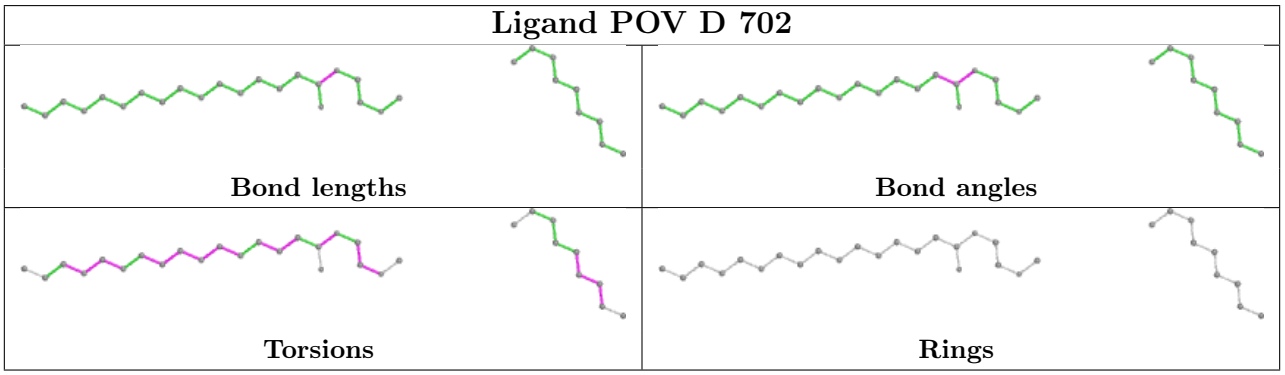
Ligand POV D 710



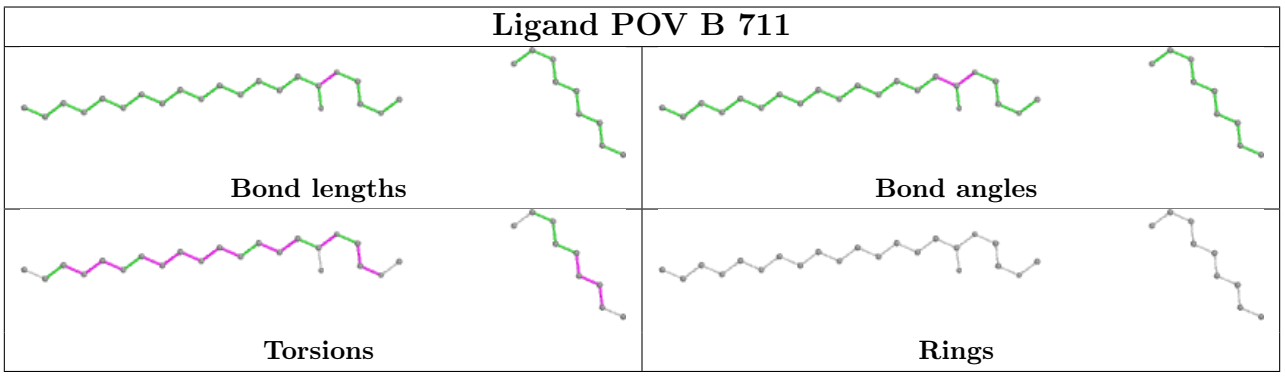
Ligand POV A 810



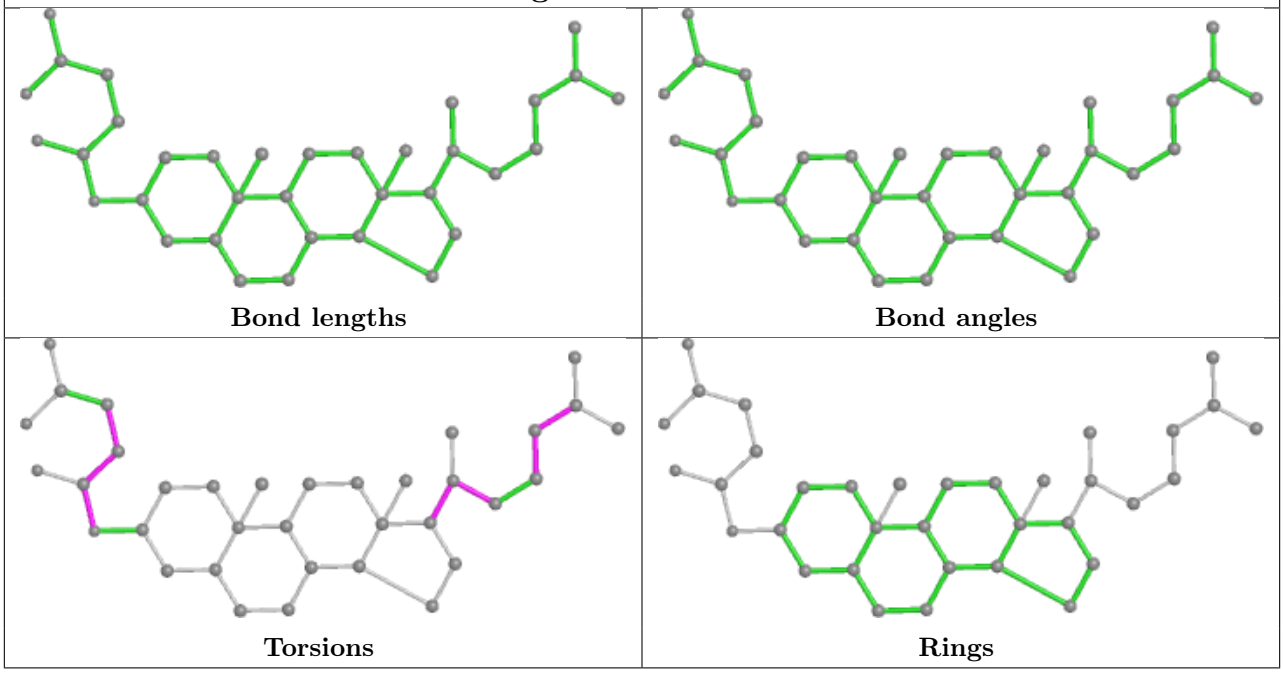
Ligand POV D 702



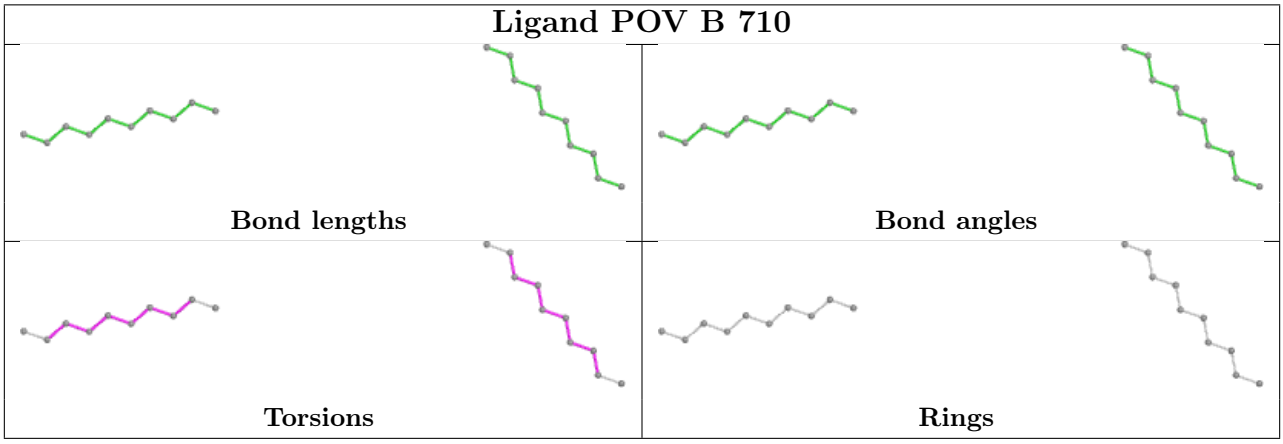
Ligand POV B 711



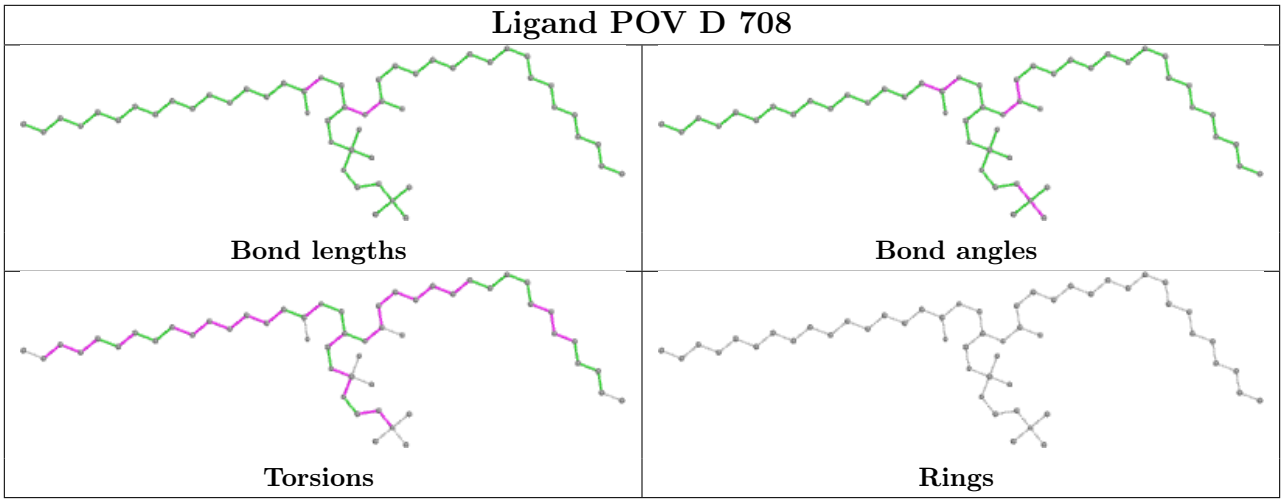
Ligand Y01 B 703



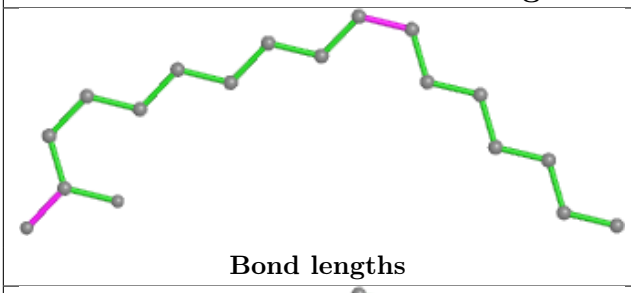
Ligand POV B 710



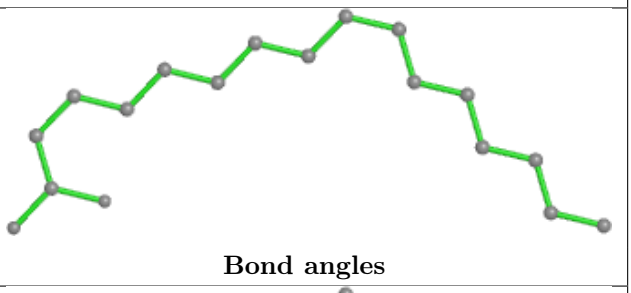
Ligand POV D 708



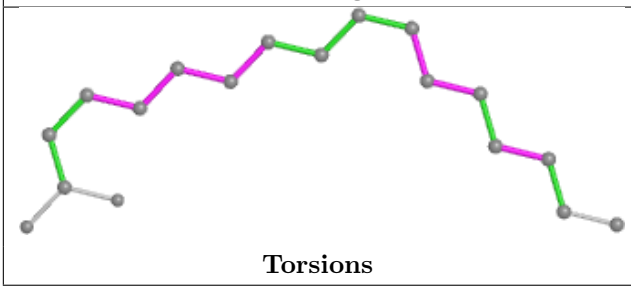
Ligand POV C 708



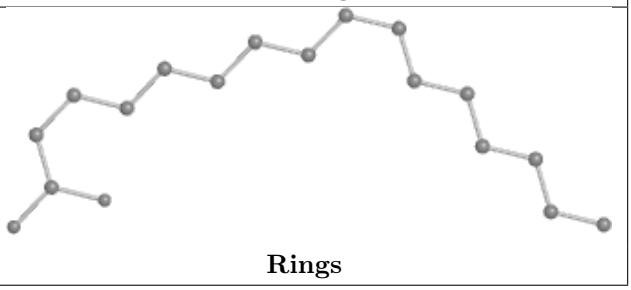
Bond lengths



Bond angles

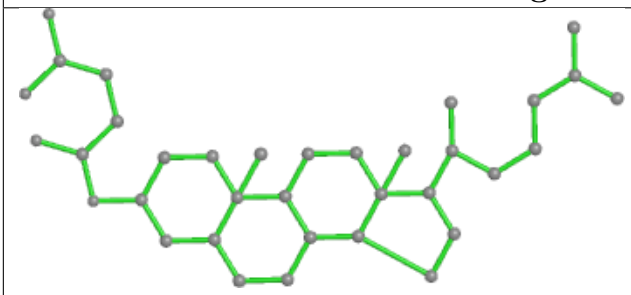


Torsions

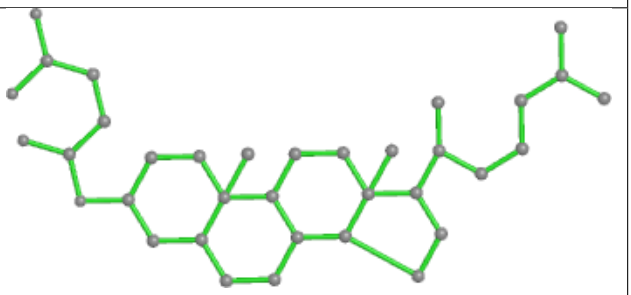


Rings

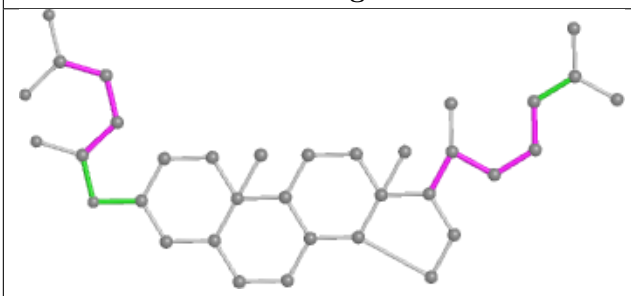
Ligand Y01 B 704



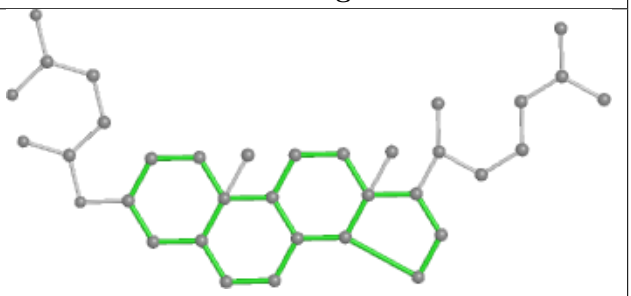
Bond lengths



Bond angles

