Full wwPDB EM Validation Report (i)

Aug 5, 2026 – 06:44 AM EDT

PDB ID	:	7S8B / pdb_00007s8b
EMDB ID	:	EMD-24892
Title	:	Cryo-EM structure of human TRPV6 in complex with channel blocker ruthenium red
Authors	:	Nadezhdin, K.D.; Neuberger, A.; Sobolevsky, A.I.
Deposited on	:	2021-09-17
Resolution	:	2.43 Å(reported)
Based on initial model	:	7K4B

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 (i) 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 (1)) were used in the production of this report:

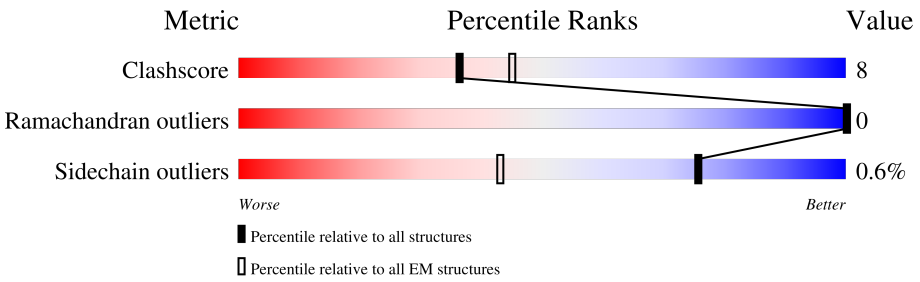
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

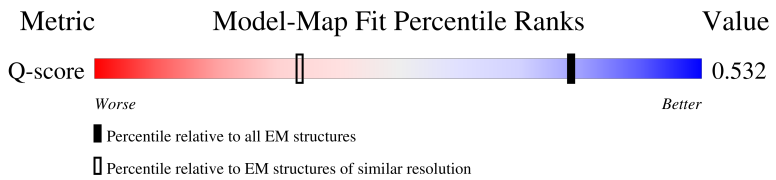
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.43 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5787 (1.94 - 2.93)

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	16% 77% 12% 10%
1	B	683	16% 77% 12% 10%
1	C	683	16% 76% 13% 10%
1	D	683	16% 77% 12% 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	Y01	B	704	-	-	X	-
2	Y01	C	704	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 21124 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
			Total	C	N	O	S		
1	A	612	4912	3173	831	868	40	0	0
1	B	612	4912	3173	831	868	40	0	0
1	C	612	4912	3173	831	868	40	0	0
1	D	612	4912	3173	831	868	40	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

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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

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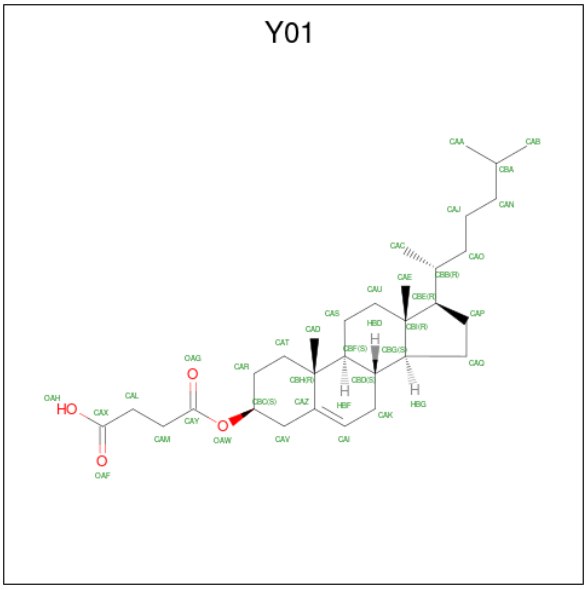
Chain	Residue	Modelled	Actual	Comment	Reference
D	683	LYS	-	expression tag	UNP Q9H1D0

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



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

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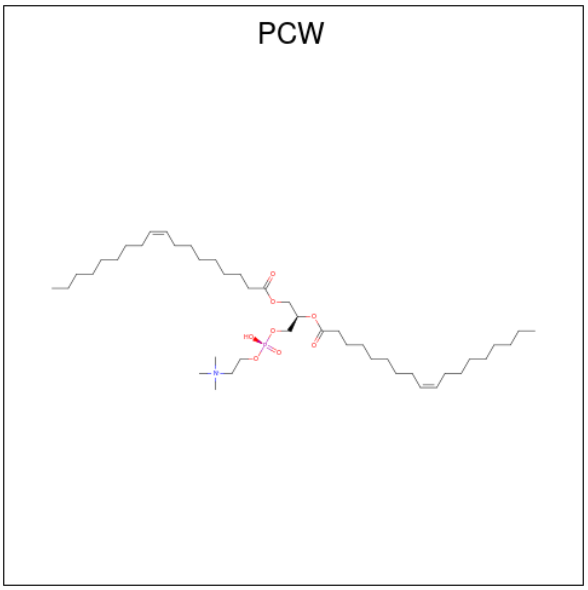
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
2	D	1	35	31	4	0

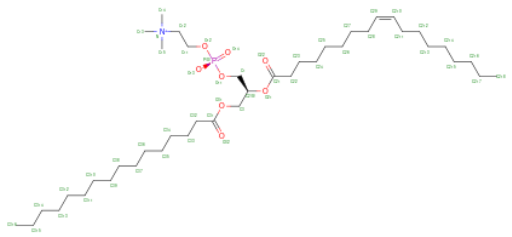
- Molecule 3 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PCW) (formula: $C_{44}H_{85}NO_8P$).



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

- Molecule 4 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (CCD ID: POV) (formula: $C_{42}H_{82}NO_8P$).

POV



Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total C 13 13	0
4	A	1	Total C O 19 17 2	0
4	A	1	Total C O 16 14 2	0
4	A	1	Total C N O P 52 42 1 8 1	0
4	A	1	Total C N O P 42 32 1 8 1	0
4	A	1	Total C N O P 52 42 1 8 1	0
4	A	1	Total C N O P 52 42 1 8 1	0
4	B	1	Total C N O P 52 42 1 8 1	0
4	B	1	Total C 13 13	0
4	B	1	Total C O 19 17 2	0
4	B	1	Total C O 16 14 2	0
4	B	1	Total C N O P 52 42 1 8 1	0
4	B	1	Total C N O P 42 32 1 8 1	0
4	B	1	Total C N O P 52 42 1 8 1	0

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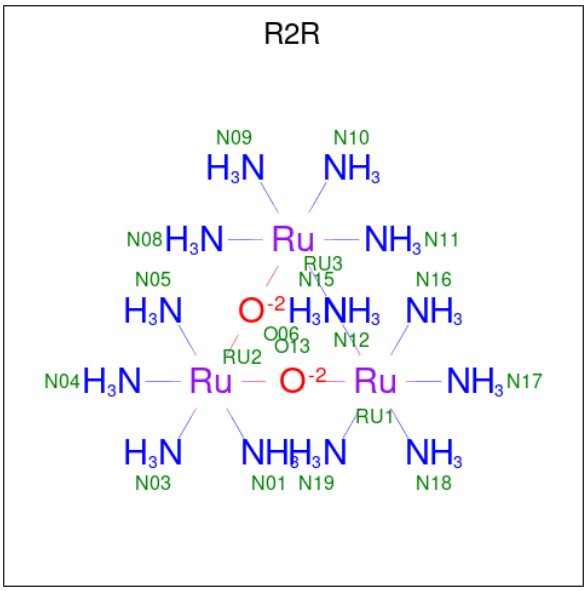
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
4	C	1	52	42	1	8	1	0
			Total	C				
4	C	1	13	13				0
			Total	C	O			
4	C	1	19	17	2			0
			Total	C	O			
4	C	1	16	14	2			0
			Total	C	N	O	P	
4	C	1	52	42	1	8	1	0
			Total	C	N	O	P	
4	C	1	42	32	1	8	1	0
			Total	C	N	O	P	
4	C	1	52	42	1	8	1	0
			Total	C	N	O	P	
4	D	1	52	42	1	8	1	0
			Total	C	N	O	P	
4	D	1	42	32	1	8	1	0
			Total	C	N	O	P	
4	D	1	52	42	1	8	1	0
			Total	C	N	O	P	
4	D	1	52	42	1	8	1	0
			Total	C				
4	D	1	13	13				0
			Total	C	O			
4	D	1	19	17	2			0
			Total	C	O			
4	D	1	16	14	2			0

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 6 is ruthenium(6+) azanide pentaamino(oxido)ruthenium (1/4/2) (CCD ID: R2R) (formula: $H_{42}N_{14}O_2Ru_3$) (labeled as "Ligand of Interest" by depositor).



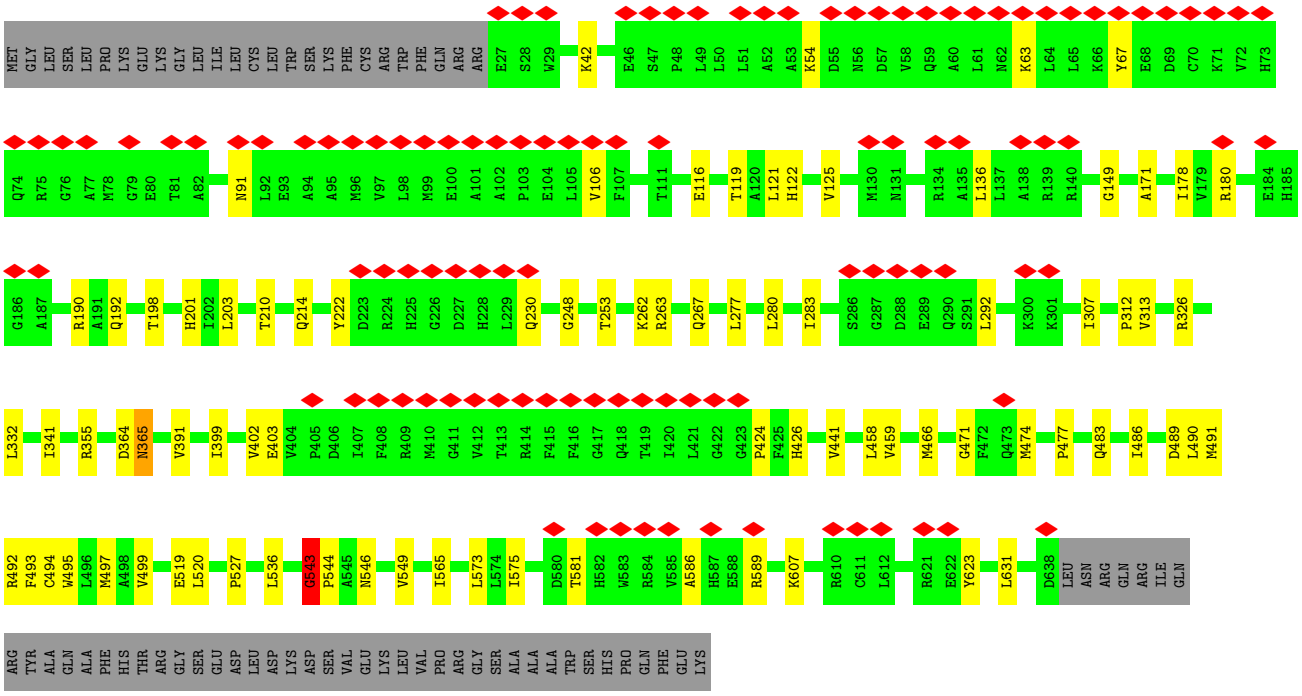
Mol	Chain	Residues	Atoms				AltConf
			Total	N	O	Ru	
6	A	1	19	14	2	3	0

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.

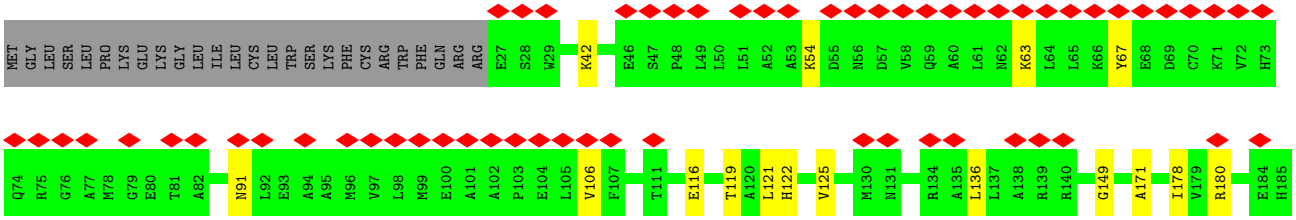
• Molecule 1: Transient receptor potential cation channel subfamily V member 6

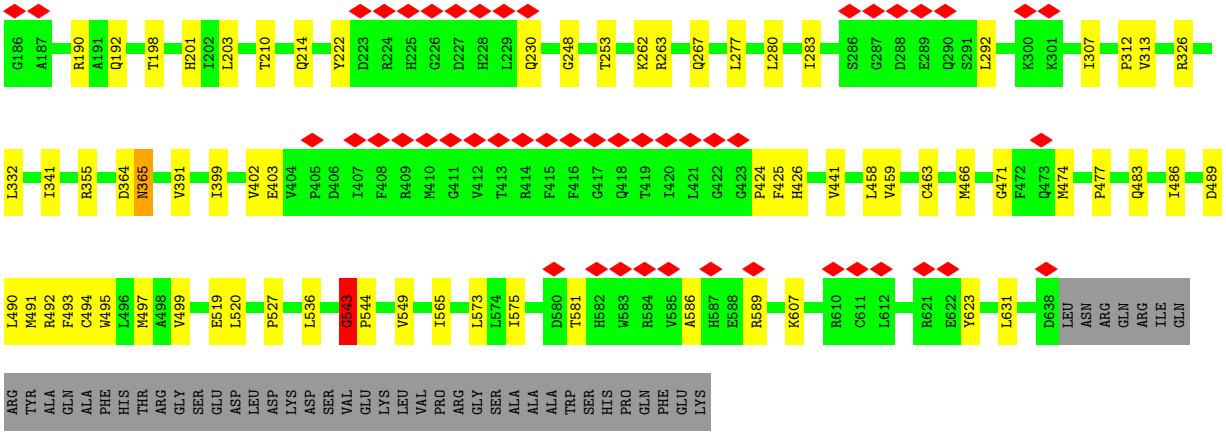
Chain A:



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

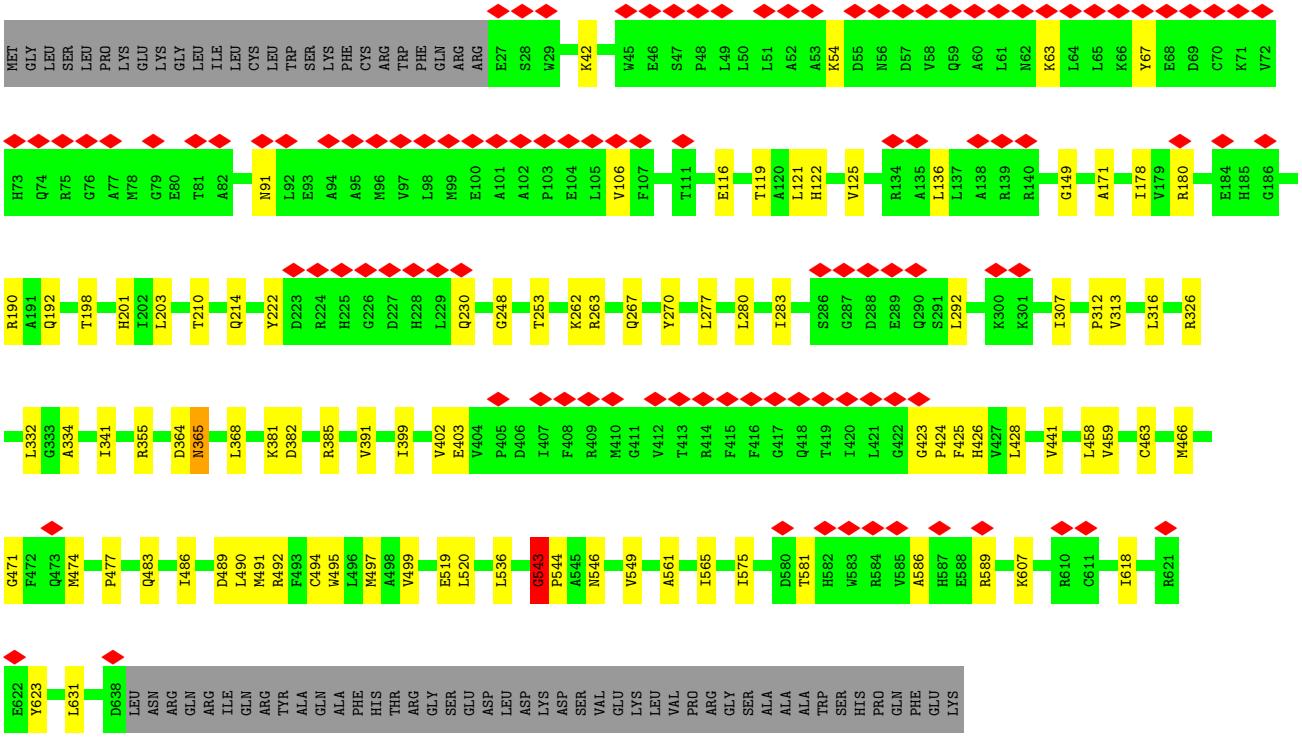
Chain B:





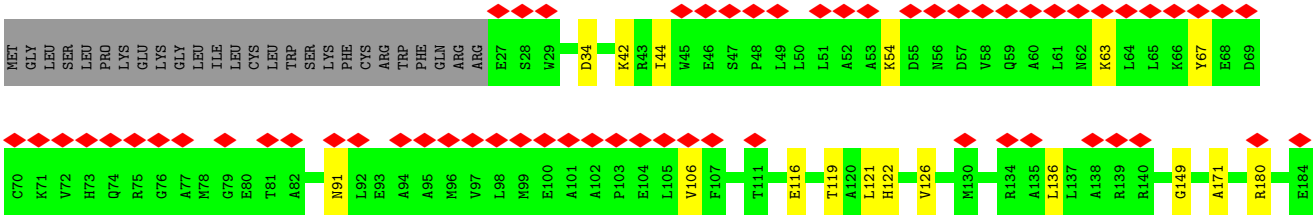
• Molecule 1: Transient receptor potential cation channel subfamily V member 6

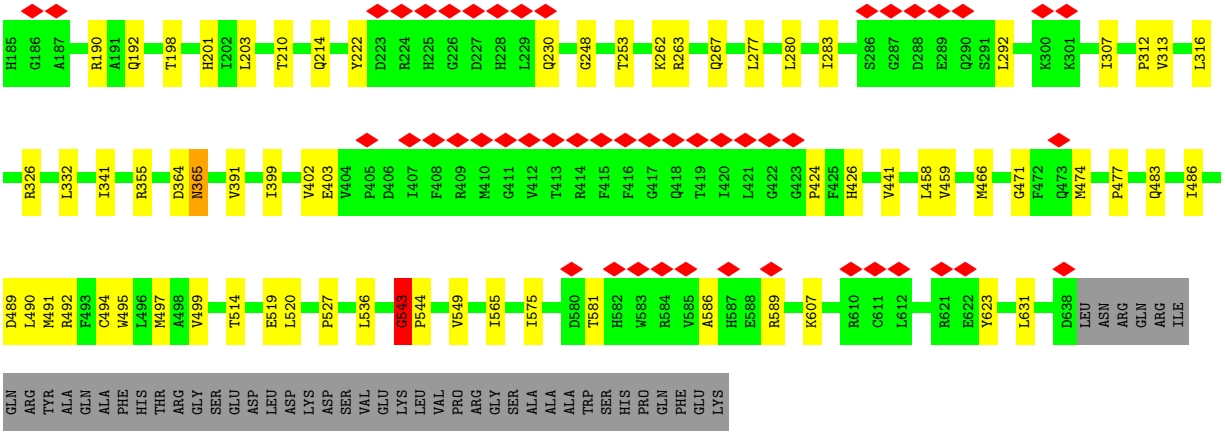
Chain C:



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

Chain D:




H185 G186 A187 R190 A191 Q192 T198 H201 I202 L203 T210 Q214 Y222 D223 R224 H225 G226 D227 H228 L229 Q230 G248 T253 K262 R263 Q267 L277 L280 I283 S286 G287 D288 E289 Q290 S291 L292 K300 K301 I307 P312 V313 L316
R326 L332 I341 R355 D364 N365 V391 I399 V402 E403 V404 P405 D406 I407 F408 R409 M410 G411 V412 T413 R414 F415 F416 G417 Q418 T419 I420 L421 G422 G423 P424 F425 H426 V441 L458 V459 M466 G471 F472 Q473 M474 P477 Q483 I486
D489 L490 M491 R492 F493 C494 W495 L496 M497 A498 V499 T514 E519 L520 P527 L536 G543 P544 V549 I565 I575 D580 T581 H582 W583 R584 V585 A586 H587 E588 R589 K607 R610 C611 L612 R621 E622 Y623 L631 D638 LEU ASN ARG GLN ARG ILE
GLN ARG TYR ALA GLN ALA PHE HIS THR ARG GLY SER GLU ASP LEU ASP LYS ASP SER VAL GLU LYS LEU VAL PRO ARG GLY SER ALA ALA ALA TRP SER HIS PRO GLN PHE GLU LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	49537	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 ($e^-/Å^2$)	58.5	Depositor
Minimum defocus (nm)	-500	Depositor
Maximum defocus (nm)	-2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.375	Depositor
Minimum map value	-0.092	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0219	Depositor
Map size (Å)	204.544, 204.544, 204.544	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.799, 0.799, 0.799	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, R2R, PCW, POV, Y01

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	0.36	0/5025	0.60	4/6818 (0.1%)
1	B	0.36	0/5025	0.60	2/6818 (0.0%)
1	C	0.36	0/5025	0.60	4/6818 (0.1%)
1	D	0.36	0/5025	0.60	2/6818 (0.0%)
All	All	0.36	0/20100	0.60	12/27272 (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	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

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	D	543	GLY	CA-C-N	6.75	127.81	119.98
1	D	543	GLY	C-N-CA	6.75	127.81	119.98
1	C	543	GLY	CA-C-N	6.73	127.78	119.98
1	C	543	GLY	C-N-CA	6.73	127.78	119.98
1	A	543	GLY	CA-C-N	6.70	127.75	119.98
1	A	543	GLY	C-N-CA	6.70	127.75	119.98
1	B	543	GLY	CA-C-N	6.69	127.74	119.98
1	B	543	GLY	C-N-CA	6.69	127.74	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	546	ASN	CA-C-N	5.01	131.11	121.54
1	A	546	ASN	C-N-CA	5.01	131.11	121.54
1	C	546	ASN	CA-C-N	5.00	131.09	121.54
1	C	546	ASN	C-N-CA	5.00	131.09	121.54

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	543	GLY	Peptide
1	B	543	GLY	Peptide
1	C	543	GLY	Peptide
1	D	543	GLY	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	64	0
1	B	4912	0	4964	66	0
1	C	4912	0	4964	80	0
1	D	4912	0	4964	66	0
2	A	105	0	147	25	0
2	B	105	0	147	37	0
2	C	105	0	147	39	0
2	D	105	0	147	23	0
3	A	13	0	20	1	0
3	B	13	0	20	1	0
3	C	13	0	20	1	0
3	D	13	0	20	1	0
4	A	246	0	373	14	0
4	B	246	0	373	14	0
4	C	246	0	373	17	0
4	D	246	0	373	14	0
5	A	1	0	0	0	0
6	A	19	0	0	0	0
All	All	21124	0	22016	330	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 8.

All (330) 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:C:459:VAL:HG12	2:C:704:Y01:HAP1	1.42	1.01
2:B:704:Y01:HAE3	1:C:565:ILE:HD11	1.57	0.87
1:A:483:GLN:HB2	2:A:802:Y01:HAL2	1.54	0.87
1:B:463:CYS:SG	2:B:704:Y01:HAQ2	2.15	0.87
1:D:483:GLN:HB2	2:D:707:Y01:HAL2	1.56	0.85
2:C:704:Y01:HAJ2	4:D:705:POV:H214	1.67	0.77
1:C:426:HIS:CD2	2:C:703:Y01:HAL1	2.22	0.75
1:D:426:HIS:CD2	2:D:706:Y01:HAL1	2.21	0.75
1:B:424:PRO:HG3	2:B:704:Y01:HAR1	1.69	0.75
1:A:426:HIS:CD2	2:A:801:Y01:HAL1	2.22	0.73
1:B:426:HIS:CD2	2:B:703:Y01:HAL1	2.23	0.73
1:C:483:GLN:HB2	2:C:704:Y01:HAL2	1.68	0.73
2:B:704:Y01:HAC2	2:B:704:Y01:HAE2	1.70	0.73
2:B:704:Y01:HAC1	1:C:565:ILE:HD11	1.70	0.72
1:C:463:CYS:HB2	2:C:704:Y01:HAQ2	1.72	0.70
1:D:424:PRO:HG3	2:D:707:Y01:HAR1	1.75	0.69
2:B:704:Y01:HAC3	1:C:561:ALA:HB1	1.75	0.67
2:C:704:Y01:CAJ	4:D:705:POV:H214	2.27	0.65
1:C:463:CYS:HB3	2:C:704:Y01:HAK1	1.77	0.64
1:A:424:PRO:HG3	2:A:802:Y01:HAR1	1.79	0.64
1:B:459:VAL:HG12	2:B:704:Y01:HAP2	1.80	0.64
1:B:483:GLN:HB2	2:B:704:Y01:HAL2	1.81	0.62
2:C:704:Y01:HAC2	2:C:704:Y01:CAE	2.31	0.61
1:A:332:LEU:HD21	2:A:801:Y01:HAD2	1.84	0.60
2:B:704:Y01:HAE3	1:C:565:ILE:CD1	2.28	0.60
1:B:332:LEU:HD21	2:B:703:Y01:HAD2	1.83	0.60
1:A:424:PRO:CG	2:A:802:Y01:HAR1	2.32	0.60
1:B:459:VAL:CG1	2:B:704:Y01:HAP2	2.32	0.59
1:D:332:LEU:HD21	2:D:706:Y01:HAD2	1.84	0.59
2:B:704:Y01:HAJ2	4:C:702:POV:H214	1.84	0.59
1:D:402:VAL:HG21	2:D:706:Y01:HAK1	1.85	0.59
1:C:402:VAL:CG2	2:C:703:Y01:HAK1	2.33	0.59
1:C:365:ASN:ND2	1:D:519:GLU:OE1	2.36	0.59
1:C:402:VAL:HG21	2:C:703:Y01:HAK1	1.85	0.59
1:A:494:CYS:HB3	2:B:701:Y01:HAA3	1.85	0.58
1:C:494:CYS:HB3	2:D:704:Y01:HAA3	1.85	0.58
1:B:402:VAL:HG21	2:B:703:Y01:HAK1	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:489:ASP:OD1	1:C:492:ARG:NH1	2.37	0.58
2:A:810:Y01:HAA3	1:D:494:CYS:HB3	1.84	0.58
1:B:536:LEU:HD21	1:B:543:GLY:HA3	1.86	0.58
1:D:536:LEU:HD21	1:D:543:GLY:HA3	1.86	0.58
1:A:402:VAL:HG21	2:A:801:Y01:HAK1	1.86	0.57
1:A:497:MET:HE3	2:B:701:Y01:HBA	1.86	0.57
1:C:428:LEU:HD21	2:C:704:Y01:HAK2	1.85	0.57
1:A:536:LEU:HD21	1:A:543:GLY:HA3	1.86	0.57
1:A:489:ASP:OD1	1:A:492:ARG:NH1	2.37	0.57
1:B:494:CYS:HB3	2:C:701:Y01:HAA3	1.86	0.57
1:D:489:ASP:OD1	1:D:492:ARG:NH1	2.37	0.57
1:B:54:LYS:O	1:B:91:ASN:ND2	2.38	0.56
1:B:497:MET:HE3	2:C:701:Y01:HBA	1.86	0.56
1:C:54:LYS:O	1:C:91:ASN:ND2	2.38	0.56
1:C:536:LEU:HD21	1:C:543:GLY:HA3	1.86	0.56
1:B:489:ASP:OD1	1:B:492:ARG:NH1	2.37	0.56
1:D:424:PRO:CG	2:D:707:Y01:HAR1	2.35	0.56
2:B:704:Y01:HAE2	2:B:704:Y01:CAC	2.36	0.55
1:D:54:LYS:O	1:D:91:ASN:ND2	2.39	0.55
2:A:810:Y01:HBA	1:D:497:MET:HE3	1.88	0.55
2:C:704:Y01:HAV1	2:C:704:Y01:HAM2	1.88	0.55
1:A:119:THR:HG23	1:A:121:LEU:H	1.72	0.55
1:B:119:THR:HG23	1:B:121:LEU:H	1.72	0.55
1:A:54:LYS:O	1:A:91:ASN:ND2	2.38	0.55
1:C:119:THR:HG23	1:C:121:LEU:H	1.72	0.55
1:D:119:THR:HG23	1:D:121:LEU:H	1.72	0.55
4:B:709:POV:H217	2:D:704:Y01:HAA2	1.88	0.55
4:A:807:POV:H217	2:C:701:Y01:HAA2	1.89	0.55
2:B:701:Y01:HAA2	4:D:701:POV:H217	1.89	0.55
1:D:402:VAL:CG2	2:D:706:Y01:HAK1	2.37	0.55
1:C:463:CYS:CB	2:C:704:Y01:HAQ2	2.37	0.54
1:C:267:GLN:HE21	1:C:277:LEU:HD22	1.72	0.54
1:D:267:GLN:HE21	1:D:277:LEU:HD22	1.72	0.54
1:A:586:ALA:HA	1:A:589:ARG:HG3	1.90	0.54
1:D:116:GLU:H	1:D:149:GLY:HA3	1.73	0.54
1:D:586:ALA:HA	1:D:589:ARG:HG3	1.90	0.54
1:A:365:ASN:ND2	1:B:519:GLU:OE1	2.40	0.54
1:B:116:GLU:H	1:B:149:GLY:HA3	1.73	0.54
1:D:119:THR:H	1:D:122:HIS:HD2	1.56	0.54
1:A:267:GLN:HE21	1:A:277:LEU:HD22	1.72	0.54
1:B:586:ALA:HA	1:B:589:ARG:HG3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:GLU:H	1:C:149:GLY:HA3	1.73	0.54
1:C:586:ALA:HA	1:C:589:ARG:HG3	1.90	0.54
2:A:810:Y01:HAA2	4:C:709:POV:H217	1.89	0.54
1:B:267:GLN:HE21	1:B:277:LEU:HD22	1.72	0.54
1:A:119:THR:H	1:A:122:HIS:HD2	1.56	0.53
1:C:119:THR:H	1:C:122:HIS:HD2	1.56	0.53
1:A:116:GLU:H	1:A:149:GLY:HA3	1.73	0.53
1:A:519:GLU:OE1	1:D:365:ASN:ND2	2.42	0.53
1:B:403:GLU:OE2	1:B:607:LYS:NZ	2.42	0.53
1:D:403:GLU:OE2	1:D:607:LYS:NZ	2.42	0.53
1:B:365:ASN:ND2	1:C:519:GLU:OE1	2.42	0.53
1:A:459:VAL:HG11	2:A:802:Y01:HAN1	1.89	0.53
1:B:402:VAL:CG2	2:B:703:Y01:HAK1	2.38	0.53
1:B:483:GLN:HB2	2:B:704:Y01:CAY	2.38	0.53
1:C:403:GLU:OE2	1:C:607:LYS:NZ	2.42	0.53
1:D:441:VAL:HG21	4:D:711:POV:H37A	1.91	0.53
1:A:403:GLU:OE2	1:A:607:LYS:NZ	2.42	0.53
1:D:459:VAL:HG11	2:D:707:Y01:HAN1	1.90	0.53
1:A:402:VAL:CG2	2:A:801:Y01:HAK1	2.38	0.53
1:B:474:MET:HE1	1:C:491:MET:HE3	1.92	0.53
1:A:441:VAL:HG21	4:A:806:POV:H37A	1.90	0.52
1:A:486:ILE:HA	1:A:490:LEU:HB3	1.92	0.52
1:B:119:THR:H	1:B:122:HIS:HD2	1.56	0.52
1:C:355:ARG:NH2	1:C:364:ASP:OD2	2.40	0.52
1:B:581:THR:HG21	1:C:575:ILE:HG21	1.91	0.52
1:B:326:ARG:NH1	1:B:471:GLY:O	2.43	0.52
1:B:441:VAL:HG21	4:B:708:POV:H37A	1.90	0.52
2:B:704:Y01:CAE	1:C:565:ILE:HD11	2.35	0.52
1:D:486:ILE:HA	1:D:490:LEU:HB3	1.92	0.52
1:A:355:ARG:NH2	1:A:364:ASP:OD2	2.40	0.52
1:D:355:ARG:NH2	1:D:364:ASP:OD2	2.40	0.52
1:D:326:ARG:NH1	1:D:471:GLY:O	2.43	0.52
1:A:326:ARG:NH1	1:A:471:GLY:O	2.43	0.51
1:C:326:ARG:NH1	1:C:471:GLY:O	2.43	0.51
1:D:198:THR:H	1:D:201:HIS:HD2	1.59	0.51
1:D:581:THR:O	1:D:586:ALA:N	2.44	0.51
1:A:466:MET:HE3	2:A:802:Y01:HAI	1.92	0.51
1:A:391:VAL:HG13	2:A:801:Y01:HAA3	1.91	0.51
1:C:198:THR:H	1:C:201:HIS:HD2	1.59	0.51
1:B:198:THR:H	1:B:201:HIS:HD2	1.59	0.51
2:C:704:Y01:HAM2	2:C:704:Y01:CAV	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:THR:H	1:A:201:HIS:HD2	1.59	0.50
1:B:486:ILE:HA	1:B:490:LEU:HB3	1.92	0.50
1:A:581:THR:O	1:A:586:ALA:N	2.44	0.50
2:B:704:Y01:HAM2	2:B:704:Y01:HAV1	1.93	0.50
1:C:486:ILE:HA	1:C:490:LEU:HB3	1.92	0.50
1:B:391:VAL:HG13	2:B:703:Y01:HAA3	1.93	0.50
1:B:520:LEU:HD11	1:B:544:PRO:HB3	1.94	0.50
1:B:581:THR:O	1:B:586:ALA:N	2.44	0.50
1:A:42:LYS:HD2	1:D:623:TYR:HA	1.94	0.50
1:C:520:LEU:HD11	1:C:544:PRO:HB3	1.94	0.50
1:B:171:ALA:HB1	1:B:203:LEU:HD21	1.94	0.50
1:C:424:PRO:HG3	2:C:704:Y01:HAR1	1.93	0.50
1:C:581:THR:O	1:C:586:ALA:N	2.44	0.50
1:C:332:LEU:HD21	2:C:703:Y01:HAD2	1.94	0.49
1:D:171:ALA:HB1	1:D:203:LEU:HD21	1.94	0.49
1:D:391:VAL:HG13	2:D:706:Y01:HAA3	1.93	0.49
2:C:704:Y01:CAE	2:C:704:Y01:CAC	2.90	0.49
1:D:520:LEU:HD11	1:D:544:PRO:HB3	1.94	0.49
1:B:424:PRO:CG	2:B:704:Y01:HAR1	2.42	0.49
1:C:426:HIS:CG	2:C:703:Y01:HAL1	2.47	0.49
1:B:355:ARG:NH2	1:B:364:ASP:OD2	2.40	0.49
1:C:425:PHE:CZ	2:C:704:Y01:HAV1	2.47	0.49
2:A:810:Y01:OAG	2:A:810:Y01:HAV1	2.13	0.49
1:B:623:TYR:HA	1:C:42:LYS:HD2	1.93	0.49
4:C:709:POV:H25	4:C:709:POV:H32	1.95	0.49
2:C:704:Y01:HAC2	2:C:704:Y01:HAE3	1.95	0.49
2:D:704:Y01:OAG	2:D:704:Y01:HAV1	2.13	0.49
1:A:520:LEU:HD11	1:A:544:PRO:HB3	1.94	0.49
2:A:802:Y01:HAU2	2:A:802:Y01:HAC1	1.95	0.49
1:A:171:ALA:HB1	1:A:203:LEU:HD21	1.94	0.48
1:C:171:ALA:HB1	1:C:203:LEU:HD21	1.94	0.48
1:C:497:MET:HE3	2:D:704:Y01:HBA	1.94	0.48
4:A:807:POV:H217	2:C:701:Y01:CAA	2.43	0.48
2:B:701:Y01:CAA	4:D:701:POV:H217	2.43	0.48
1:C:341:ILE:HG12	4:C:709:POV:H37	1.95	0.48
1:D:495:TRP:CE2	3:D:708:PCW:H20	2.48	0.48
2:D:707:Y01:HAC1	2:D:707:Y01:HAU2	1.94	0.48
1:B:341:ILE:HG12	4:B:709:POV:H37	1.96	0.48
1:B:495:TRP:CE2	3:B:705:PCW:H20	2.49	0.48
1:C:474:MET:HE1	1:D:491:MET:HE3	1.95	0.48
4:D:701:POV:H25	4:D:701:POV:H32	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:THR:O	1:C:214:GLN:NE2	2.47	0.48
1:D:210:THR:O	1:D:214:GLN:NE2	2.47	0.48
1:A:210:THR:O	1:A:214:GLN:NE2	2.47	0.48
2:A:810:Y01:CAA	4:C:709:POV:H217	2.43	0.48
1:B:210:THR:O	1:B:214:GLN:NE2	2.47	0.48
1:C:399:ILE:HG12	2:C:703:Y01:HBG	1.96	0.48
2:D:707:Y01:HAM2	2:D:707:Y01:HBC	1.45	0.48
4:B:709:POV:H32	4:B:709:POV:H25	1.95	0.48
2:C:703:Y01:HAB1	2:C:703:Y01:HAJ2	1.73	0.48
2:B:701:Y01:OAG	2:B:701:Y01:HAV1	2.13	0.47
2:C:704:Y01:HAN1	2:C:704:Y01:HBB	1.37	0.47
4:C:709:POV:H31B	4:C:709:POV:H21C	1.96	0.47