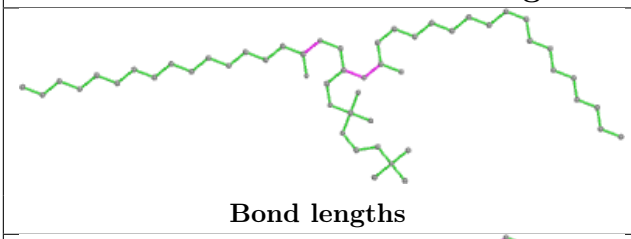


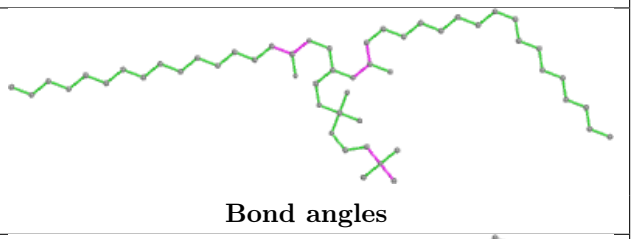
Torsions

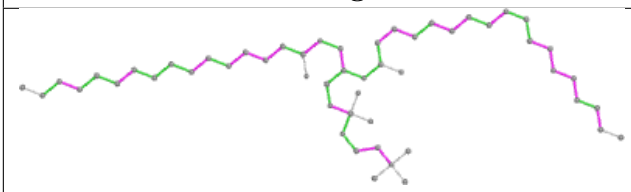


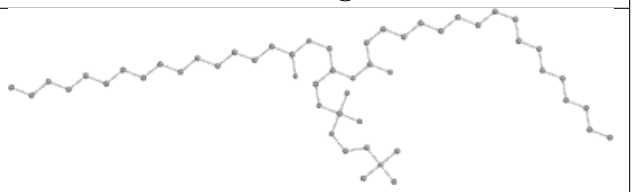
Rings

Ligand POV B 702


Bond lengths


Bond angles

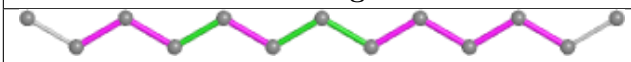

Torsions


Rings

Ligand POV B 705

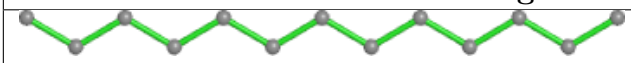

Bond lengths

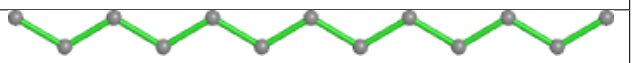

Bond angles

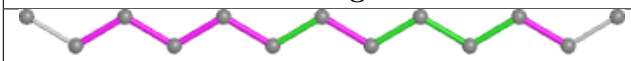

Torsions

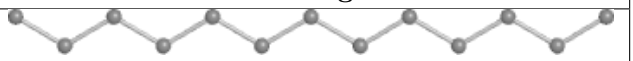

Rings

Ligand PCW D 701

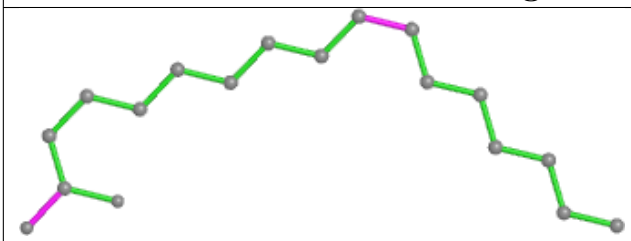

Bond lengths

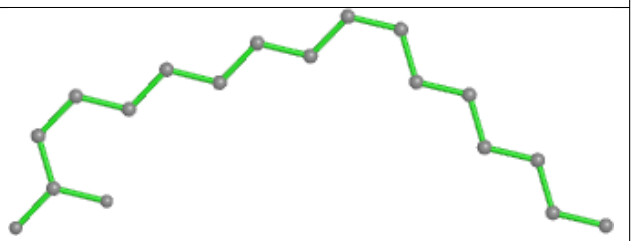

Bond angles

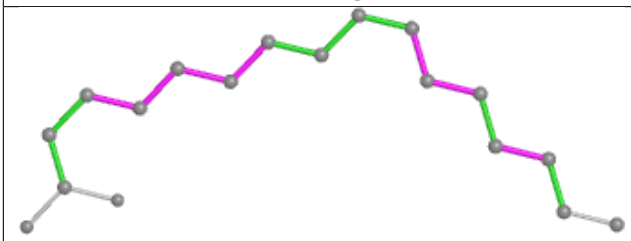

Torsions

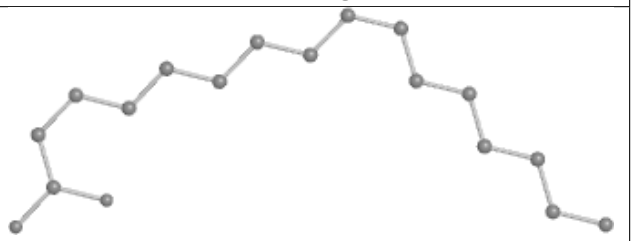

Rings

Ligand POV A 807

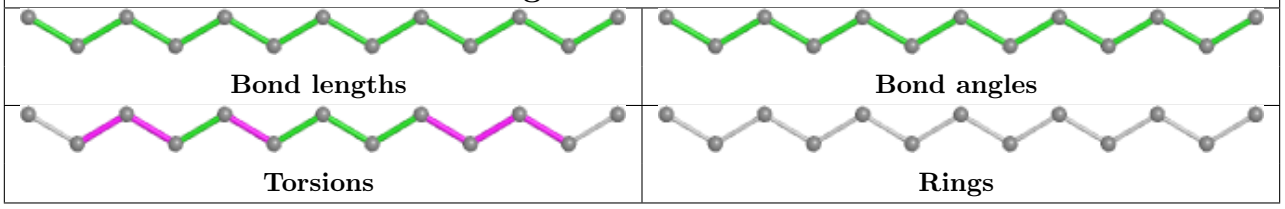