4:A:811:POV:C214	2:D:707:Y01:HAC3	2.43	0.47
4:B:709:POV:H217	2:D:704:Y01:CAA	2.44	0.47
1:C:618:ILE:HD11	1:D:34:ASP:HB3	1.96	0.47
1:C:441:VAL:HG21	4:C:708:POV:H37A	1.96	0.47
4:D:703:POV:H35	4:D:703:POV:H32A	1.59	0.47
1:A:495:TRP:CE2	3:A:803:PCW:H20	2.50	0.47
2:A:802:Y01:HAC3	4:B:702:POV:C214	2.44	0.47
4:A:807:POV:H25	4:A:807:POV:H32	1.96	0.47
1:C:190:ARG:HH22	1:C:230:GLN:HB2	1.80	0.47
2:C:704:Y01:HAC2	2:C:704:Y01:HAE2	1.96	0.47
2:C:701:Y01:HAV1	2:C:701:Y01:OAG	2.14	0.47
4:C:711:POV:H210	4:C:711:POV:H213	1.70	0.47
1:D:341:ILE:HG12	4:D:701:POV:H37	1.96	0.47
1:D:190:ARG:HH22	1:D:230:GLN:HB2	1.80	0.47
4:B:709:POV:H21C	4:B:709:POV:H31B	1.96	0.46
4:D:701:POV:H21C	4:D:701:POV:H31B	1.97	0.46
1:A:341:ILE:HG12	4:A:807:POV:H37	1.97	0.46
4:A:807:POV:H31B	4:A:807:POV:H21C	1.97	0.46
4:B:711:POV:H210	4:B:711:POV:H213	1.69	0.46
1:C:495:TRP:CE2	3:C:705:PCW:H20	2.50	0.46
1:C:391:VAL:HG13	2:C:703:Y01:HAA3	1.97	0.46
1:D:520:LEU:HD21	1:D:544:PRO:HB3	1.98	0.46
1:A:190:ARG:HH22	1:A:230:GLN:HB2	1.80	0.46
1:C:520:LEU:HD21	1:C:544:PRO:HB3	1.98	0.46
1:B:520:LEU:HD21	1:B:544:PRO:HB3	1.98	0.46
2:D:706:Y01:HAB1	2:D:706:Y01:HAJ2	1.74	0.46
1:A:520:LEU:HD21	1:A:544:PRO:HB3	1.98	0.46
1:B:190:ARG:HH22	1:B:230:GLN:HB2	1.80	0.46
1:B:425:PHE:CZ	2:B:704:Y01:HAV1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:270:TYR:CZ	1:D:126:VAL:HG21	2.51	0.46
1:C:581:THR:HG21	1:D:575:ILE:HG21	1.97	0.46
1:A:565:ILE:HD11	2:D:707:Y01:HAE3	1.98	0.45
1:C:106:VAL:HG13	1:C:136:LEU:HD22	1.98	0.45
1:C:423:GLY:HA3	2:C:703:Y01:CAX	2.46	0.45
1:A:283:ILE:HG23	1:A:292:LEU:HD23	1.98	0.45
1:A:491:MET:HE3	1:D:474:MET:HE1	1.97	0.45
1:A:623:TYR:HA	1:B:42:LYS:HD2	1.99	0.45
2:A:801:Y01:HAB1	2:A:801:Y01:HAJ2	1.74	0.45
4:A:804:POV:H312	4:A:804:POV:H39A	1.70	0.45
1:A:106:VAL:HG13	1:A:136:LEU:HD22	1.98	0.45
1:B:466:MET:HG3	1:C:499:VAL:HG11	1.98	0.45
2:A:802:Y01:HAC3	4:B:702:POV:H21D	1.99	0.45
4:A:809:POV:H35	4:A:809:POV:H32A	1.59	0.45
2:B:704:Y01:CAC	2:B:704:Y01:CAE	2.94	0.45
1:A:399:ILE:HG12	2:A:801:Y01:HBG	1.99	0.45
4:A:805:POV:H212	4:A:805:POV:H215	1.80	0.45
2:B:704:Y01:HAB1	4:C:702:POV:H21C	1.99	0.45
1:C:623:TYR:HA	1:D:42:LYS:HD2	1.98	0.45
1:D:106:VAL:HG13	1:D:136:LEU:HD22	1.98	0.45
1:D:192:GLN:HG2	1:D:198:THR:HG22	1.99	0.45
1:A:575:ILE:HG21	1:D:581:THR:HG21	1.99	0.45
1:D:283:ILE:HG23	1:D:292:LEU:HD23	1.98	0.45
1:B:283:ILE:HG23	1:B:292:LEU:HD23	1.98	0.44
1:B:399:ILE:HG12	2:B:703:Y01:HBG	2.00	0.44
4:D:710:POV:H215	4:D:710:POV:H212	1.80	0.44
1:A:180:ARG:NH2	1:A:222:TYR:OH	2.51	0.44
2:B:704:Y01:HAN1	2:B:704:Y01:HBB	1.49	0.44
1:C:192:GLN:HG2	1:C:198:THR:HG22	1.99	0.44
1:C:283:ILE:HG23	1:C:292:LEU:HD23	1.98	0.44
1:C:428:LEU:CD2	2:C:704:Y01:HAK2	2.47	0.44
2:C:704:Y01:HAC2	1:D:565:ILE:HD11	1.99	0.44
2:A:802:Y01:HAM2	2:A:802:Y01:HBC	1.37	0.44
4:B:702:POV:H34	4:B:702:POV:H37	1.71	0.44
1:D:466:MET:HE3	2:D:707:Y01:HAI	1.98	0.44
4:D:709:POV:H39A	4:D:709:POV:H312	1.70	0.44
2:B:701:Y01:HAB3	2:B:701:Y01:HAJ1	1.85	0.44
1:C:248:GLY:HA2	1:C:307:ILE:HD13	1.99	0.44
1:D:248:GLY:HA2	1:D:307:ILE:HD13	1.99	0.44
1:A:192:GLN:HG2	1:A:198:THR:HG22	1.99	0.44
1:C:198:THR:H	1:C:201:HIS:CD2	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:198:THR:H	1:D:201:HIS:CD2	2.36	0.44
1:A:198:THR:H	1:A:201:HIS:CD2	2.36	0.44
1:A:312:PRO:HG2	1:A:313:VAL:HG23	2.00	0.44
4:A:811:POV:H37	4:A:811:POV:H34	1.71	0.44
1:B:192:GLN:HG2	1:B:198:THR:HG22	1.99	0.44
1:B:280:LEU:HD22	1:B:631:LEU:HB2	2.00	0.44
1:D:399:ILE:HG12	2:D:706:Y01:HBG	1.99	0.44
1:A:280:LEU:HD22	1:A:631:LEU:HB2	2.00	0.44
1:A:499:VAL:HG11	1:D:466:MET:HG3	2.00	0.44
1:B:106:VAL:HG13	1:B:136:LEU:HD22	1.98	0.44
1:B:248:GLY:HA3	1:B:292:LEU:HD11	2.00	0.44
1:C:248:GLY:HA3	1:C:292:LEU:HD11	2.00	0.44
1:C:428:LEU:HD21	2:C:704:Y01:HBF	2.00	0.44
4:C:711:POV:H211	4:C:711:POV:H28A	1.76	0.44
1:B:180:ARG:NH2	1:B:222:TYR:OH	2.51	0.43
1:D:312:PRO:HG2	1:D:313:VAL:HG23	2.00	0.43
1:A:248:GLY:HA2	1:A:307:ILE:HD13	1.99	0.43
1:A:474:MET:HE1	1:B:491:MET:HE3	2.00	0.43
1:C:312:PRO:HG2	1:C:313:VAL:HG23	2.00	0.43
1:B:312:PRO:HG2	1:B:313:VAL:HG23	2.00	0.43
4:B:711:POV:H32A	4:B:711:POV:H35	1.59	0.43
1:C:180:ARG:NH2	1:C:222:TYR:OH	2.51	0.43
1:D:180:ARG:NH2	1:D:222:TYR:OH	2.51	0.43
1:D:280:LEU:HD22	1:D:631:LEU:HB2	2.00	0.43
4:B:707:POV:H212	4:B:707:POV:H215	1.79	0.43
4:B:708:POV:H34A	4:B:708:POV:H37	1.86	0.43
1:B:248:GLY:HA2	1:B:307:ILE:HD13	1.99	0.43
4:B:706:POV:H312	4:B:706:POV:H39A	1.70	0.43
1:C:280:LEU:HD22	1:C:631:LEU:HB2	2.00	0.43
1:B:262:LYS:HD2	1:B:263:ARG:HE	1.84	0.42
1:A:63:LYS:HG3	1:A:67:TYR:HE2	1.85	0.42
1:A:248:GLY:HA3	1:A:292:LEU:HD11	2.00	0.42
1:B:63:LYS:HG3	1:B:67:TYR:HE2	1.85	0.42
4:C:708:POV:H34A	4:C:708:POV:H37	1.89	0.42
2:C:704:Y01:CAC	2:C:704:Y01:HAE3	2.49	0.42
4:C:711:POV:H32A	4:C:711:POV:H35	1.65	0.42
1:A:581:THR:HG21	1:B:575:ILE:HG21	2.00	0.42
4:A:811:POV:H21D	2:D:707:Y01:HAC3	2.01	0.42
2:B:704:Y01:HAJ2	2:B:704:Y01:HAB1	1.71	0.42
2:C:704:Y01:HAE3	1:D:565:ILE:HD11	2.02	0.42
1:D:248:GLY:HA3	1:D:292:LEU:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:LYS:HD2	1:A:263:ARG:HE	1.84	0.42
1:B:527:PRO:HB3	2:C:701:Y01:HAD2	2.01	0.42
2:A:802:Y01:HAE3	1:B:565:ILE:HD11	2.02	0.42
2:B:704:Y01:HAM2	2:B:704:Y01:HBC	1.67	0.42
1:D:63:LYS:HG3	1:D:67:TYR:HE2	1.85	0.42
4:D:701:POV:H23	4:D:701:POV:H26	1.92	0.42
1:A:466:MET:HG3	1:B:499:VAL:HG11	2.02	0.41
1:B:253:THR:HG22	1:B:307:ILE:HG13	2.03	0.41
1:C:63:LYS:HG3	1:C:67:TYR:HE2	1.85	0.41
1:D:262:LYS:HD2	1:D:263:ARG:HE	1.84	0.41
4:D:703:POV:H28A	4:D:703:POV:H211	1.78	0.41
1:C:382:ASP:OD1	1:C:385:ARG:NH2	2.47	0.41
1:C:477:PRO:HB3	1:C:589:ARG:HB3	2.02	0.41
1:C:368:LEU:HB2	1:D:514:THR:HA	2.03	0.41
2:A:810:Y01:HAD2	1:D:527:PRO:HB3	2.01	0.41
2:B:704:Y01:CAB	4:C:702:POV:H21C	2.50	0.41
1:A:459:VAL:CG1	2:A:802:Y01:HAP2	2.50	0.41
1:A:527:PRO:HB3	2:B:701:Y01:HAD2	2.01	0.41
1:B:477:PRO:HB3	1:B:589:ARG:HB3	2.02	0.41
1:C:262:LYS:HD2	1:C:263:ARG:HE	1.84	0.41
1:C:334:ALA:HB2	4:C:710:POV:H28	2.02	0.41
1:C:466:MET:HG3	1:D:499:VAL:HG11	2.03	0.41
1:D:253:THR:HG22	1:D:307:ILE:HG13	2.02	0.41
4:A:807:POV:H24A	1:B:527:PRO:HG3	2.03	0.41
1:B:198:THR:H	1:B:201:HIS:CD2	2.36	0.41
1:B:493:PHE:HB2	1:B:573:LEU:HD13	2.03	0.41
1:C:253:THR:HG22	1:C:307:ILE:HG13	2.03	0.41
1:C:381:LYS:HG2	4:C:711:POV:H1	2.03	0.41
2:D:704:Y01:HAB3	2:D:704:Y01:HAJ1	1.85	0.41
1:A:253:THR:HG22	1:A:307:ILE:HG13	2.03	0.41
2:A:810:Y01:HAB3	2:A:810:Y01:HAJ1	1.85	0.41
2:B:704:Y01:HAM2	2:B:704:Y01:CAV	2.36	0.41
1:A:125:VAL:HG22	1:A:178:ILE:HG21	2.04	0.40
4:A:809:POV:H213	4:A:809:POV:H210	1.69	0.40
1:C:425:PHE:HB2	2:C:703:Y01:HAL2	2.03	0.40
4:C:707:POV:H215	4:C:707:POV:H212	1.80	0.40
1:D:280:LEU:HD11	1:D:316:LEU:HD13	2.04	0.40
1:B:125:VAL:HG22	1:B:178:ILE:HG21	2.04	0.40
4:C:702:POV:H34	4:C:702:POV:H37	1.70	0.40
1:A:477:PRO:HB3	1:A:589:ARG:HB3	2.02	0.40
1:A:493:PHE:HB2	1:A:573:LEU:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:VAL:HG22	1:C:178:ILE:HG21	2.04	0.40
1:C:280:LEU:HD11	1:C:316:LEU:HD13	2.04	0.40
1:D:44:ILE:HG21	1:D:54:LYS:HD2	2.03	0.40
1:A:527:PRO:HG3	4:D:701:POV:H24A	2.04	0.40
1:C:483:GLN:HB2	2:C:704:Y01:CAY	2.52	0.40
1:D:477:PRO:HB3	1:D:589:ARG:HB3	2.02	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	610/683 (89%)	580 (95%)	30 (5%)	0	100	100
1	B	610/683 (89%)	581 (95%)	29 (5%)	0	100	100
1	C	610/683 (89%)	580 (95%)	30 (5%)	0	100	100
1	D	610/683 (89%)	580 (95%)	30 (5%)	0	100	100
All	All	2440/2732 (89%)	2321 (95%)	119 (5%)	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	531/593 (90%)	528 (99%)	3 (1%)	78	85
1	B	531/593 (90%)	528 (99%)	3 (1%)	78	85
1	C	531/593 (90%)	528 (99%)	3 (1%)	78	85
1	D	531/593 (90%)	528 (99%)	3 (1%)	78	85
All	All	2124/2372 (90%)	2112 (99%)	12 (1%)	76	85