Bond lengths


Bond angles

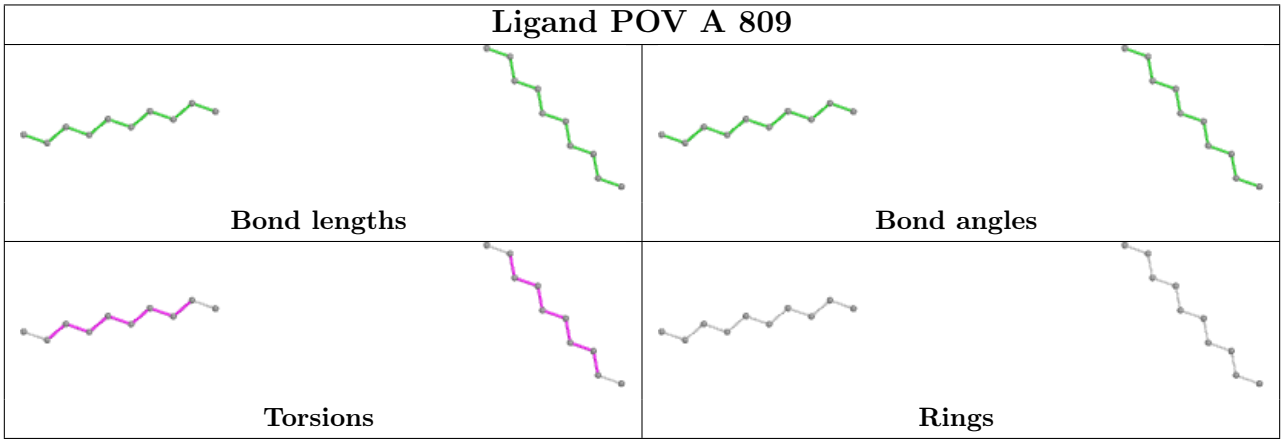

Torsions


Rings

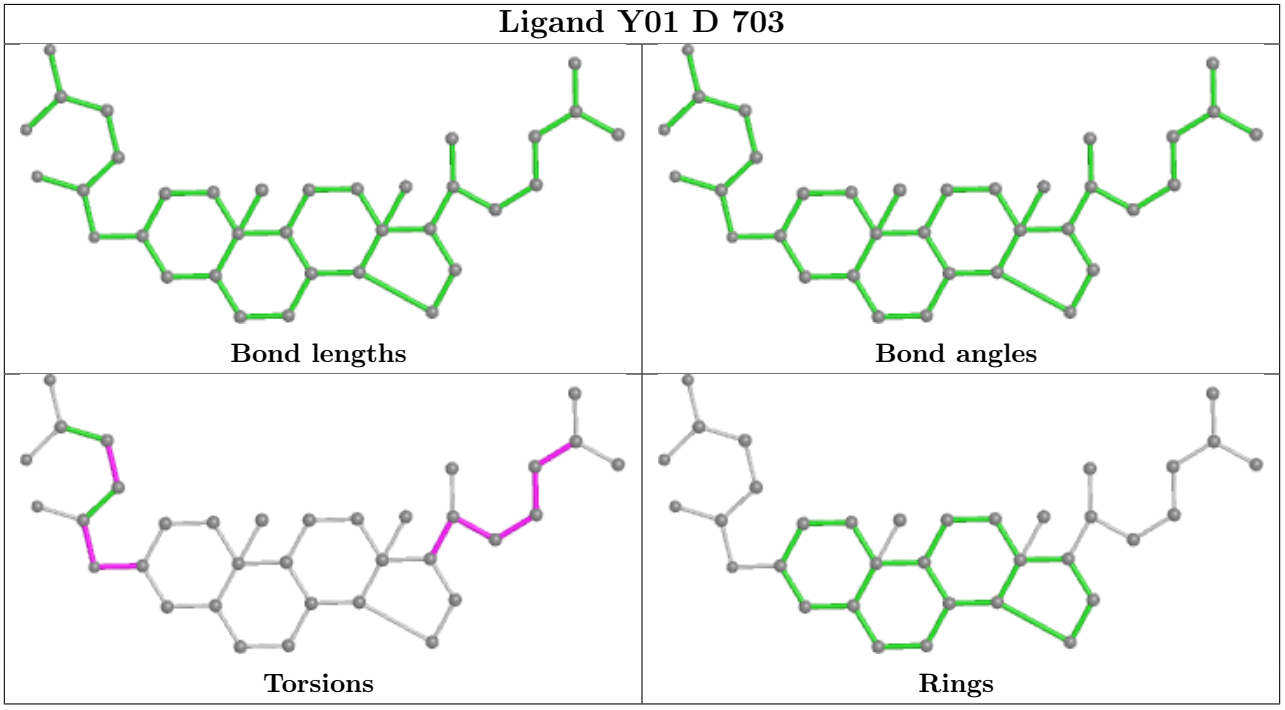
Ligand POV A 803



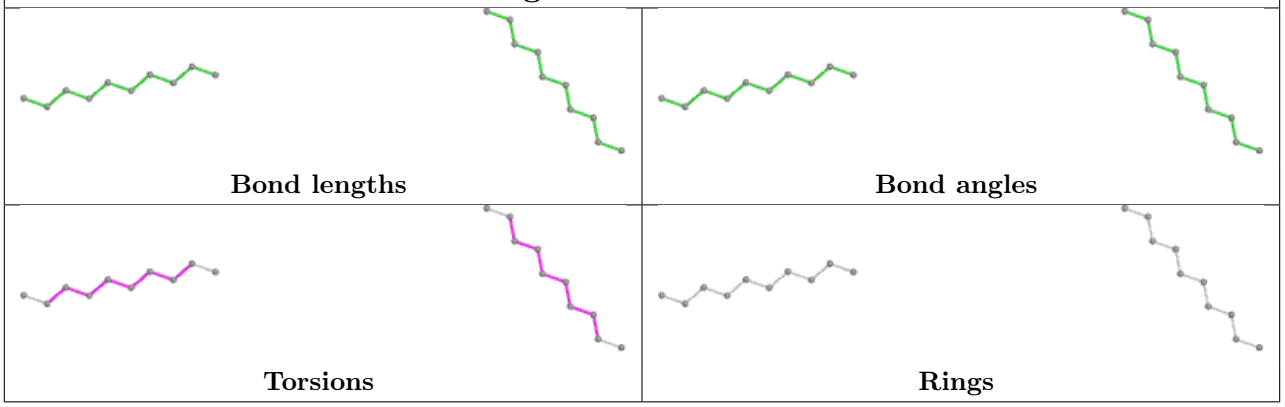
Ligand POV A 809



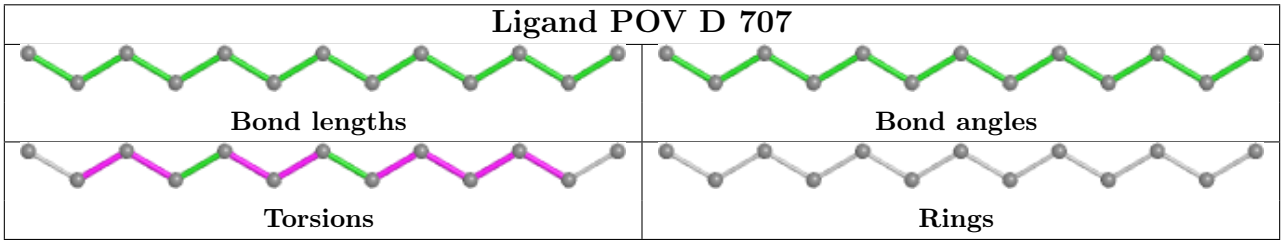
Ligand Y01 D 703



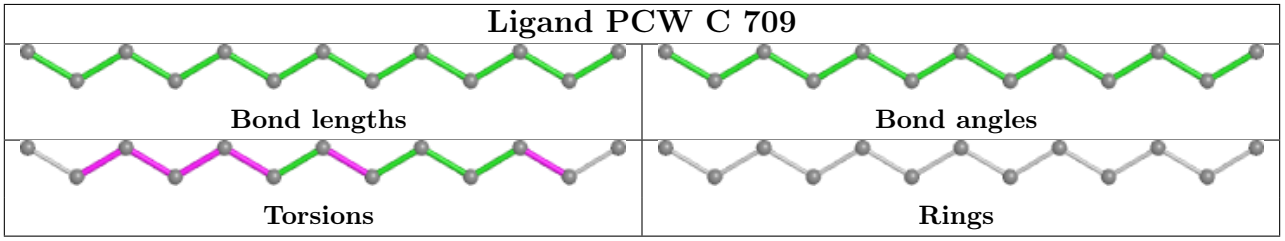
Ligand POV A 805



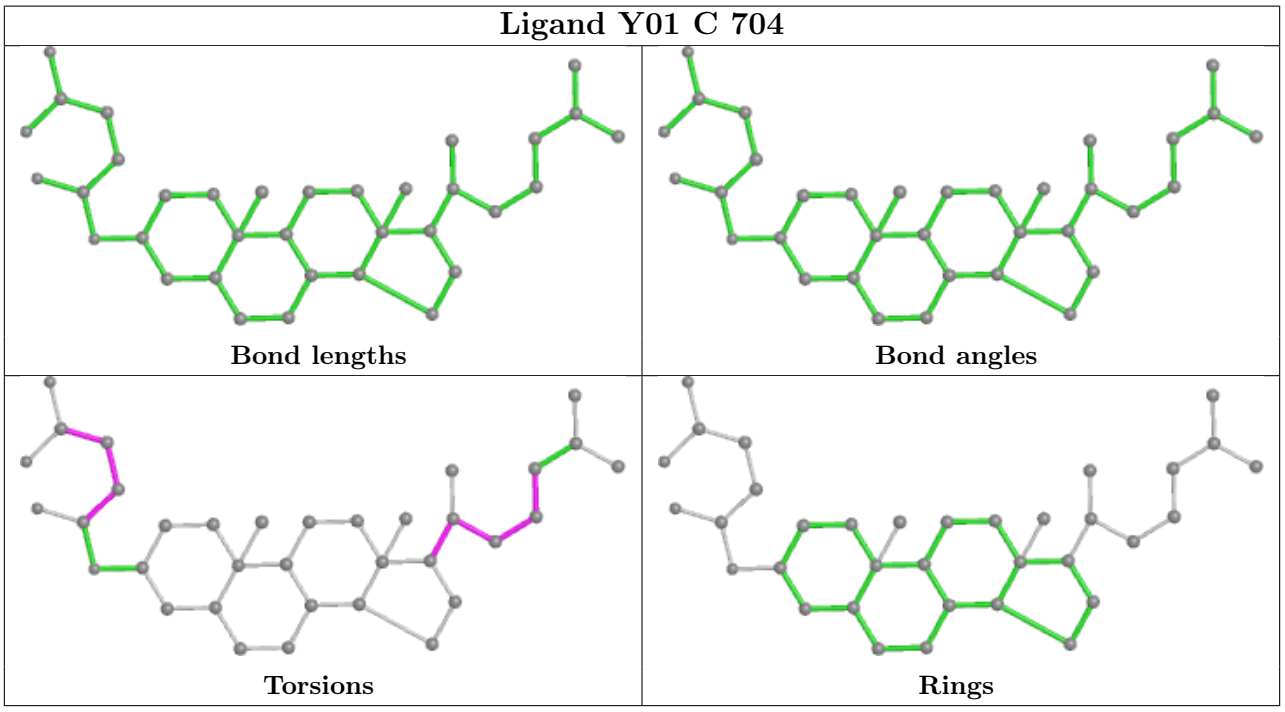
Ligand POV D 707

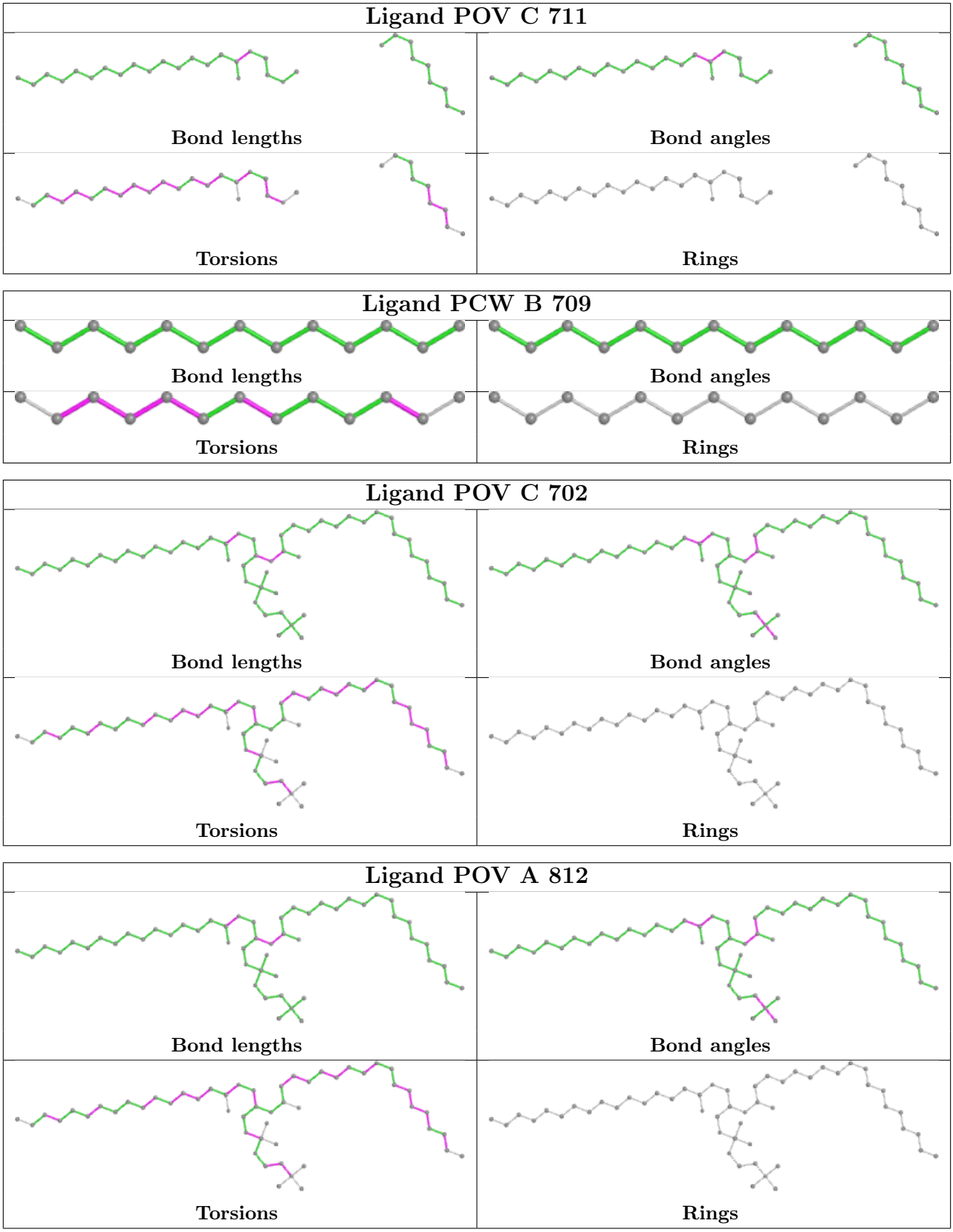


Ligand PCW C 709

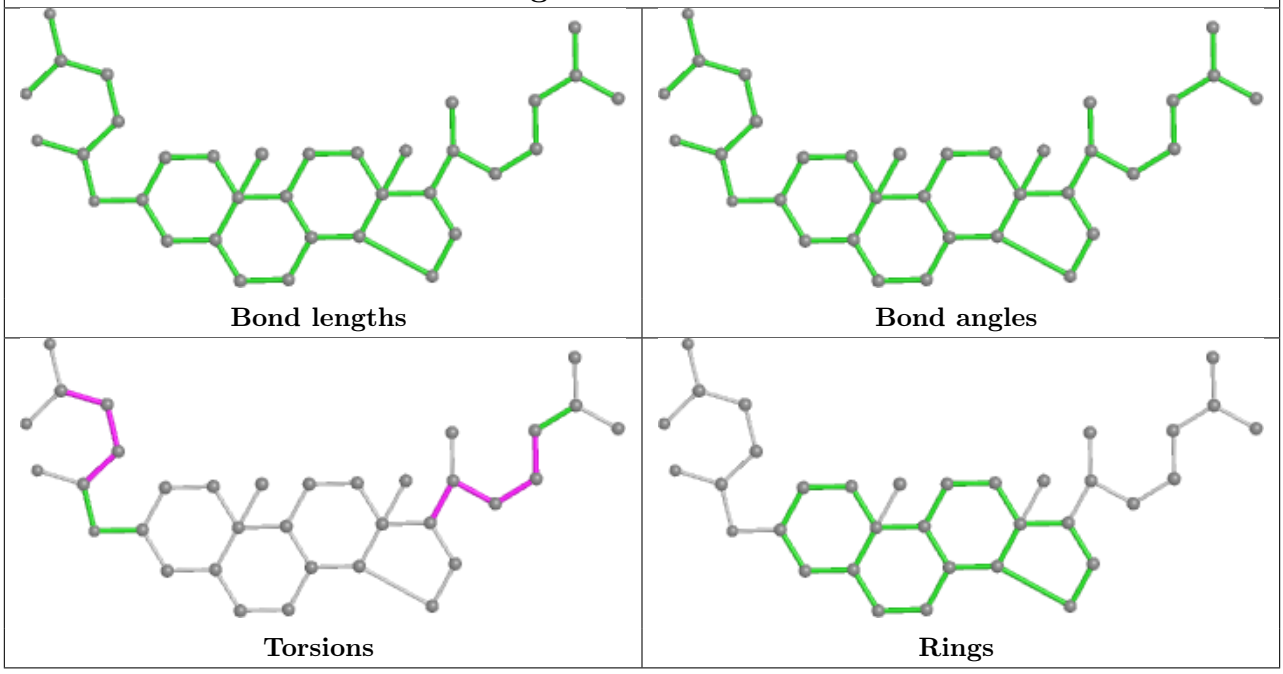


Ligand Y01 C 704

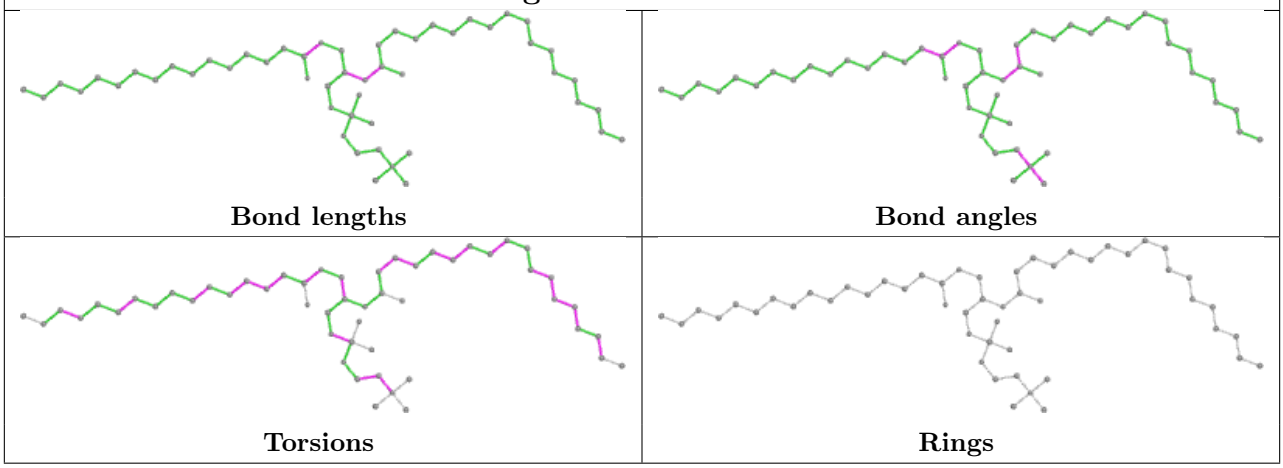



Ligand POV C 711
Bond lengths
Bond angles
Torsions
Rings
Ligand PCW B 709
Bond lengths
Bond angles
Torsions
Rings
Ligand POV C 702
Bond lengths
Bond angles
Torsions
Rings
Ligand POV A 812
Bond lengths
Bond angles
Torsions
Rings

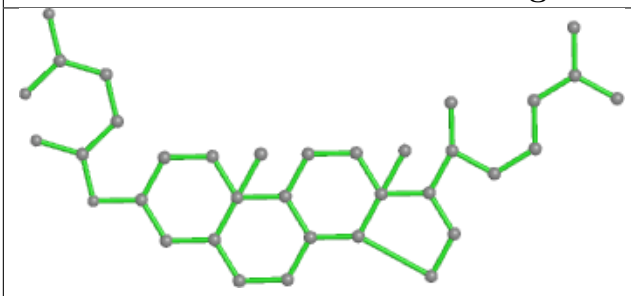
Ligand Y01 A 802



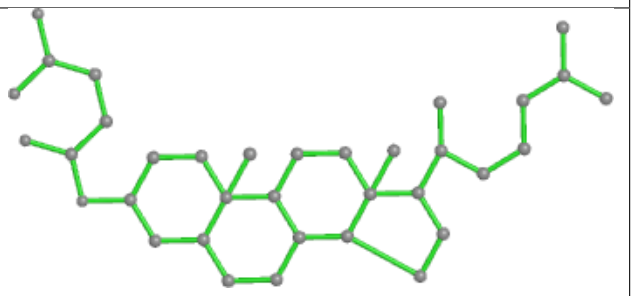
Ligand POV D 704



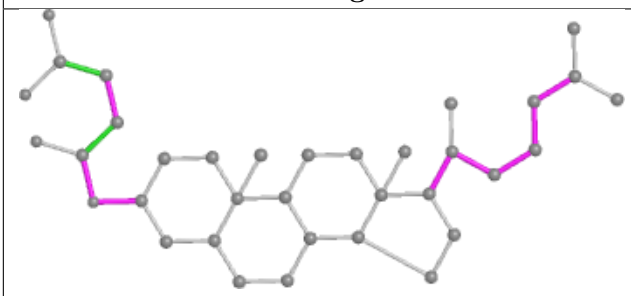
Ligand Y01 A 811



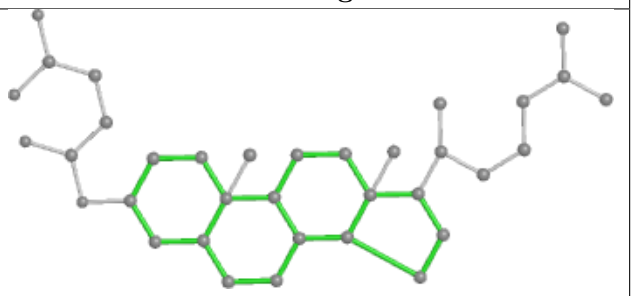
Bond lengths



Bond angles

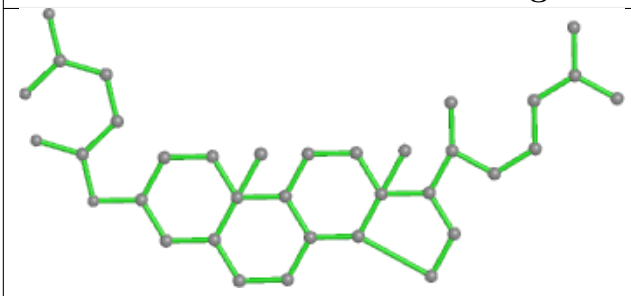


Torsions

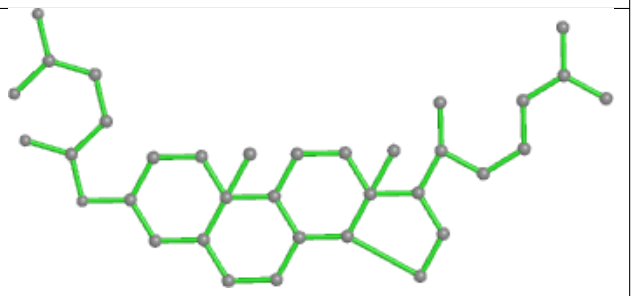


Rings

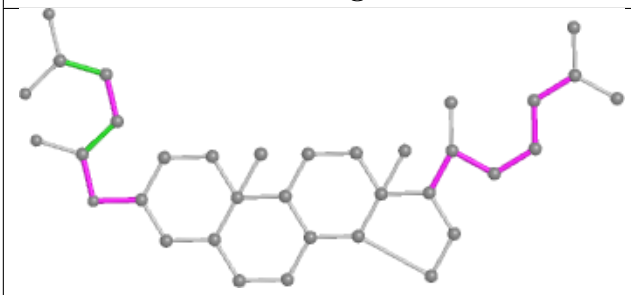
Ligand Y01 C 701



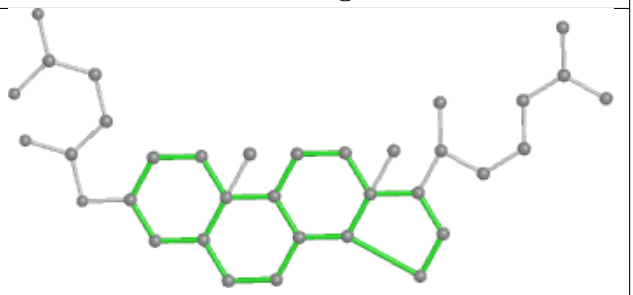
Bond lengths



Bond angles

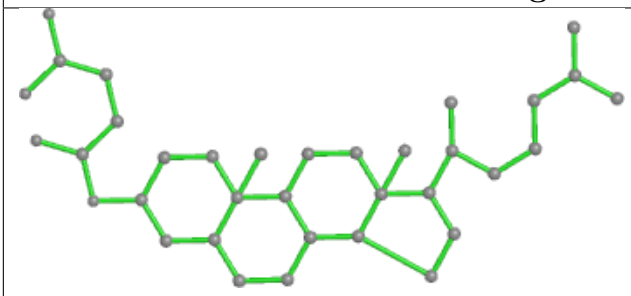


Torsions

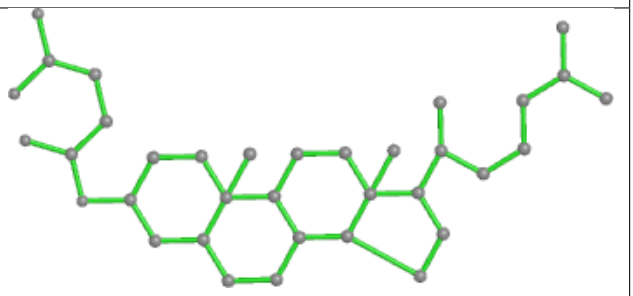


Rings

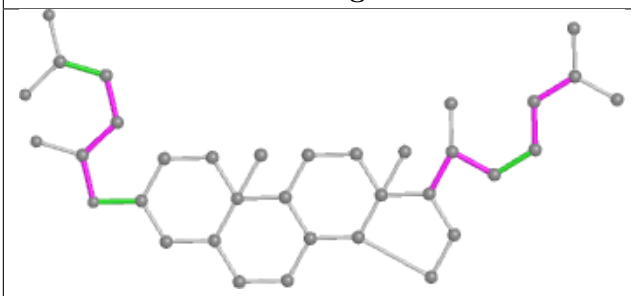
Ligand Y01 A 801



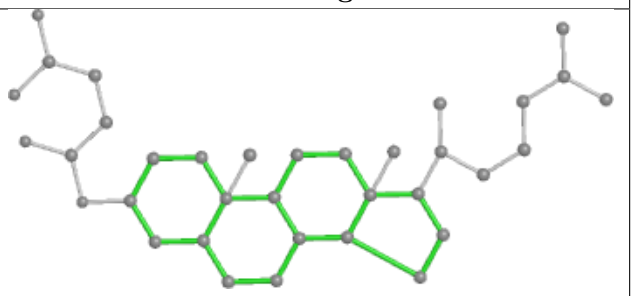
Bond lengths



Bond angles