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	365	ASN
1	A	458	LEU
1	A	549	VAL
1	B	365	ASN
1	B	458	LEU
1	B	549	VAL
1	C	365	ASN
1	C	458	LEU
1	C	549	VAL
1	D	365	ASN
1	D	458	LEU
1	D	549	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	62	ASN
1	A	91	ASN
1	A	122	HIS
1	A	267	GLN
1	A	290	GLN
1	A	365	ASN
1	A	369	GLN
1	A	596	GLN
1	B	37	ASN
1	B	56	ASN
1	B	62	ASN
1	B	84	HIS
1	B	91	ASN
1	B	122	HIS

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Mol	Chain	Res	Type
1	B	290	GLN
1	B	365	ASN
1	B	596	GLN
1	C	37	ASN
1	C	56	ASN
1	C	62	ASN
1	C	91	ASN
1	C	122	HIS
1	C	290	GLN
1	C	365	ASN
1	C	596	GLN
1	D	37	ASN
1	D	62	ASN
1	D	91	ASN
1	D	122	HIS
1	D	267	GLN
1	D	290	GLN
1	D	365	ASN
1	D	369	GLN
1	D	596	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 46 ligands modelled in this entry, 1 is monoatomic - leaving 45 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	$\#\|Z\| > 2$
4	POV	B	708	-	15,15,51	1.07	1 (6%)	15,15,59	1.00	1 (6%)
4	POV	C	706	-	12,12,51	0.68	0	11,11,59	0.41	0
2	Y01	C	701	-	38,38,38	0.46	0	57,57,57	0.49	0
2	Y01	D	704	-	38,38,38	0.46	0	57,57,57	0.48	0
3	PCW	C	705	-	12,12,53	0.93	0	11,11,61	0.32	0
3	PCW	A	803	-	12,12,53	0.93	0	11,11,61	0.32	0
4	POV	A	808	-	41,41,51	1.15	3 (7%)	47,49,59	1.02	3 (6%)
4	POV	C	707	-	18,18,51	1.41	2 (11%)	18,18,59	0.90	1 (5%)
4	POV	C	708	-	15,15,51	1.07	1 (6%)	15,15,59	1.00	1 (6%)
4	POV	A	811	-	51,51,51	1.07	3 (5%)	57,59,59	0.91	3 (5%)
4	POV	D	705	-	51,51,51	1.07	3 (5%)	57,59,59	0.92	3 (5%)
3	PCW	B	705	-	12,12,53	0.93	0	11,11,61	0.32	0
4	POV	C	702	-	51,51,51	1.07	3 (5%)	57,59,59	0.89	3 (5%)
4	POV	B	707	-	18,18,51	1.42	2 (11%)	18,18,59	0.87	1 (5%)
4	POV	B	709	-	51,51,51	1.04	4 (7%)	57,59,59	1.00	3 (5%)
4	POV	A	804	-	12,12,51	0.68	0	11,11,59	0.44	0
2	Y01	B	703	-	38,38,38	0.46	0	57,57,57	0.55	0
4	POV	B	706	-	12,12,51	0.67	0	11,11,59	0.43	0
2	Y01	A	802	-	38,38,38	0.44	0	57,57,57	0.73	0
4	POV	A	807	-	51,51,51	1.03	3 (5%)	57,59,59	1.00	3 (5%)
6	R2R	A	813	-	14,18,18	4.31	14 (100%)	-		
4	POV	A	805	-	18,18,51	1.42	2 (11%)	18,18,59	0.87	1 (5%)
4	POV	C	710	-	41,41,51	1.14	3 (7%)	47,49,59	1.04	3 (6%)
2	Y01	C	703	-	38,38,38	0.46	0	57,57,57	0.57	0
2	Y01	C	704	-	38,38,38	0.52	0	57,57,57	1.06	3 (5%)
4	POV	C	709	-	51,51,51	1.03	3 (5%)	57,59,59	0.99	3 (5%)
4	POV	A	806	-	15,15,51	1.07	1 (6%)	15,15,59	1.00	1 (6%)
4	POV	D	710	-	18,18,51	1.41	2 (11%)	18,18,59	0.87	1 (5%)
4	POV	B	711	-	51,51,51	1.10	3 (5%)	57,59,59	0.99	4 (7%)
2	Y01	A	801	-	38,38,38	0.45	0	57,57,57	0.55	0
4	POV	C	711	-	51,51,51	1.09	3 (5%)	57,59,59	0.96	4 (7%)
4	POV	D	711	-	15,15,51	1.08	1 (6%)	15,15,59	1.00	1 (6%)
2	Y01	B	704	-	38,38,38	0.49	0	57,57,57	0.97	5 (8%)
4	POV	D	703	-	51,51,51	1.09	3 (5%)	57,59,59	0.99	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	Y01	A	810	-	38,38,38	0.46	0	57,57,57	0.48	0
2	Y01	D	706	-	38,38,38	0.46	0	57,57,57	0.55	0
2	Y01	B	701	-	38,38,38	0.45	0	57,57,57	0.48	0
4	POV	B	710	-	41,41,51	1.14	3 (7%)	47,49,59	1.02	3 (6%)
4	POV	B	702	-	51,51,51	1.07	3 (5%)	57,59,59	0.90	3 (5%)
4	POV	D	701	-	51,51,51	1.04	3 (5%)	57,59,59	1.00	3 (5%)
4	POV	D	702	-	41,41,51	1.15	3 (7%)	47,49,59	1.02	3 (6%)
4	POV	D	709	-	12,12,51	0.67	0	11,11,59	0.43	0
3	PCW	D	708	-	12,12,53	0.93	0	11,11,61	0.27	0
2	Y01	D	707	-	38,38,38	0.44	0	57,57,57	0.73	1 (1%)
4	POV	A	809	-	51,51,51	1.09	4 (7%)	57,59,59	0.99	4 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	POV	B	708	-	-	7/14/14/55	-
4	POV	C	706	-	-	8/10/10/55	-
2	Y01	C	701	-	-	8/19/77/77	0/4/4/4
2	Y01	D	704	-	-	8/19/77/77	0/4/4/4
3	PCW	C	705	-	-	5/10/10/57	-
3	PCW	A	803	-	-	5/10/10/57	-
4	POV	A	808	-	-	27/45/45/55	-
4	POV	C	707	-	-	10/17/17/55	-
4	POV	C	708	-	-	7/14/14/55	-
4	POV	A	811	-	-	24/55/55/55	-
4	POV	D	705	-	-	25/55/55/55	-
3	PCW	B	705	-	-	5/10/10/57	-
4	POV	C	702	-	-	23/55/55/55	-
4	POV	B	707	-	-	10/17/17/55	-
4	POV	B	709	-	-	34/55/55/55	-
4	POV	A	804	-	-	8/10/10/55	-
2	Y01	B	703	-	-	9/19/77/77	0/4/4/4
4	POV	B	706	-	-	8/10/10/55	-
2	Y01	A	802	-	-	9/19/77/77	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	POV	A	807	-	-	34/55/55/55	-
4	POV	A	805	-	-	10/17/17/55	-
4	POV	C	710	-	-	27/45/45/55	-
2	Y01	C	703	-	-	10/19/77/77	0/4/4/4
2	Y01	C	704	-	-	13/19/77/77	0/4/4/4
4	POV	C	709	-	-	34/55/55/55	-
4	POV	A	806	-	-	7/14/14/55	-
4	POV	D	710	-	-	10/17/17/55	-
4	POV	B	711	-	-	32/55/55/55	-
2	Y01	A	801	-	-	9/19/77/77	0/4/4/4
4	POV	C	711	-	-	32/55/55/55	-
4	POV	D	711	-	-	7/14/14/55	-
2	Y01	B	704	-	-	13/19/77/77	0/4/4/4
4	POV	D	703	-	-	32/55/55/55	-
2	Y01	A	810	-	-	8/19/77/77	0/4/4/4
2	Y01	D	706	-	-	9/19/77/77	0/4/4/4
2	Y01	B	701	-	-	8/19/77/77	0/4/4/4
4	POV	B	710	-	-	27/45/45/55	-
4	POV	B	702	-	-	24/55/55/55	-
4	POV	D	701	-	-	34/55/55/55	-
4	POV	D	702	-	-	27/45/45/55	-
4	POV	D	709	-	-	8/10/10/55	-
3	PCW	D	708	-	-	6/10/10/57	-
2	Y01	D	707	-	-	8/19/77/77	0/4/4/4
4	POV	A	809	-	-	32/55/55/55	-

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	813	R2R	RU2-N01	-5.56	2.04	2.11
6	A	813	R2R	RU2-N05	-5.45	2.04	2.11
6	A	813	R2R	RU2-N03	-5.29	2.04	2.11
6	A	813	R2R	RU2-N04	-5.26	2.04	2.11
4	A	805	POV	C29-C210	4.19	1.55	1.31
4	D	710	POV	C29-C210	4.18	1.55	1.31
4	B	707	POV	C29-C210	4.18	1.55	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	707	POV	C29-C210	4.17	1.55	1.31
6	A	813	R2R	RU3-N12	-3.88	2.04	2.10
6	A	813	R2R	RU1-N17	-3.87	2.04	2.10
6	A	813	R2R	RU1-N18	-3.86	2.04	2.10
6	A	813	R2R	RU3-N10	-3.85	2.04	2.10
6	A	813	R2R	RU3-N08	-3.80	2.04	2.10
6	A	813	R2R	RU1-N19	-3.80	2.04	2.10
6	A	813	R2R	RU3-N09	-3.76	2.04	2.10
6	A	813	R2R	RU3-N11	-3.75	2.04	2.10
6	A	813	R2R	RU1-N15	-3.74	2.04	2.10
6	A	813	R2R	RU1-N16	-3.69	2.04	2.10
4	D	711	POV	O31-C31	2.86	1.41	1.33
4	A	808	POV	O21-C21	2.84	1.42	1.34
4	D	702	POV	O21-C21	2.82	1.42	1.34
4	A	806	POV	O31-C31	2.82	1.41	1.33
4	B	708	POV	O31-C31	2.82	1.41	1.33
4	A	807	POV	O21-C2	-2.82	1.40	1.46
4	D	701	POV	O21-C2	-2.82	1.40	1.46
4	B	710	POV	O21-C21	2.81	1.42	1.34
4	C	710	POV	O21-C21	2.81	1.42	1.34
4	C	708	POV	O31-C31	2.81	1.41	1.33
4	C	711	POV	O21-C2	-2.79	1.40	1.46
4	C	709	POV	O21-C2	-2.79	1.40	1.46
4	D	703	POV	O21-C2	-2.79	1.40	1.46
4	B	702	POV	O21-C21	2.78	1.42	1.34
4	A	809	POV	O21-C2	-2.77	1.40	1.46
4	B	711	POV	O21-C2	-2.77	1.40	1.46
4	C	702	POV	O31-C31	2.76	1.41	1.33
4	D	705	POV	O31-C31	2.76	1.41	1.33
4	B	709	POV	O21-C2	-2.75	1.40	1.46
4	A	811	POV	O21-C21	2.74	1.42	1.34
4	D	705	POV	O21-C21	2.74	1.42	1.34
4	A	805	POV	O21-C21	2.74	1.41	1.33
4	B	707	POV	O21-C21	2.74	1.41	1.33
4	D	710	POV	O21-C21	2.74	1.41	1.33
4	C	702	POV	O21-C21	2.73	1.42	1.34
4	C	707	POV	O21-C21	2.72	1.41	1.33
4	A	811	POV	O31-C31	2.72	1.41	1.33
4	B	702	POV	O31-C31	2.72	1.41	1.33
4	B	711	POV	O31-C31	2.72	1.41	1.33
4	D	703	POV	O31-C31	2.71	1.41	1.33
4	C	711	POV	O21-C21	2.71	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	711	POV	O31-C31	2.70	1.41	1.33
4	D	703	POV	O21-C21	2.70	1.41	1.34
4	B	711	POV	O21-C21	2.70	1.41	1.34
4	A	809	POV	O31-C31	2.70	1.41	1.33
4	A	809	POV	O21-C21	2.67	1.41	1.34
4	A	808	POV	O21-C2	-2.66	1.40	1.46
4	B	710	POV	O21-C2	-2.63	1.40	1.46
4	D	702	POV	O21-C2	-2.63	1.40	1.46
4	C	710	POV	O21-C2	-2.63	1.40	1.46
4	A	808	POV	O31-C31	2.55	1.40	1.33
4	C	702	POV	O21-C2	-2.55	1.40	1.46
4	D	705	POV	O21-C2	-2.54	1.40	1.46
4	C	710	POV	O31-C31	2.54	1.40	1.33
4	B	702	POV	O21-C2	-2.53	1.40	1.46
4	B	709	POV	O31-C31	2.51	1.40	1.33
4	B	710	POV	O31-C31	2.50	1.40	1.33
4	A	807	POV	O31-C31	2.50	1.40	1.33
4	D	702	POV	O31-C31	2.50	1.40	1.33
4	A	811	POV	O21-C2	-2.49	1.40	1.46
4	D	701	POV	O31-C31	2.48	1.40	1.33
4	C	709	POV	O31-C31	2.43	1.40	1.33
4	C	709	POV	O21-C21	2.42	1.41	1.34
4	A	807	POV	O21-C21	2.39	1.41	1.34
4	B	709	POV	O21-C21	2.39	1.41	1.34
4	D	701	POV	O21-C21	2.39	1.41	1.34
4	A	809	POV	P-O12	2.01	1.67	1.59
4	B	709	POV	P-O12	2.00	1.67	1.59

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	703	POV	O21-C21-C22	3.89	119.90	111.48
4	B	711	POV	O21-C21-C22	3.88	119.87	111.48
4	A	809	POV	O21-C21-C22	3.87	119.85	111.48
4	C	710	POV	O21-C21-C22	3.75	119.59	111.48
4	A	808	POV	O21-C21-C22	3.73	119.54	111.48
4	D	702	POV	O21-C21-C22	3.71	119.50	111.48
4	B	710	POV	O21-C21-C22	3.70	119.49	111.48
4	B	709	POV	O21-C21-C22	3.70	119.49	111.48
4	D	701	POV	O21-C21-C22	3.70	119.49	111.48
4	D	705	POV	O21-C21-C22	3.69	119.47	111.48
4	A	811	POV	O21-C21-C22	3.67	119.43	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	807	POV	O21-C21-C22	3.67	119.42	111.48
4	C	709	POV	O21-C21-C22	3.63	119.34	111.48
4	B	702	POV	O21-C21-C22	3.59	119.25	111.48
4	C	711	POV	O21-C21-C22	3.56	119.19	111.48
4	C	702	POV	O21-C21-C22	3.47	118.98	111.48
4	C	708	POV	O31-C31-C32	2.89	120.63	111.83
4	B	708	POV	O31-C31-C32	2.87	120.60	111.83
4	D	711	POV	O31-C31-C32	2.87	120.59	111.83
4	A	806	POV	O31-C31-C32	2.87	120.57	111.83
4	C	711	POV	C14-N-C12	2.79	120.98	109.91
4	B	709	POV	O31-C31-C32	2.75	120.22	111.83
4	D	701	POV	O31-C31-C32	2.73	120.15	111.83
4	A	807	POV	O31-C31-C32	2.72	120.14	111.83
4	D	703	POV	C14-N-C12	2.72	120.73	109.91
4	B	711	POV	C14-N-C12	2.72	120.71	109.91
4	A	809	POV	C14-N-C12	2.71	120.69	109.91
4	A	811	POV	O31-C31-C32	2.70	120.06	111.83
4	B	702	POV	O31-C31-C32	2.70	120.06	111.83
4	D	705	POV	O31-C31-C32	2.69	120.05	111.83
4	C	702	POV	O31-C31-C32	2.69	120.03	111.83
4	A	807	POV	C14-N-C12	2.69	120.60	109.91
4	D	701	POV	C14-N-C12	2.68	120.58	109.91
4	C	710	POV	O31-C31-C32	2.68	120.00	111.83
4	B	709	POV	C14-N-C12	2.67	120.54	109.91
4	C	709	POV	C14-N-C12	2.66	120.48	109.91
4	A	809	POV	C2-O21-C21	-2.63	111.51	117.80
4	D	703	POV	C2-O21-C21	-2.61	111.54	117.80
2	C	704	Y01	CAP-CAQ-CBG	-2.61	100.03	105.14
4	B	711	POV	C2-O21-C21	-2.60	111.58	117.80
4	D	702	POV	O31-C31-C32	2.59	119.72	111.83
4	A	808	POV	O31-C31-C32	2.57	119.66	111.83
4	B	710	POV	O31-C31-C32	2.56	119.64	111.83
4	B	711	POV	O31-C31-C32	2.55	119.60	111.83
4	A	809	POV	O31-C31-C32	2.53	119.56	111.83
4	C	711	POV	O31-C31-C32	2.53	119.55	111.83
4	C	709	POV	O31-C31-C32	2.52	119.52	111.83
4	D	703	POV	O31-C31-C32	2.50	119.46	111.83
4	C	711	POV	C2-O21-C21	-2.43	111.99	117.80
4	D	702	POV	C14-N-C12	2.38	119.39	109.91
4	A	808	POV	C14-N-C12	2.37	119.35	109.91
4	B	710	POV	C14-N-C12	2.37	119.33	109.91
4	C	710	POV	C14-N-C12	2.37	119.31	109.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	704	Y01	CAT-CBH-CBF	2.33	111.82	108.74
2	C	704	Y01	CAC-CBB-CBE	2.31	116.35	112.88
2	B	704	Y01	CBI-CBE-CBB	2.30	123.06	119.50
2	B	704	Y01	CBF-CBH-CAZ	-2.29	106.30	109.65
4	B	702	POV	C14-N-C12	2.23	118.78	109.91
4	A	811	POV	C14-N-C12	2.23	118.77	109.91
4	C	702	POV	C14-N-C12	2.22	118.75	109.91
2	B	704	Y01	CBH-CBF-CBD	-2.22	109.47	112.71
4	D	705	POV	C14-N-C12	2.22	118.72	109.91
2	B	704	Y01	CAC-CBB-CBE	2.08	116.01	112.88
2	D	707	Y01	CBF-CBH-CAZ	-2.05	106.66	109.65
4	C	707	POV	O21-C21-C22	2.04	119.85	112.14
2	C	704	Y01	CBG-CBI-CBE	2.02	102.42	100.10
4	D	710	POV	O21-C21-C22	2.01	119.75	112.14
4	A	805	POV	O21-C21-C22	2.01	119.73	112.14
4	B	707	POV	O21-C21-C22	2.01	119.73	112.14

There are no chirality outliers.

All (701) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	802	Y01	OAG-CAY-OAW-CBC
2	A	802	Y01	CAM-CAY-OAW-CBC
2	B	704	Y01	OAG-CAY-OAW-CBC
2	B	704	Y01	CAM-CAY-OAW-CBC
2	C	704	Y01	OAG-CAY-OAW-CBC
2	C	704	Y01	CAM-CAY-OAW-CBC
2	D	707	Y01	OAG-CAY-OAW-CBC
2	D	707	Y01	CAM-CAY-OAW-CBC
4	A	807	POV	O12-C11-C12-N
4	A	808	POV	C1-O11-P-O12
4	A	808	POV	C1-O11-P-O13
4	A	808	POV	C11-O12-P-O11
4	A	808	POV	O12-C11-C12-N
4	A	808	POV	C22-C21-O21-C2
4	A	809	POV	C1-O11-P-O12
4	A	809	POV	C1-O11-P-O13
4	A	809	POV	C1-O11-P-O14
4	A	809	POV	C11-O12-P-O11
4	A	809	POV	C11-O12-P-O13
4	B	709	POV	O12-C11-C12-N
4	B	710	POV	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
4	B	710	POV	C1-O11-P-O13
4	B	710	POV	C11-O12-P-O11
4	B	710	POV	O12-C11-C12-N
4	B	710	POV	C22-C21-O21-C2
4	B	711	POV	C1-O11-P-O12
4	B	711	POV	C1-O11-P-O13
4	B	711	POV	C1-O11-P-O14
4	B	711	POV	C11-O12-P-O11
4	B	711	POV	C11-O12-P-O13
4	C	709	POV	O12-C11-C12-N
4	C	710	POV	C1-O11-P-O12
4	C	710	POV	C1-O11-P-O13
4	C	710	POV	C11-O12-P-O11
4	C	710	POV	O12-C11-C12-N
4	C	710	POV	C22-C21-O21-C2
4	C	711	POV	C1-O11-P-O12
4	C	711	POV	C1-O11-P-O13
4	C	711	POV	C11-O12-P-O11
4	C	711	POV	C11-O12-P-O13
4	D	701	POV	O12-C11-C12-N
4	D	702	POV	C1-O11-P-O12
4	D	702	POV	C1-O11-P-O13
4	D	702	POV	C11-O12-P-O11
4	D	702	POV	O12-C11-C12-N
4	D	702	POV	C22-C21-O21-C2
4	D	703	POV	C1-O11-P-O12
4	D	703	POV	C1-O11-P-O13
4	D	703	POV	C1-O11-P-O14
4	D	703	POV	C11-O12-P-O11
4	D	703	POV	C11-O12-P-O13
2	C	704	Y01	CAN-CAJ-CAO-CBB
2	A	810	Y01	CAV-CBC-OAW-CAY
2	B	701	Y01	CAV-CBC-OAW-CAY
2	C	701	Y01	CAV-CBC-OAW-CAY
2	D	704	Y01	CAV-CBC-OAW-CAY
2	B	704	Y01	CAN-CAJ-CAO-CBB
4	A	808	POV	O22-C21-O21-C2
4	B	710	POV	O22-C21-O21-C2
4	C	710	POV	O22-C21-O21-C2
4	D	702	POV	O22-C21-O21-C2
2	B	704	Y01	CAO-CBB-CBE-CAP
2	C	704	Y01	CAO-CBB-CBE-CAP

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Mol	Chain	Res	Type	Atoms
2	A	810	Y01	CAJ-CAO-CBB-CBE
4	A	811	POV	C32-C31-O31-C3
4	B	702	POV	C32-C31-O31-C3
4	C	702	POV	C32-C31-O31-C3
4	D	705	POV	C32-C31-O31-C3
2	B	701	Y01	CAJ-CAO-CBB-CBE
2	C	701	Y01	CAJ-CAO-CBB-CBE
2	C	704	Y01	CAJ-CAO-CBB-CBE
2	D	704	Y01	CAJ-CAO-CBB-CBE
4	A	804	POV	C39-C310-C311-C312
4	B	706	POV	C39-C310-C311-C312
4	C	706	POV	C39-C310-C311-C312
4	D	709	POV	C39-C310-C311-C312
2	A	810	Y01	CAJ-CAO-CBB-CAC
4	A	811	POV	O32-C31-O31-C3
4	B	702	POV	O32-C31-O31-C3
4	C	702	POV	O32-C31-O31-C3
4	D	705	POV	O32-C31-O31-C3
4	A	806	POV	C32-C31-O31-C3
4	B	708	POV	C32-C31-O31-C3
4	C	708	POV	C32-C31-O31-C3
4	D	711	POV	C32-C31-O31-C3
4	C	711	POV	C11-C12-N-C14
2	A	802	Y01	CAJ-CAO-CBB-CBE
2	A	801	Y01	CAX-CAL-CAM-CAY
2	B	701	Y01	CAJ-CAO-CBB-CAC
2	C	701	Y01	CAJ-CAO-CBB-CAC
2	D	704	Y01	CAJ-CAO-CBB-CAC
4	A	806	POV	O32-C31-O31-C3
4	B	708	POV	O32-C31-O31-C3
4	C	708	POV	O32-C31-O31-C3
4	D	711	POV	O32-C31-O31-C3
4	A	807	POV	O21-C2-C3-O31
4	B	709	POV	O21-C2-C3-O31
4	D	701	POV	O21-C2-C3-O31
2	B	704	Y01	CAO-CBB-CBE-CBI
4	D	703	POV	C32-C33-C34-C35
2	B	704	Y01	CAJ-CAO-CBB-CBE
2	D	707	Y01	CAJ-CAO-CBB-CBE
4	A	809	POV	C32-C33-C34-C35
2	B	703	Y01	CAX-CAL-CAM-CAY
2	D	706	Y01	CAX-CAL-CAM-CAY

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Mol	Chain	Res	Type	Atoms
4	B	711	POV	C32-C33-C34-C35
4	C	710	POV	C32-C33-C34-C35
2	B	704	Y01	CAC-CBB-CBE-CAP
4	A	809	POV	C11-C12-N-C14
4	B	711	POV	C11-C12-N-C14
4	C	711	POV	C11-C12-N-C13
4	D	703	POV	C11-C12-N-C14
4	A	805	POV	C21-C22-C23-C24
4	A	806	POV	C31-C32-C33-C34
4	B	707	POV	C21-C22-C23-C24
4	B	708	POV	C31-C32-C33-C34
4	C	707	POV	C21-C22-C23-C24
4	D	710	POV	C21-C22-C23-C24
2	B	704	Y01	CAO-CAJ-CAN-CBA
2	C	704	Y01	CAO-CBB-CBE-CBI
2	A	802	Y01	CAJ-CAO-CBB-CAC
4	D	711	POV	C31-C32-C33-C34
2	C	704	Y01	CAO-CAJ-CAN-CBA
2	C	704	Y01	CAC-CBB-CBE-CAP
4	C	708	POV	C31-C32-C33-C34
2	D	707	Y01	CAJ-CAO-CBB-CAC
4	A	805	POV	C211-C210-C29-C28
4	B	707	POV	C211-C210-C29-C28
4	C	707	POV	C211-C210-C29-C28
4	D	710	POV	C211-C210-C29-C28
2	C	701	Y01	CAO-CAJ-CAN-CBA
2	D	706	Y01	CAO-CAJ-CAN-CBA
4	A	807	POV	C11-C12-N-C14
4	A	807	POV	C11-C12-N-C15
4	A	809	POV	C11-C12-N-C13
4	B	709	POV	C11-C12-N-C14
4	B	709	POV	C11-C12-N-C15
4	B	711	POV	C11-C12-N-C13
4	C	709	POV	C11-C12-N-C14
4	C	709	POV	C11-C12-N-C15
4	D	701	POV	C11-C12-N-C14
4	D	701	POV	C11-C12-N-C15
4	D	703	POV	C11-C12-N-C13
2	B	701	Y01	CAO-CAJ-CAN-CBA
2	A	801	Y01	CAO-CAJ-CAN-CBA
2	B	703	Y01	CAO-CAJ-CAN-CBA
2	C	703	Y01	CAO-CAJ-CAN-CBA

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Mol	Chain	Res	Type	Atoms
2	D	704	Y01	CAO-CAJ-CAN-CBA
2	A	802	Y01	CAX-CAL-CAM-CAY
2	C	704	Y01	CAX-CAL-CAM-CAY
2	D	707	Y01	CAX-CAL-CAM-CAY
2	A	810	Y01	CAO-CAJ-CAN-CBA
4	A	809	POV	C210-C211-C212-C213
4	B	711	POV	C210-C211-C212-C213
4	C	711	POV	C210-C211-C212-C213
4	D	703	POV	C210-C211-C212-C213
2	B	704	Y01	CAX-CAL-CAM-CAY
4	A	807	POV	C11-C12-N-C13
4	B	709	POV	C11-C12-N-C13
4	C	709	POV	C11-C12-N-C13
4	D	701	POV	C11-C12-N-C13
3	A	803	PCW	C22-C23-C24-C25
3	B	705	PCW	C22-C23-C24-C25
4	B	710	POV	C212-C213-C214-C215
4	B	706	POV	C32-C33-C34-C35
4	B	710	POV	C24-C25-C26-C27
4	B	710	POV	C32-C33-C34-C35
4	C	706	POV	C32-C33-C34-C35
4	C	710	POV	C24-C25-C26-C27
4	C	711	POV	C213-C214-C215-C216
4	D	705	POV	C25-C26-C27-C28
3	C	705	PCW	C22-C23-C24-C25
4	A	804	POV	C32-C33-C34-C35
4	A	808	POV	C212-C213-C214-C215
4	A	808	POV	C24-C25-C26-C27
4	A	811	POV	C25-C26-C27-C28
4	C	702	POV	C25-C26-C27-C28
4	D	702	POV	C212-C213-C214-C215
4	D	702	POV	C24-C25-C26-C27
4	D	709	POV	C32-C33-C34-C35
3	D	708	PCW	C22-C23-C24-C25
4	A	807	POV	C24-C25-C26-C27
4	A	808	POV	C211-C212-C213-C214
4	A	809	POV	C213-C214-C215-C216
4	B	702	POV	C25-C26-C27-C28
4	B	709	POV	C24-C25-C26-C27
4	B	711	POV	C213-C214-C215-C216
4	C	709	POV	C24-C25-C26-C27
4	C	711	POV	C312-C313-C314-C315