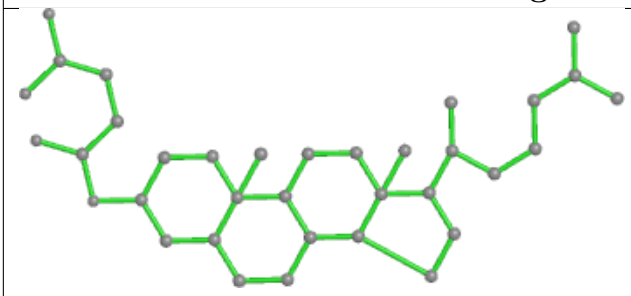


Torsions

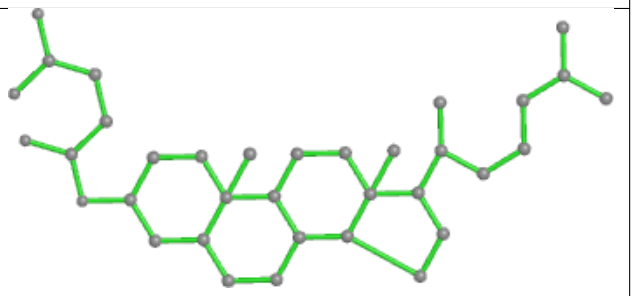


Rings

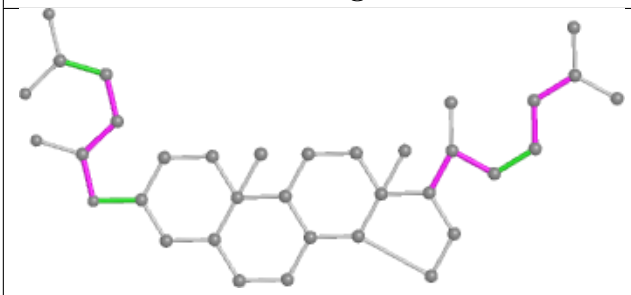
Ligand Y01 C 703



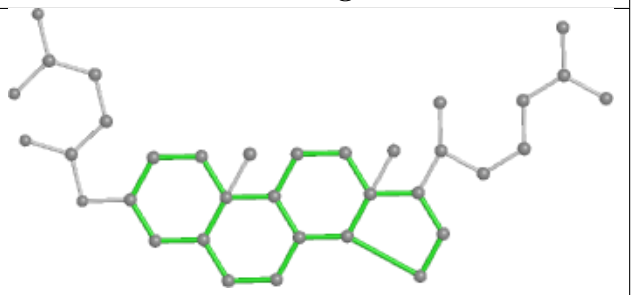
Bond lengths



Bond angles

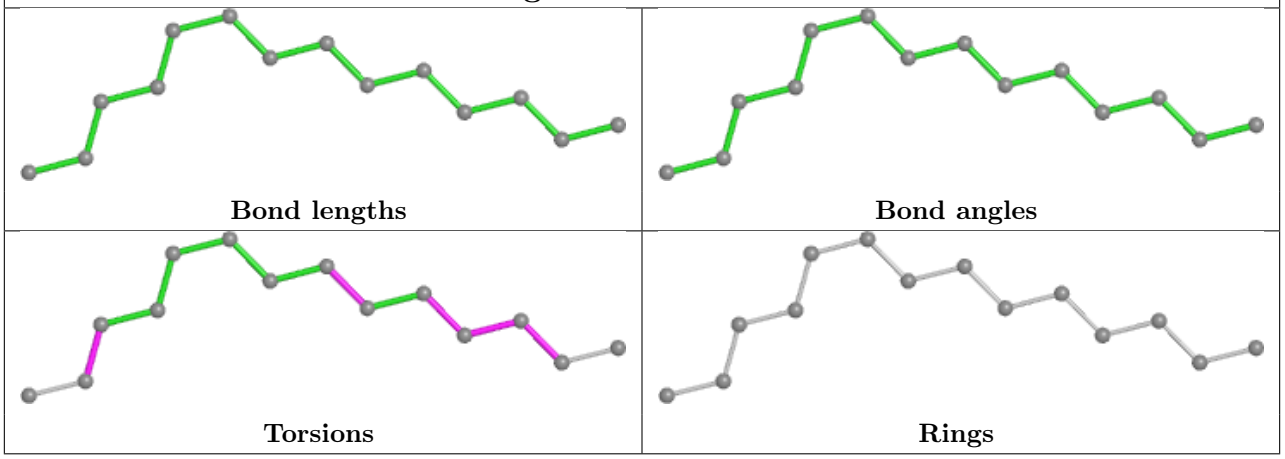


Torsions

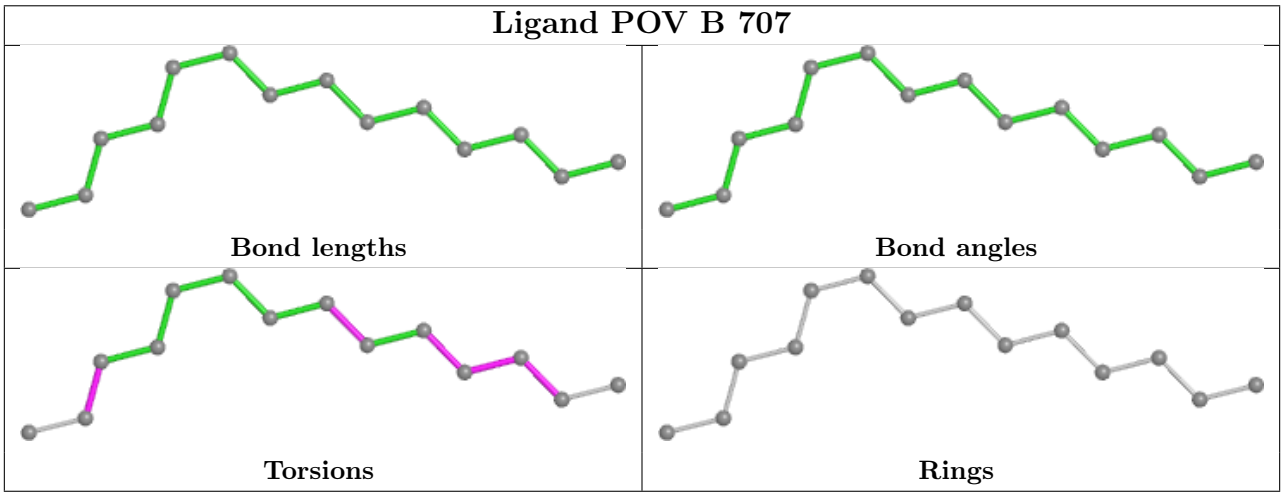


Rings

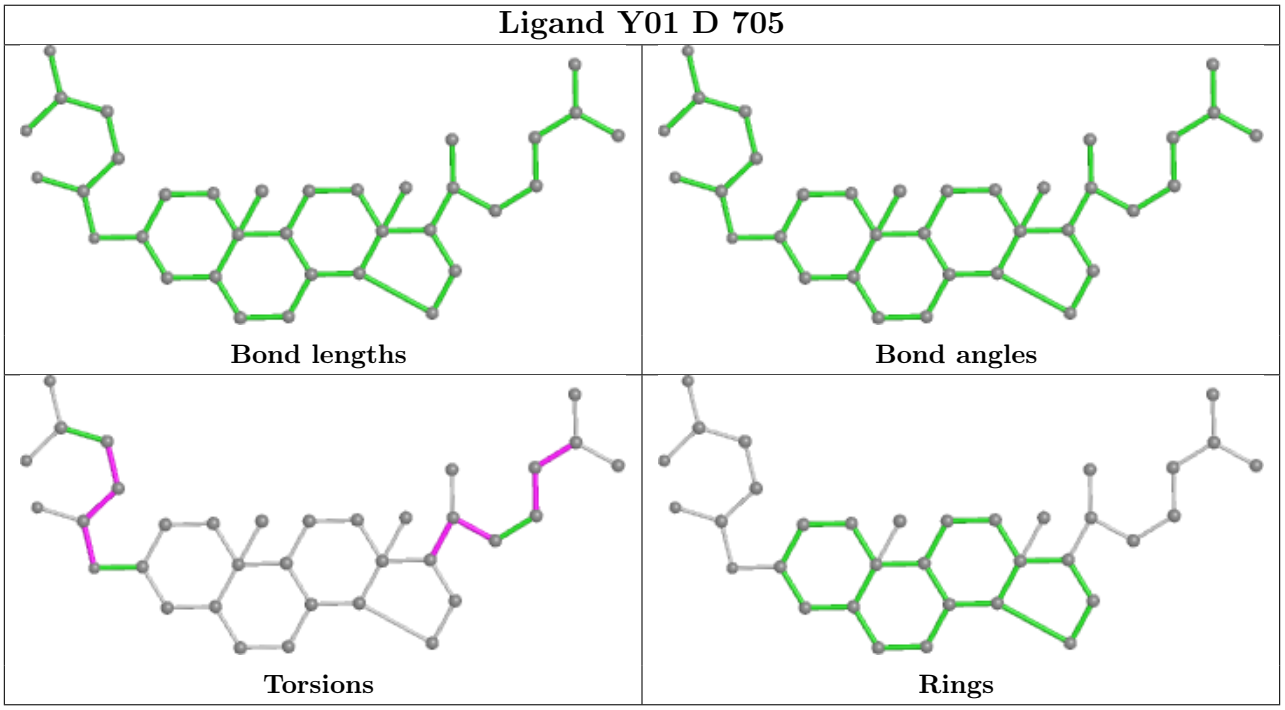
Ligand POV C 707



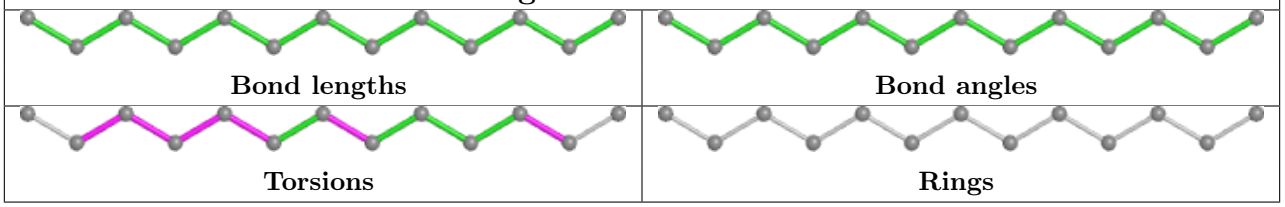
Ligand POV B 707



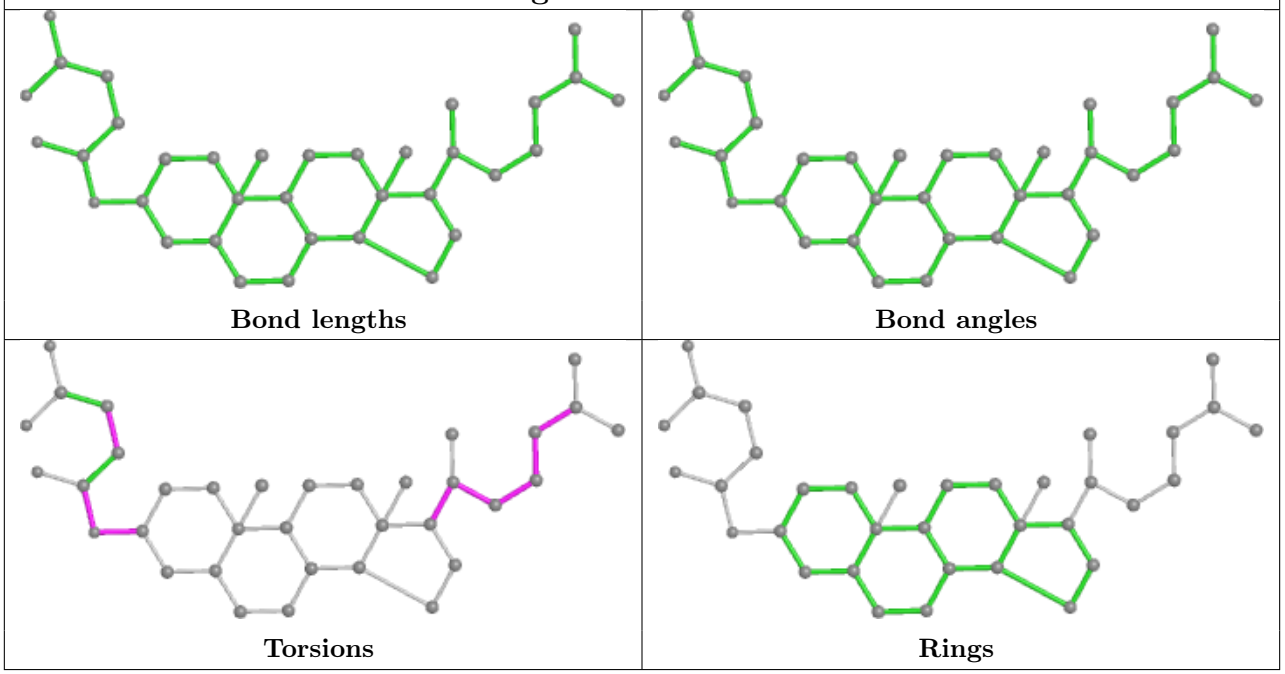
Ligand Y01 D 705



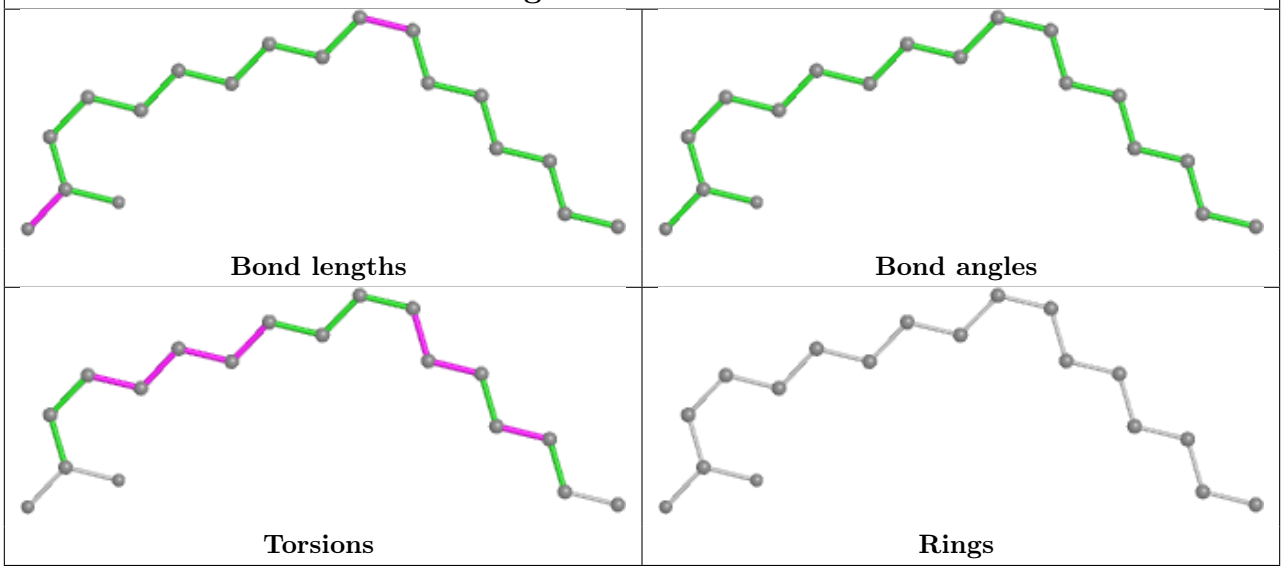
Ligand PCW A 808



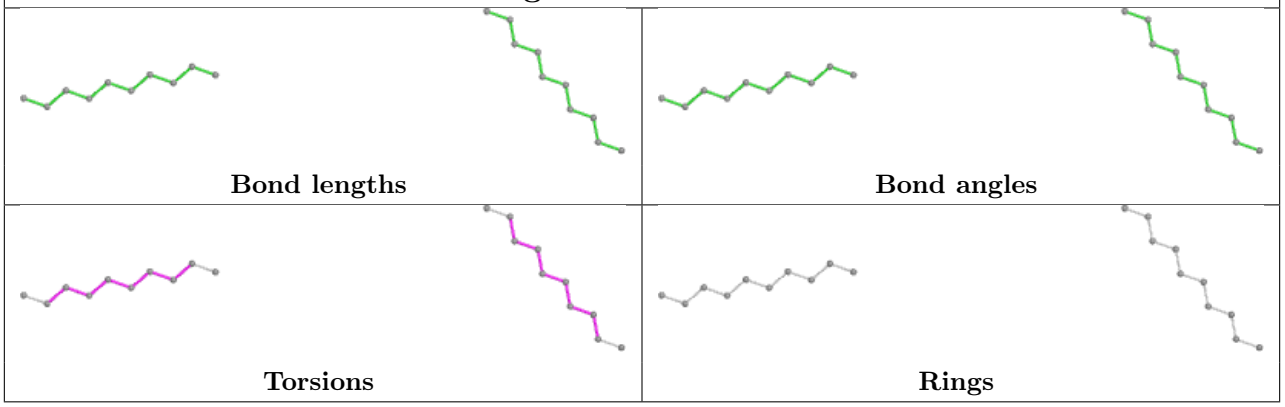
Ligand Y01 B 701



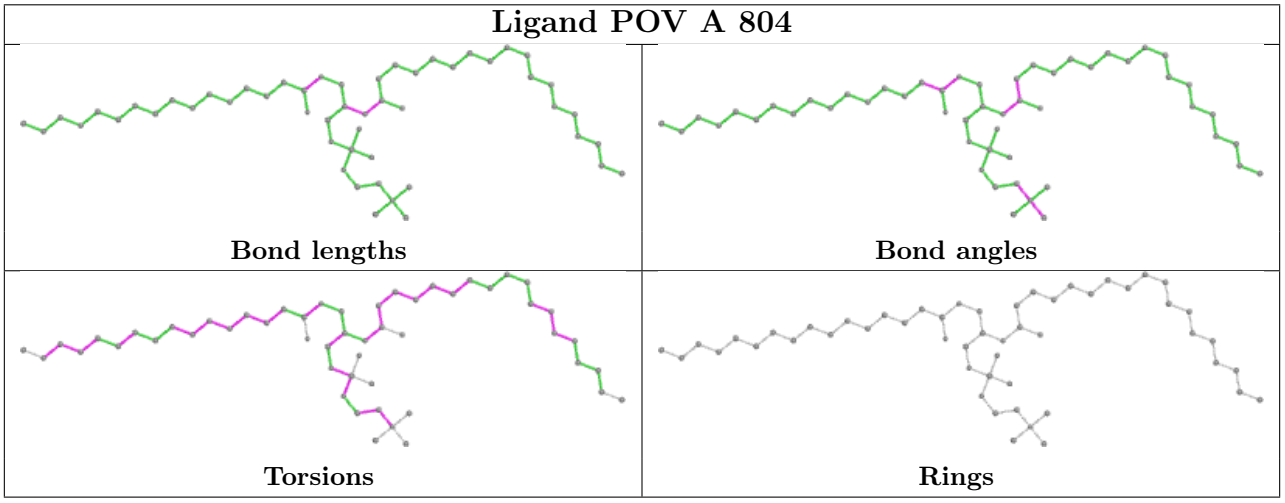
Ligand POV B 708