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Mol	Chain	Res	Type	Atoms
4	D	701	POV	C24-C25-C26-C27
4	D	702	POV	C211-C212-C213-C214
4	D	703	POV	C213-C214-C215-C216
4	D	705	POV	C23-C24-C25-C26
4	A	809	POV	C312-C313-C314-C315
4	B	710	POV	C211-C212-C213-C214
4	A	811	POV	C23-C24-C25-C26
4	B	711	POV	C312-C313-C314-C315
4	D	703	POV	C312-C313-C314-C315
4	A	805	POV	C23-C24-C25-C26
4	B	707	POV	C23-C24-C25-C26
4	D	710	POV	C23-C24-C25-C26
4	A	808	POV	C32-C33-C34-C35
4	C	707	POV	C23-C24-C25-C26
4	D	702	POV	C32-C33-C34-C35
4	A	808	POV	C21-C22-C23-C24
4	B	710	POV	C21-C22-C23-C24
4	C	710	POV	C21-C22-C23-C24
4	D	702	POV	C21-C22-C23-C24
4	B	702	POV	C23-C24-C25-C26
4	C	709	POV	C37-C38-C39-C310
4	C	710	POV	C211-C212-C213-C214
4	D	703	POV	C23-C24-C25-C26
4	C	710	POV	C212-C213-C214-C215
4	B	709	POV	C37-C38-C39-C310
2	A	802	Y01	CAN-CAJ-CAO-CBB
2	D	707	Y01	CAN-CAJ-CAO-CBB
4	A	807	POV	C31-C32-C33-C34
4	A	809	POV	C23-C24-C25-C26
4	B	709	POV	C212-C213-C214-C215
4	A	809	POV	C37-C38-C39-C310
4	B	711	POV	C23-C24-C25-C26
4	B	711	POV	C37-C38-C39-C310
4	D	703	POV	C37-C38-C39-C310
4	D	701	POV	C31-C32-C33-C34
4	D	703	POV	C31-C32-C33-C34
4	A	807	POV	C37-C38-C39-C310
4	A	809	POV	C24-C25-C26-C27
4	B	711	POV	C24-C25-C26-C27
4	C	702	POV	C211-C212-C213-C214
4	C	702	POV	C23-C24-C25-C26
4	C	707	POV	C211-C212-C213-C214

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Mol	Chain	Res	Type	Atoms
4	C	709	POV	C36-C37-C38-C39
4	C	711	POV	C24-C25-C26-C27
4	C	711	POV	C37-C38-C39-C310
4	D	701	POV	C212-C213-C214-C215
4	D	701	POV	C37-C38-C39-C310
4	D	703	POV	C24-C25-C26-C27
4	A	807	POV	C212-C213-C214-C215
4	A	811	POV	C36-C37-C38-C39
4	B	702	POV	C36-C37-C38-C39
4	C	702	POV	C36-C37-C38-C39
4	C	709	POV	C212-C213-C214-C215
4	C	711	POV	C23-C24-C25-C26
4	D	705	POV	C36-C37-C38-C39
4	C	711	POV	C32-C33-C34-C35
4	A	809	POV	C11-C12-N-C15
4	B	711	POV	C11-C12-N-C15
4	D	703	POV	C11-C12-N-C15
4	A	807	POV	C36-C37-C38-C39
4	B	702	POV	C211-C212-C213-C214
4	C	711	POV	C211-C212-C213-C214
4	D	701	POV	C36-C37-C38-C39
4	C	711	POV	C22-C21-O21-C2
4	A	809	POV	C211-C212-C213-C214
4	B	711	POV	C211-C212-C213-C214
4	B	709	POV	C36-C37-C38-C39
4	A	809	POV	C31-C32-C33-C34
4	B	709	POV	C31-C32-C33-C34
4	B	711	POV	C31-C32-C33-C34
4	A	811	POV	C211-C212-C213-C214
4	D	703	POV	C211-C212-C213-C214
4	A	811	POV	C37-C38-C39-C310
4	B	702	POV	C37-C38-C39-C310
4	C	702	POV	C37-C38-C39-C310
4	D	705	POV	C37-C38-C39-C310
4	C	709	POV	C31-C32-C33-C34
4	B	709	POV	C311-C312-C313-C314
4	D	705	POV	C211-C212-C213-C214
4	D	705	POV	C212-C213-C214-C215
4	C	702	POV	C212-C213-C214-C215
4	C	709	POV	C35-C36-C37-C38
4	D	701	POV	C311-C312-C313-C314
4	A	811	POV	C212-C213-C214-C215

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Mol	Chain	Res	Type	Atoms
4	B	702	POV	C212-C213-C214-C215
4	C	711	POV	C311-C312-C313-C314
3	A	803	PCW	C23-C24-C25-C26
4	A	807	POV	C311-C312-C313-C314
4	B	707	POV	C211-C212-C213-C214
4	C	709	POV	C311-C312-C313-C314
4	D	710	POV	C211-C212-C213-C214
2	D	707	Y01	CAJ-CAN-CBA-CAA
4	A	809	POV	C22-C21-O21-C2
4	B	711	POV	C22-C21-O21-C2
4	D	703	POV	C22-C21-O21-C2
4	A	811	POV	C33-C34-C35-C36
4	B	702	POV	C33-C34-C35-C36
4	C	702	POV	C33-C34-C35-C36
4	D	705	POV	C33-C34-C35-C36
4	A	809	POV	O22-C21-O21-C2
4	D	703	POV	O22-C21-O21-C2
3	B	705	PCW	C23-C24-C25-C26
4	A	805	POV	C211-C212-C213-C214
4	A	811	POV	C26-C27-C28-C29
4	B	702	POV	C26-C27-C28-C29
4	C	702	POV	C26-C27-C28-C29
3	C	705	PCW	C23-C24-C25-C26
4	C	709	POV	C311-C310-C39-C38
4	D	701	POV	C35-C36-C37-C38
2	A	802	Y01	CAJ-CAN-CBA-CAA
3	D	708	PCW	C23-C24-C25-C26
4	A	807	POV	C35-C36-C37-C38
4	C	711	POV	C11-C12-N-C15
4	B	709	POV	C311-C310-C39-C38
4	B	709	POV	C35-C36-C37-C38
4	A	805	POV	C22-C23-C24-C25
4	B	707	POV	C22-C23-C24-C25
4	B	709	POV	C22-C21-O21-C2
4	C	709	POV	C22-C21-O21-C2
4	D	710	POV	C22-C23-C24-C25
4	A	805	POV	C25-C26-C27-C28
4	A	809	POV	C311-C312-C313-C314
4	B	711	POV	C311-C312-C313-C314
4	D	710	POV	C25-C26-C27-C28
4	A	811	POV	C31-C32-C33-C34
4	B	702	POV	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
4	C	702	POV	C31-C32-C33-C34
4	D	705	POV	C31-C32-C33-C34
4	D	703	POV	C311-C312-C313-C314
4	C	709	POV	O21-C2-C3-O31
4	B	707	POV	C25-C26-C27-C28
4	A	806	POV	C1-C2-C3-O31
4	B	708	POV	C1-C2-C3-O31
4	C	707	POV	C22-C23-C24-C25
4	D	701	POV	C311-C310-C39-C38
4	A	807	POV	C311-C310-C39-C38
4	D	711	POV	C1-C2-C3-O31
4	B	711	POV	O22-C21-O21-C2
4	C	707	POV	C25-C26-C27-C28
4	C	711	POV	C25-C26-C27-C28
4	D	702	POV	C22-C23-C24-C25
4	A	808	POV	C22-C23-C24-C25
4	B	710	POV	C22-C23-C24-C25
4	B	702	POV	C22-C21-O21-C2
4	B	706	POV	C36-C37-C38-C39
4	D	709	POV	C36-C37-C38-C39
4	A	804	POV	C36-C37-C38-C39
4	C	706	POV	C36-C37-C38-C39
4	C	710	POV	C22-C23-C24-C25
3	A	803	PCW	C20-C21-C22-C23
3	B	705	PCW	C20-C21-C22-C23
3	C	705	PCW	C16-C17-C18-C19
4	B	709	POV	C210-C211-C212-C213
4	C	707	POV	C26-C27-C28-C29
4	D	705	POV	C26-C27-C28-C29
2	C	703	Y01	CAO-CBB-CBE-CBI
4	A	808	POV	O11-C1-C2-C3
4	A	811	POV	O11-C1-C2-C3
4	B	702	POV	O11-C1-C2-C3
4	B	710	POV	O11-C1-C2-C3
4	C	702	POV	O11-C1-C2-C3
4	C	710	POV	O11-C1-C2-C3
4	D	702	POV	O11-C1-C2-C3
4	D	705	POV	O11-C1-C2-C3
4	C	711	POV	O22-C21-O21-C2
4	D	703	POV	C25-C26-C27-C28
4	B	711	POV	C25-C26-C27-C28
4	C	708	POV	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
4	A	809	POV	C25-C26-C27-C28
4	A	811	POV	C22-C21-O21-C2
4	C	702	POV	C22-C21-O21-C2
4	D	705	POV	C22-C21-O21-C2
4	A	807	POV	C25-C26-C27-C28
4	D	701	POV	C25-C26-C27-C28
4	C	709	POV	C25-C26-C27-C28
4	C	709	POV	C1-C2-C3-O31
3	A	803	PCW	C16-C17-C18-C19
3	C	705	PCW	C20-C21-C22-C23
4	A	805	POV	C26-C27-C28-C29
4	B	707	POV	C26-C27-C28-C29
4	C	709	POV	C210-C211-C212-C213
4	D	710	POV	C26-C27-C28-C29
4	B	706	POV	C35-C36-C37-C38
4	B	709	POV	C25-C26-C27-C28
4	C	706	POV	C35-C36-C37-C38
4	A	804	POV	C35-C36-C37-C38
4	D	709	POV	C35-C36-C37-C38
2	C	703	Y01	CAX-CAL-CAM-CAY
4	A	807	POV	C39-C310-C311-C312
2	C	703	Y01	CAC-CBB-CBE-CAP
2	C	703	Y01	CAC-CBB-CBE-CBI
4	B	708	POV	C37-C38-C39-C310
4	D	701	POV	C39-C310-C311-C312
3	B	705	PCW	C16-C17-C18-C19
4	A	806	POV	C37-C38-C39-C310
4	A	807	POV	C34-C35-C36-C37
4	D	711	POV	C37-C38-C39-C310
4	A	811	POV	C312-C313-C314-C315
4	B	702	POV	C312-C313-C314-C315
4	C	702	POV	C312-C313-C314-C315
4	D	705	POV	C312-C313-C314-C315
2	B	704	Y01	CAJ-CAN-CBA-CAA
2	D	704	Y01	CAJ-CAN-CBA-CAA
4	A	811	POV	C213-C214-C215-C216
4	B	702	POV	C213-C214-C215-C216
4	C	702	POV	C213-C214-C215-C216
4	D	701	POV	C34-C35-C36-C37
4	A	808	POV	O21-C2-C3-O31
4	B	710	POV	O21-C2-C3-O31
4	C	710	POV	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
4	C	711	POV	O21-C2-C3-O31
4	D	702	POV	O21-C2-C3-O31
4	B	709	POV	C34-C35-C36-C37
4	B	709	POV	C39-C310-C311-C312
4	D	705	POV	C213-C214-C215-C216
4	A	804	POV	C31-C32-C33-C34
4	B	706	POV	C31-C32-C33-C34
4	C	709	POV	C39-C310-C311-C312
4	D	709	POV	C31-C32-C33-C34
4	A	804	POV	C37-C38-C39-C310
4	A	807	POV	C210-C211-C212-C213
4	D	701	POV	C210-C211-C212-C213
4	D	709	POV	C37-C38-C39-C310
4	B	706	POV	C37-C38-C39-C310
4	C	706	POV	C37-C38-C39-C310
4	C	706	POV	C31-C32-C33-C34
4	C	708	POV	C311-C310-C39-C38
4	C	708	POV	C37-C38-C39-C310
4	A	806	POV	C311-C310-C39-C38
4	B	708	POV	C311-C310-C39-C38
4	D	711	POV	C311-C310-C39-C38
3	B	705	PCW	C15-C16-C17-C18
4	A	806	POV	C35-C36-C37-C38
4	B	708	POV	C35-C36-C37-C38
3	A	803	PCW	C15-C16-C17-C18
4	C	709	POV	O22-C21-O21-C2
3	C	705	PCW	C15-C16-C17-C18
4	B	709	POV	C215-C216-C217-C218
4	D	711	POV	C35-C36-C37-C38
4	B	709	POV	C211-C212-C213-C214
4	C	709	POV	C33-C34-C35-C36
4	C	709	POV	C34-C35-C36-C37
3	D	708	PCW	C15-C16-C17-C18
4	C	709	POV	C211-C212-C213-C214
4	C	711	POV	C39-C310-C311-C312
4	C	709	POV	C215-C216-C217-C218
4	C	711	POV	C31-C32-C33-C34
2	B	701	Y01	CAJ-CAN-CBA-CAA
2	C	701	Y01	CAJ-CAN-CBA-CAA
4	A	807	POV	C215-C216-C217-C218
4	D	701	POV	C215-C216-C217-C218
4	B	710	POV	C213-C214-C215-C216

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Mol	Chain	Res	Type	Atoms
2	B	703	Y01	CAC-CBB-CBE-CBI
2	D	706	Y01	CAC-CBB-CBE-CBI
4	D	701	POV	C211-C212-C213-C214
4	A	807	POV	C211-C212-C213-C214
3	D	708	PCW	C20-C21-C22-C23
4	A	808	POV	C213-C214-C215-C216
4	A	809	POV	C39-C310-C311-C312
4	D	703	POV	C39-C310-C311-C312
4	B	709	POV	O22-C21-O21-C2
4	B	711	POV	C39-C310-C311-C312
4	A	807	POV	C1-C2-C3-O31
4	B	709	POV	C1-C2-C3-O31
4	C	711	POV	C1-C2-C3-O31
4	D	701	POV	C1-C2-C3-O31
2	A	801	Y01	CAC-CBB-CBE-CBI
2	A	810	Y01	CAJ-CAN-CBA-CAA
4	D	702	POV	C213-C214-C215-C216
4	D	703	POV	C33-C34-C35-C36
2	B	704	Y01	CAJ-CAN-CBA-CAB
4	A	808	POV	O11-C1-C2-O21
4	A	811	POV	O11-C1-C2-O21
4	B	702	POV	O11-C1-C2-O21
4	B	710	POV	O11-C1-C2-O21
4	C	702	POV	O11-C1-C2-O21
4	C	710	POV	O11-C1-C2-O21
4	D	702	POV	O11-C1-C2-O21
4	D	705	POV	O11-C1-C2-O21
2	C	703	Y01	CAO-CBB-CBE-CAP
3	D	708	PCW	C16-C17-C18-C19
2	A	801	Y01	CAO-CBB-CBE-CBI
2	B	703	Y01	CAO-CBB-CBE-CBI
2	D	706	Y01	CAO-CBB-CBE-CBI
4	A	809	POV	C33-C34-C35-C36
4	C	711	POV	C22-C23-C24-C25
4	A	807	POV	C313-C314-C315-C316
4	A	809	POV	O21-C2-C3-O31
4	B	711	POV	O21-C2-C3-O31
4	D	703	POV	O21-C2-C3-O31
4	D	701	POV	C313-C314-C315-C316
4	D	705	POV	C21-C22-C23-C24
4	B	711	POV	C33-C34-C35-C36
2	A	802	Y01	CAJ-CAN-CBA-CAB