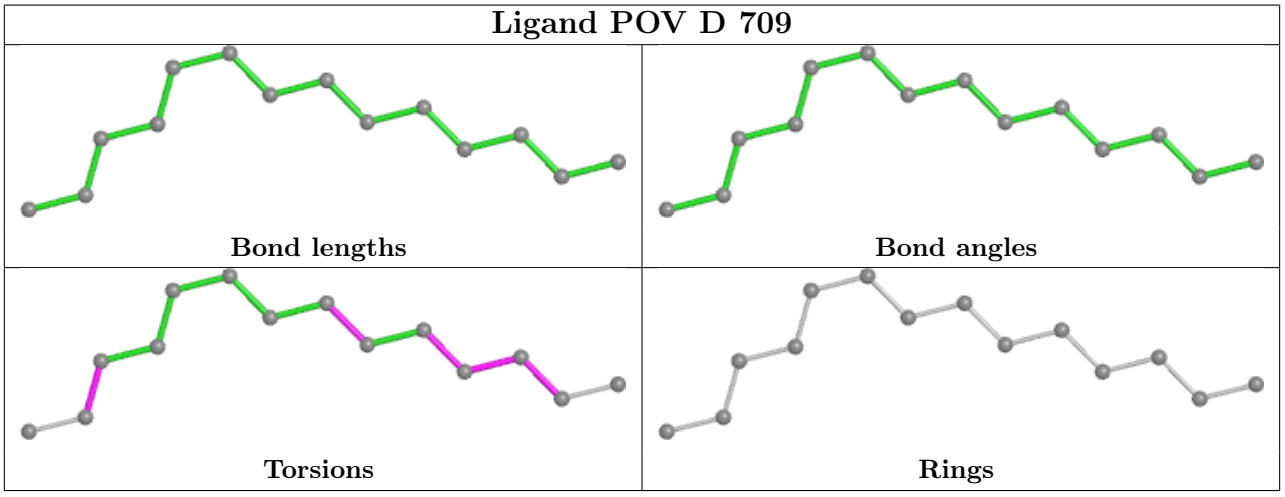
Ligand POV C 710

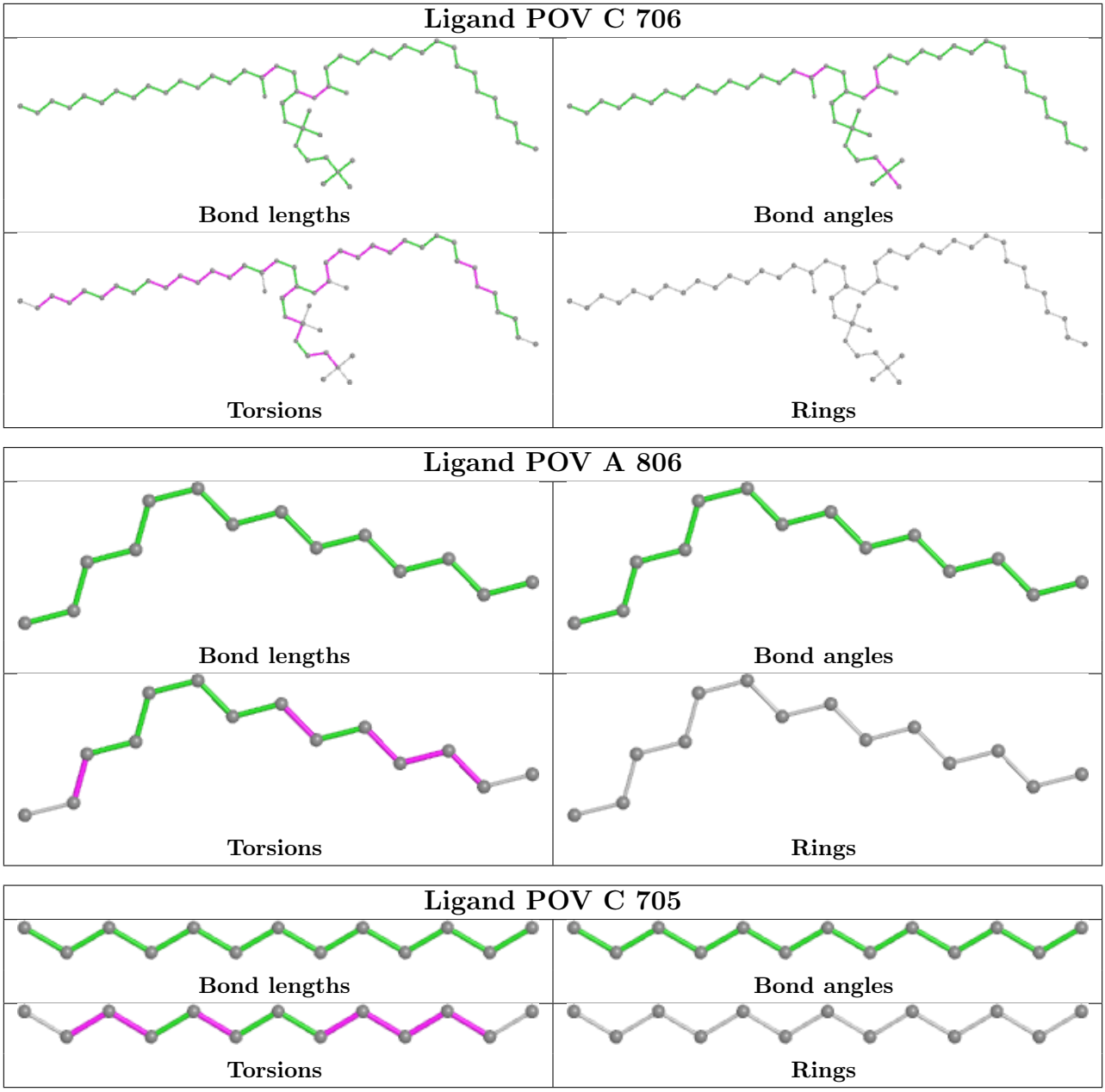


Ligand POV A 804



Ligand POV D 709





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.

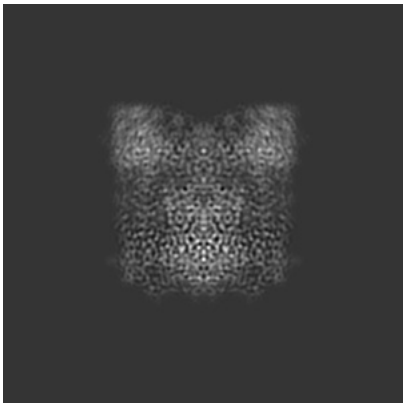
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24891. These allow visual inspection of the internal detail of the map and identification of artifacts.

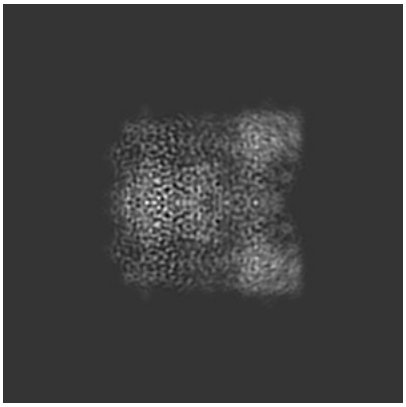
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

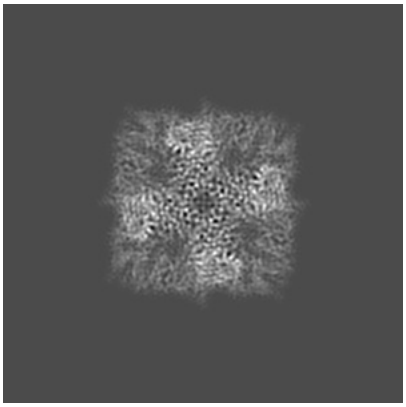
6.1.1 Primary map



X



Y

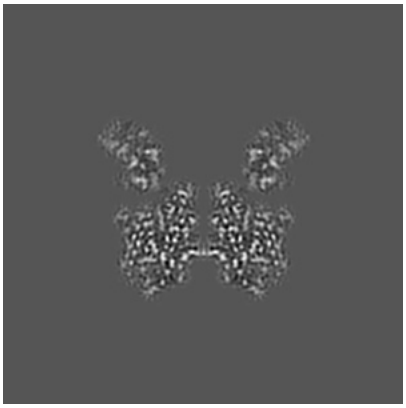


Z

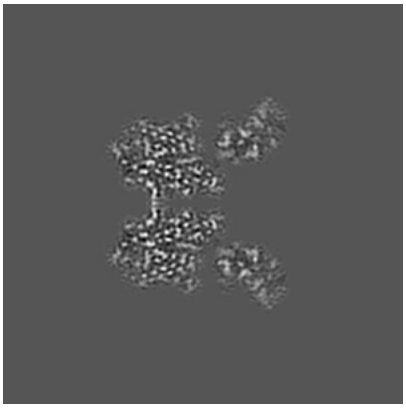
The images above show the map projected in three orthogonal directions.

6.2 Central slices

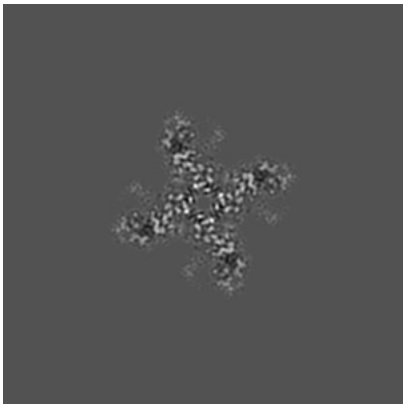
6.2.1 Primary map



X Index: 128



Y Index: 128

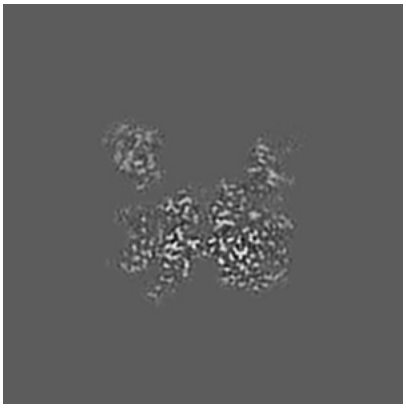


Z Index: 128

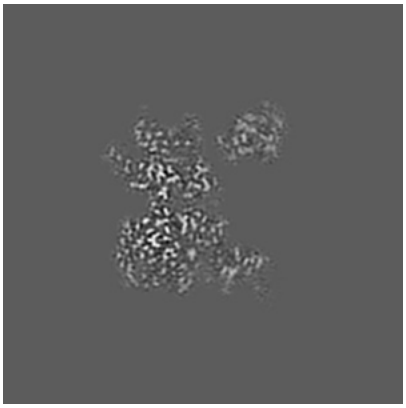
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

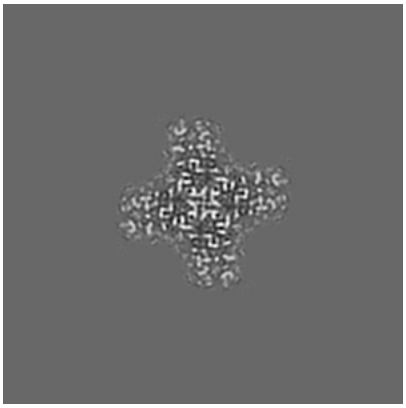
6.3.1 Primary map



X Index: 124



Y Index: 124

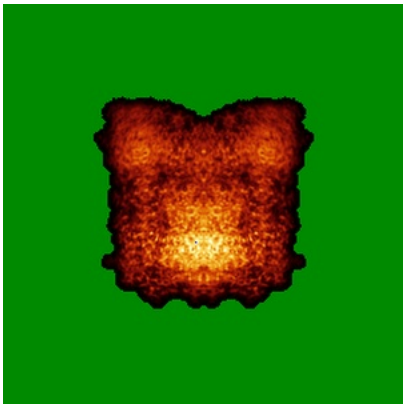


Z Index: 97

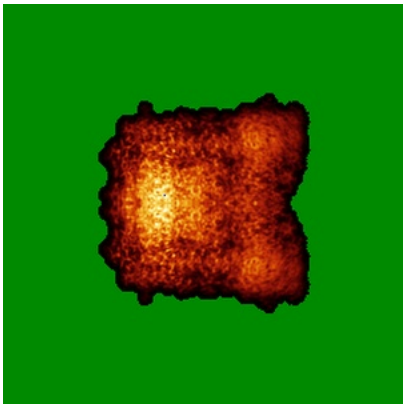
The images above show the largest variance slices of the map in three orthogonal directions.

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

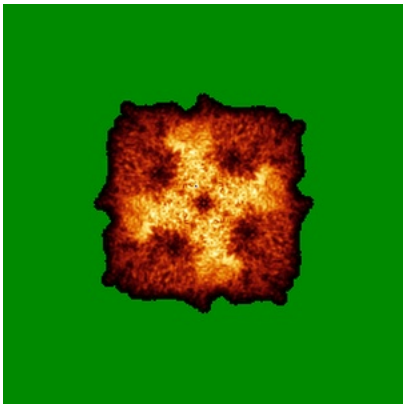
6.4.1 Primary map



X



Y

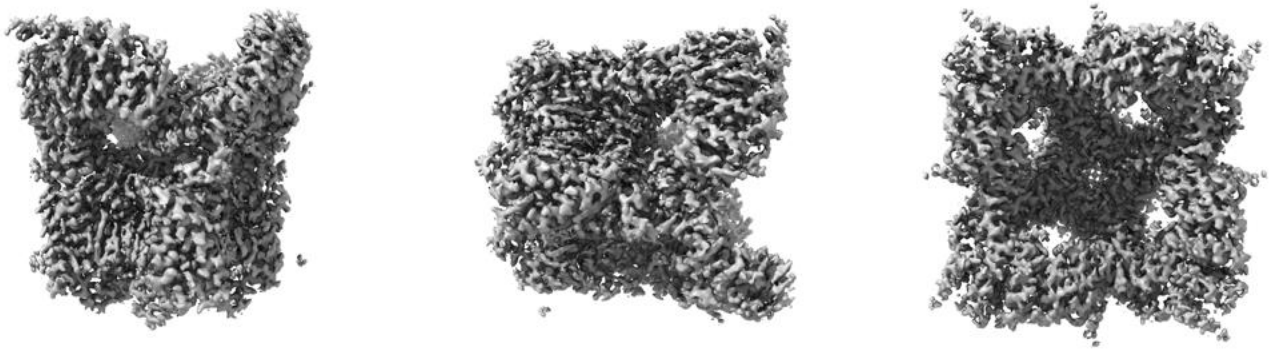


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

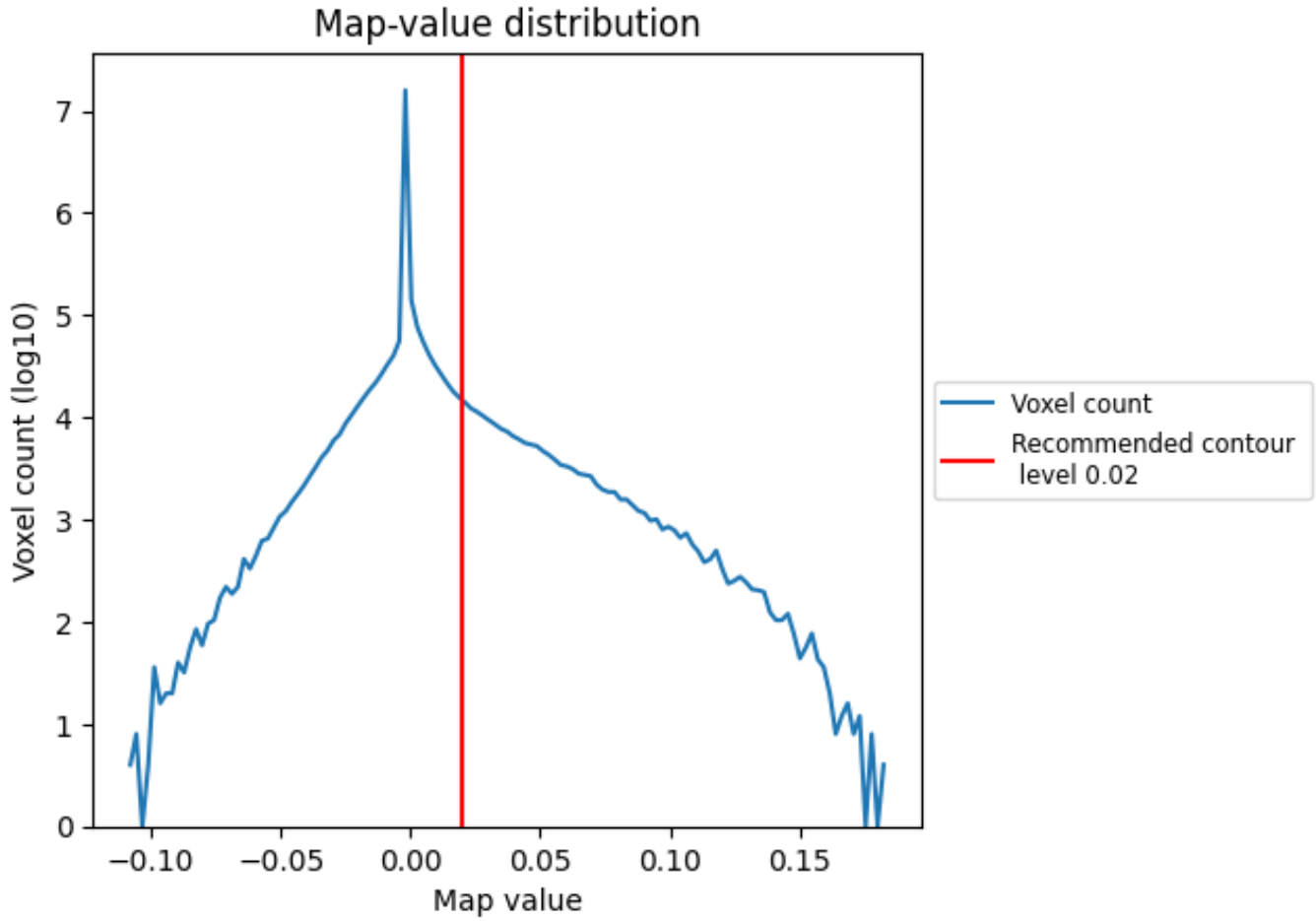
6.6 Mask visualisation (i)

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

7 Map analysis

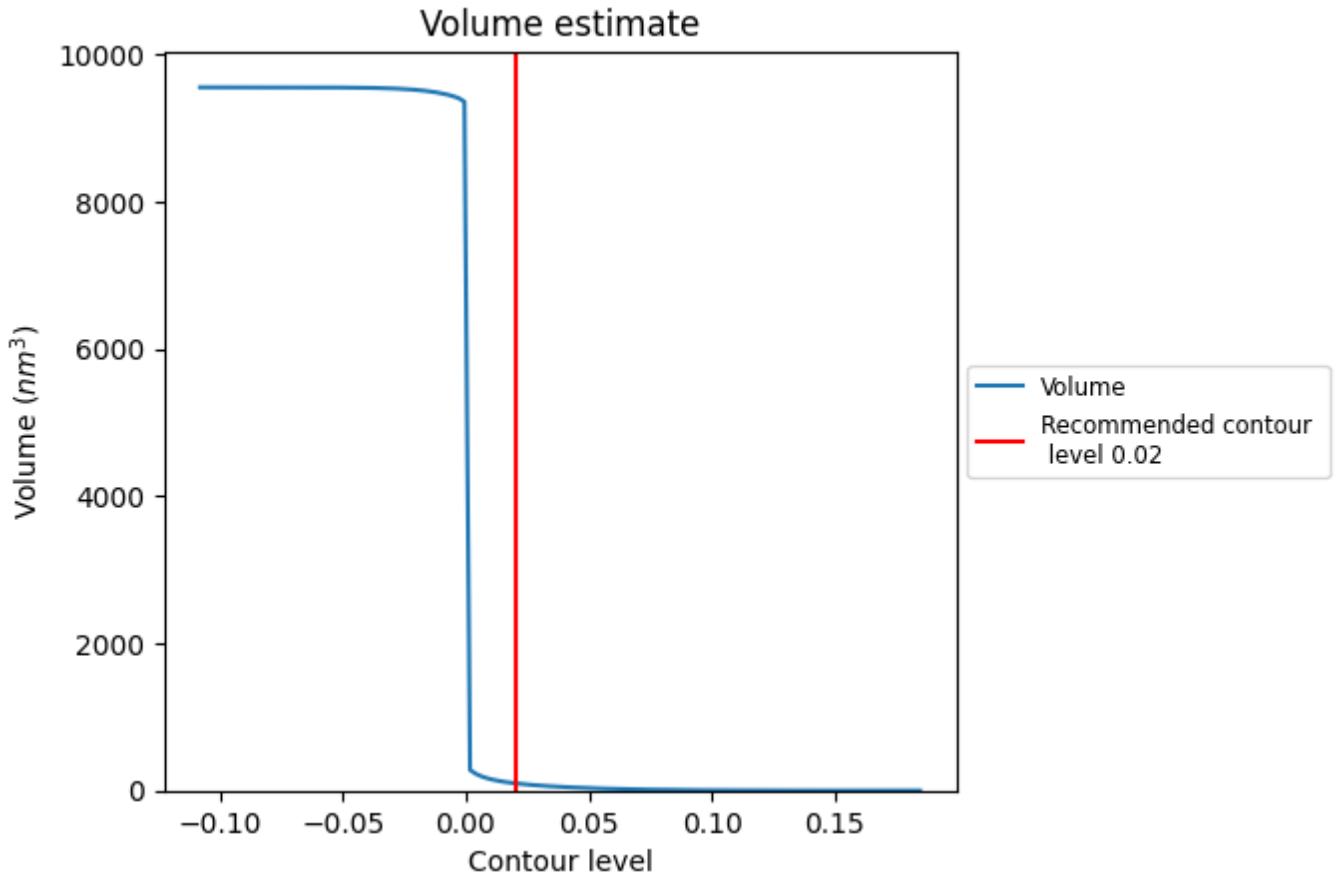
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

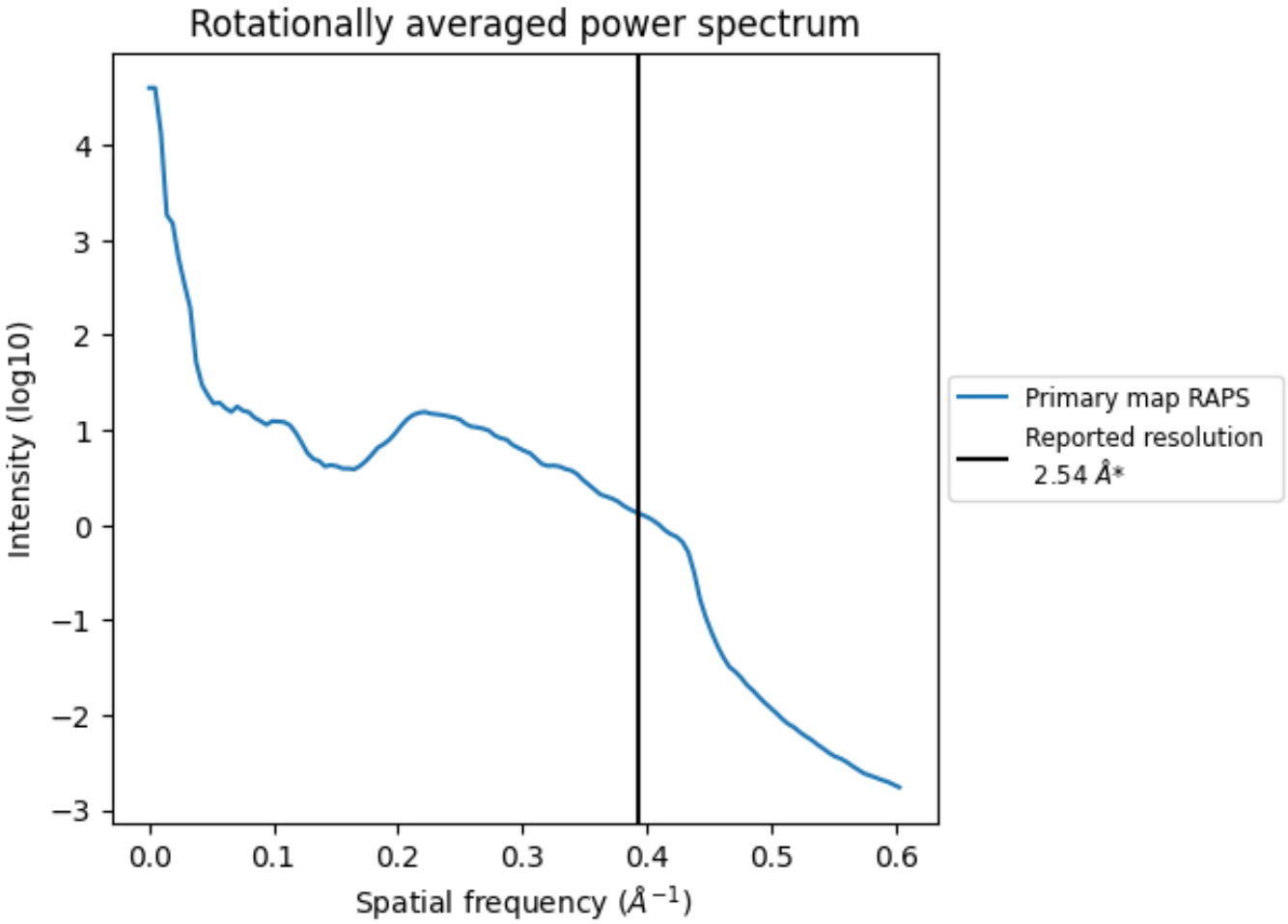
7.2 Volume estimate



The volume at the recommended contour level is 99 nm^3; this corresponds to an approximate mass of 89 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 0.394 Å^{-1}

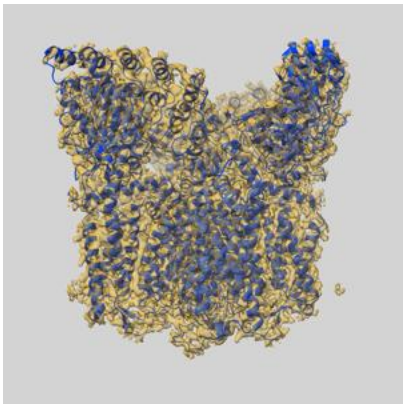
8 Fourier-Shell correlation

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

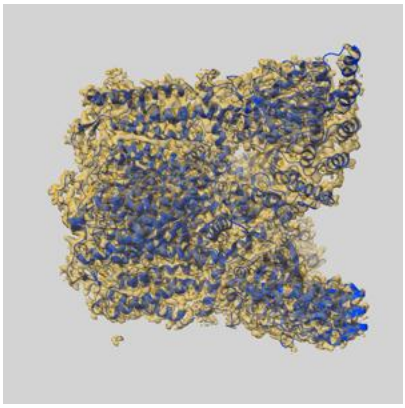
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-24891 and PDB model 7S89. Per-residue inclusion information can be found in section 3 on page 9.

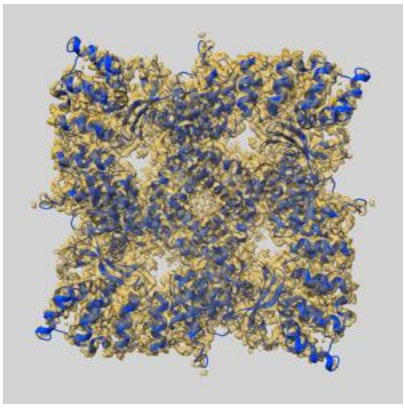
9.1 Map-model overlay



X



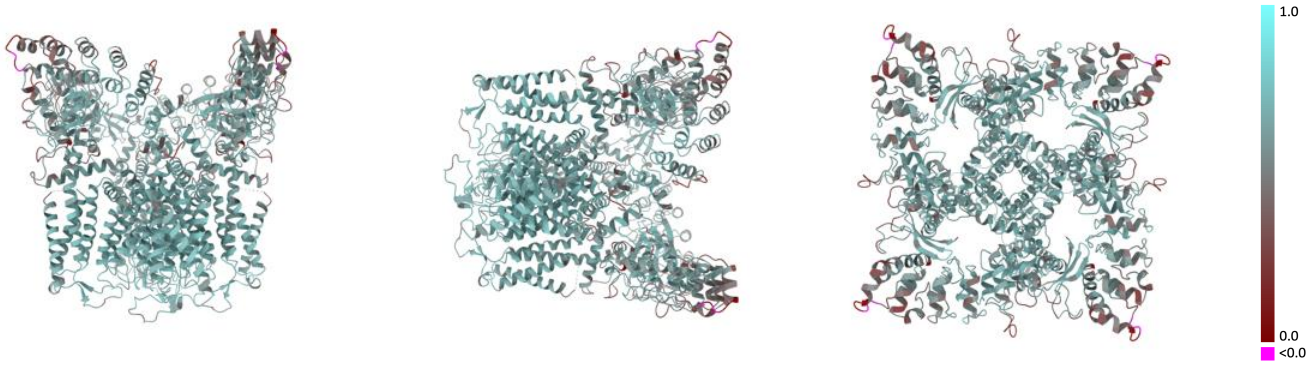
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

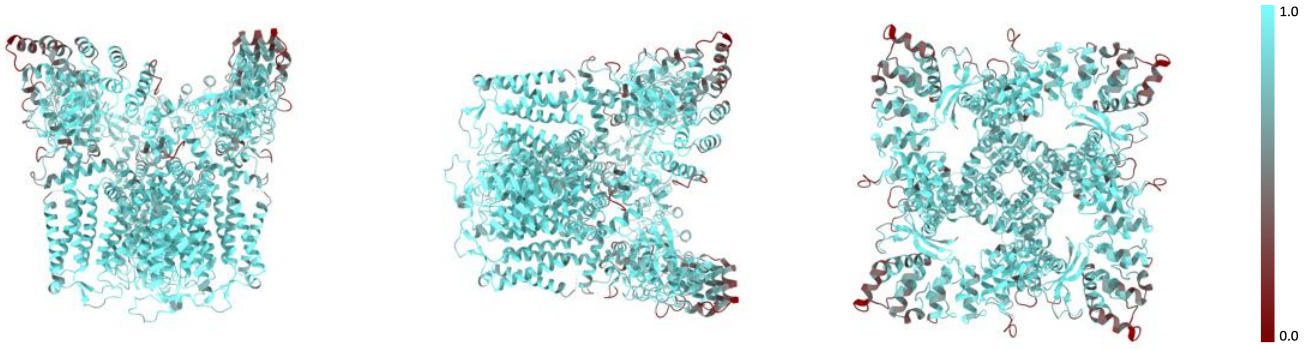
9.2 Q-score mapped to coordinate model (i)



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.

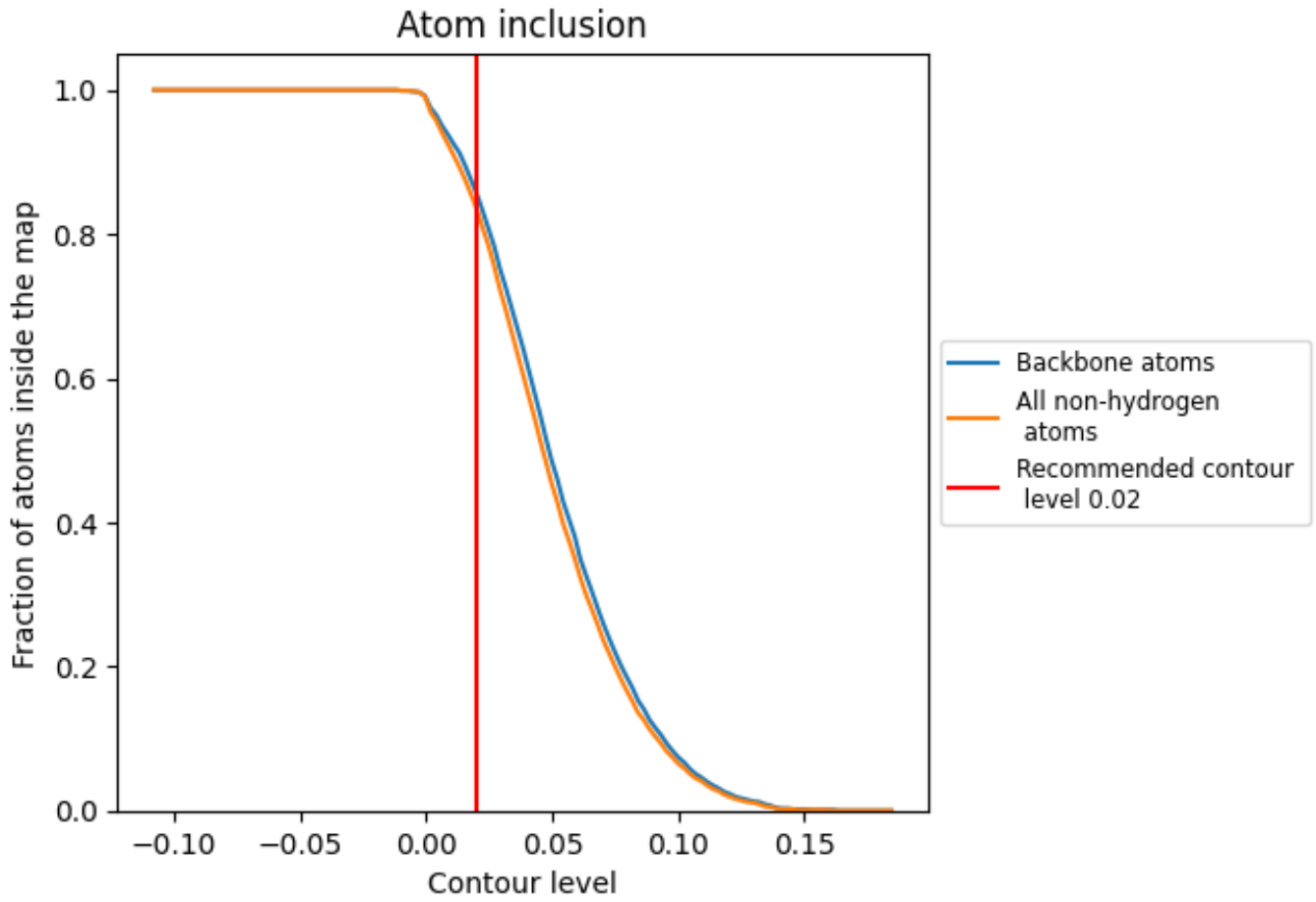
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 84% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8350	0.5960
A	0.8410	0.5960
B	0.8400	0.5960
C	0.8400	0.5960
D	0.8410	0.5950