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Mol	Chain	Res	Type	Atoms
4	B	709	POV	C32-C33-C34-C35
4	C	710	POV	C213-C214-C215-C216
4	D	701	POV	C32-C33-C34-C35
2	D	707	Y01	CAJ-CAN-CBA-CAB
4	C	708	POV	C35-C36-C37-C38
2	C	704	Y01	CAJ-CAO-CBB-CAC
2	B	703	Y01	CAC-CBB-CBE-CAP
2	D	706	Y01	CAC-CBB-CBE-CAP
2	D	704	Y01	CAJ-CAN-CBA-CAB
4	D	701	POV	C22-C21-O21-C2
4	C	709	POV	C313-C314-C315-C316
4	B	709	POV	C313-C314-C315-C316
4	A	811	POV	C21-C22-C23-C24
2	A	801	Y01	CAC-CBB-CBE-CAP
4	A	807	POV	C32-C33-C34-C35
4	C	709	POV	C32-C33-C34-C35
4	C	702	POV	C34-C35-C36-C37
4	D	705	POV	C34-C35-C36-C37
4	C	709	POV	C32-C31-O31-C3
4	C	710	POV	C32-C31-O31-C3
4	B	702	POV	C34-C35-C36-C37
4	A	811	POV	C34-C35-C36-C37
4	A	807	POV	C22-C21-O21-C2
4	A	811	POV	O22-C21-O21-C2
4	B	702	POV	O22-C21-O21-C2
4	C	702	POV	O22-C21-O21-C2
4	D	705	POV	O22-C21-O21-C2
2	B	703	Y01	CAO-CBB-CBE-CAP
2	D	706	Y01	CAO-CBB-CBE-CAP
4	D	701	POV	O22-C21-O21-C2
2	A	801	Y01	CAO-CBB-CBE-CAP
4	B	711	POV	C22-C23-C24-C25
2	A	810	Y01	CAJ-CAN-CBA-CAB
2	C	701	Y01	CAJ-CAN-CBA-CAB
2	B	701	Y01	CAJ-CAN-CBA-CAB
2	C	704	Y01	CAJ-CAN-CBA-CAB
4	B	706	POV	C311-C310-C39-C38
4	D	703	POV	C22-C23-C24-C25
4	A	804	POV	C311-C310-C39-C38
4	A	809	POV	C22-C23-C24-C25
4	C	709	POV	O32-C31-O31-C3
4	C	710	POV	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
4	C	706	POV	C311-C310-C39-C38
4	D	709	POV	C311-C310-C39-C38
4	A	811	POV	O12-C11-C12-N
4	B	702	POV	O12-C11-C12-N
4	C	702	POV	O12-C11-C12-N
4	D	705	POV	O12-C11-C12-N
4	A	807	POV	O22-C21-O21-C2
4	B	709	POV	C23-C24-C25-C26
4	B	709	POV	C21-C22-C23-C24
4	C	709	POV	C21-C22-C23-C24
4	C	711	POV	C34-C35-C36-C37
4	C	707	POV	C213-C214-C215-C216
4	C	709	POV	C23-C24-C25-C26
4	A	808	POV	C1-C2-C3-O31
4	A	809	POV	C1-C2-C3-O31
4	B	710	POV	C1-C2-C3-O31
4	B	711	POV	C1-C2-C3-O31
4	D	702	POV	C1-C2-C3-O31
4	D	703	POV	C1-C2-C3-O31
2	B	704	Y01	CAJ-CAO-CBB-CAC
4	C	710	POV	C27-C28-C29-C210
4	B	709	POV	C310-C311-C312-C313
4	A	807	POV	C11-O12-P-O14
4	A	808	POV	C1-O11-P-O14
4	A	808	POV	C11-O12-P-O14
4	A	809	POV	C11-O12-P-O14
4	B	709	POV	C11-O12-P-O14
4	B	710	POV	C1-O11-P-O14
4	B	710	POV	C11-O12-P-O14
4	B	711	POV	C11-O12-P-O14
4	C	709	POV	C11-O12-P-O14
4	C	710	POV	C1-O11-P-O14
4	C	710	POV	C11-O12-P-O14
4	C	711	POV	C1-O11-P-O14
4	C	711	POV	C11-O12-P-O14
4	D	701	POV	C11-O12-P-O14
4	D	702	POV	C1-O11-P-O14
4	D	702	POV	C11-O12-P-O14
4	D	703	POV	C11-O12-P-O14
4	D	701	POV	C21-C22-C23-C24
4	D	701	POV	C23-C24-C25-C26
4	C	707	POV	C212-C213-C214-C215

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Mol	Chain	Res	Type	Atoms
4	A	807	POV	C21-C22-C23-C24
4	A	807	POV	C23-C24-C25-C26
4	C	709	POV	C310-C311-C312-C313
4	D	710	POV	C213-C214-C215-C216
4	B	707	POV	C213-C214-C215-C216
4	A	808	POV	C27-C28-C29-C210
4	B	710	POV	C27-C28-C29-C210
4	D	702	POV	C27-C28-C29-C210
4	B	702	POV	C21-C22-C23-C24
4	C	711	POV	C214-C215-C216-C217
4	A	805	POV	C213-C214-C215-C216
4	D	705	POV	O21-C21-C22-C23
4	D	702	POV	O32-C31-O31-C3
4	C	711	POV	C313-C314-C315-C316
4	A	809	POV	C214-C215-C216-C217
4	B	711	POV	C214-C215-C216-C217
4	C	710	POV	C1-C2-C3-O31
4	A	811	POV	O21-C21-C22-C23
4	D	703	POV	C214-C215-C216-C217
2	C	703	Y01	CAJ-CAN-CBA-CAB
4	B	710	POV	C32-C31-O31-C3
4	D	702	POV	C32-C31-O31-C3
4	B	710	POV	O32-C31-O31-C3
4	B	702	POV	O21-C21-C22-C23
4	B	709	POV	C33-C34-C35-C36
4	A	808	POV	O32-C31-O31-C3
4	A	808	POV	C32-C31-O31-C3
4	B	709	POV	C32-C31-O31-C3
2	C	703	Y01	CAJ-CAO-CBB-CAC
4	B	707	POV	C212-C213-C214-C215
4	B	709	POV	O32-C31-O31-C3
4	D	701	POV	C310-C311-C312-C313
4	D	710	POV	C212-C213-C214-C215
4	A	807	POV	C310-C311-C312-C313
4	A	805	POV	C212-C213-C214-C215
2	D	706	Y01	CAJ-CAN-CBA-CAB
4	C	711	POV	C33-C34-C35-C36
4	C	702	POV	O21-C21-C22-C23
2	A	810	Y01	CAM-CAL-CAX-OAF
2	C	701	Y01	CAM-CAL-CAX-OAF
2	B	701	Y01	CAM-CAL-CAX-OAF
2	D	704	Y01	CAM-CAL-CAX-OAF

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Mol	Chain	Res	Type	Atoms
4	A	809	POV	C310-C311-C312-C313
2	A	801	Y01	CAJ-CAN-CBA-CAB
2	B	703	Y01	CAJ-CAN-CBA-CAB
4	D	703	POV	C310-C311-C312-C313
4	B	711	POV	C310-C311-C312-C313
4	D	701	POV	C33-C34-C35-C36
2	C	703	Y01	CAM-CAL-CAX-OAF
2	C	701	Y01	CAM-CAL-CAX-OAH
2	A	801	Y01	CAM-CAL-CAX-OAF
2	A	810	Y01	CAM-CAL-CAX-OAH
2	B	701	Y01	CAM-CAL-CAX-OAH
2	D	704	Y01	CAM-CAL-CAX-OAH
4	D	701	POV	O32-C31-O31-C3
4	C	710	POV	C29-C210-C211-C212
2	C	703	Y01	CAM-CAL-CAX-OAH
2	D	706	Y01	CAM-CAL-CAX-OAF
2	B	703	Y01	CAM-CAL-CAX-OAF
4	A	807	POV	C33-C34-C35-C36
4	D	701	POV	C32-C31-O31-C3
2	A	801	Y01	CAM-CAL-CAX-OAH
4	C	707	POV	C24-C25-C26-C27
4	C	706	POV	C310-C311-C312-C313
4	D	709	POV	C310-C311-C312-C313
4	A	804	POV	C310-C311-C312-C313
2	D	706	Y01	CAM-CAL-CAX-OAH
4	B	706	POV	C310-C311-C312-C313
4	A	807	POV	O32-C31-O31-C3
4	A	811	POV	C27-C28-C29-C210
2	B	703	Y01	CAM-CAL-CAX-OAH
4	B	711	POV	C34-C35-C36-C37
4	A	805	POV	C24-C25-C26-C27
4	B	702	POV	C27-C28-C29-C210
4	D	705	POV	C27-C28-C29-C210
4	B	710	POV	C2-C1-O11-P
4	D	710	POV	C24-C25-C26-C27
4	B	707	POV	C24-C25-C26-C27
4	B	709	POV	C29-C210-C211-C212
4	C	702	POV	C27-C28-C29-C210
4	A	809	POV	C34-C35-C36-C37
4	A	809	POV	C215-C216-C217-C218
4	D	703	POV	C34-C35-C36-C37
4	B	711	POV	C215-C216-C217-C218

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Mol	Chain	Res	Type	Atoms
4	D	703	POV	C215-C216-C217-C218
4	A	808	POV	C215-C216-C217-C218
4	A	807	POV	C32-C31-O31-C3
4	A	808	POV	C29-C210-C211-C212
4	C	709	POV	C29-C210-C211-C212
4	A	808	POV	C2-C1-O11-P
4	C	710	POV	C2-C1-O11-P
4	D	702	POV	C2-C1-O11-P
4	C	711	POV	C310-C311-C312-C313
4	D	705	POV	C12-C11-O12-P
4	B	711	POV	C313-C314-C315-C316
4	D	703	POV	C313-C314-C315-C316
4	A	807	POV	C29-C210-C211-C212
4	B	709	POV	C27-C28-C29-C210
4	B	710	POV	C29-C210-C211-C212
4	C	709	POV	C27-C28-C29-C210
4	D	701	POV	C29-C210-C211-C212
4	D	702	POV	C29-C210-C211-C212
4	A	809	POV	C313-C314-C315-C316
4	B	710	POV	C215-C216-C217-C218
3	D	708	PCW	C19-C20-C21-C22
4	A	807	POV	C27-C28-C29-C210
4	D	701	POV	C27-C28-C29-C210
4	D	702	POV	C215-C216-C217-C218
4	C	710	POV	C215-C216-C217-C218
2	C	704	Y01	CAL-CAM-CAY-OAW
4	C	710	POV	O21-C21-C22-C23
4	B	710	POV	O21-C21-C22-C23
4	D	702	POV	O21-C21-C22-C23
4	A	808	POV	O21-C21-C22-C23
4	D	705	POV	O31-C31-C32-C33
4	A	811	POV	O31-C31-C32-C33
4	B	702	POV	O31-C31-C32-C33
4	C	702	POV	O31-C31-C32-C33
4	C	711	POV	C215-C216-C217-C218
2	A	802	Y01	CAO-CAJ-CAN-CBA
4	A	808	POV	O22-C21-C22-C23
4	A	811	POV	O32-C31-C32-C33
4	B	702	POV	O32-C31-C32-C33
4	C	702	POV	O32-C31-C32-C33
4	D	702	POV	O22-C21-C22-C23
4	D	705	POV	O32-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
4	B	710	POV	O22-C21-C22-C23
4	A	807	POV	O21-C21-C22-C23
4	C	710	POV	O22-C21-C22-C23
2	B	704	Y01	CAL-CAM-CAY-OAW
4	D	701	POV	O21-C21-C22-C23
2	C	704	Y01	CAL-CAM-CAY-OAG
4	C	709	POV	O21-C21-C22-C23
4	B	709	POV	O21-C21-C22-C23

There are no ring outliers.

40 monomers are involved in 170 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	708	POV	2	0
2	C	701	Y01	6	0
2	D	704	Y01	6	0
3	C	705	PCW	1	0
3	A	803	PCW	1	0
4	C	707	POV	1	0
4	C	708	POV	2	0
4	A	811	POV	3	0
4	D	705	POV	2	0
3	B	705	PCW	1	0
4	C	702	POV	4	0
4	B	707	POV	1	0
4	B	709	POV	5	0
4	A	804	POV	1	0
2	B	703	Y01	6	0
4	B	706	POV	1	0
2	A	802	Y01	11	0
4	A	807	POV	6	0
4	A	805	POV	1	0
4	C	710	POV	1	0
2	C	703	Y01	10	0
2	C	704	Y01	23	0
4	C	709	POV	5	0
4	A	806	POV	1	0
4	D	710	POV	1	0
4	B	711	POV	2	0
2	A	801	Y01	7	0
4	C	711	POV	4	0
4	D	711	POV	1	0

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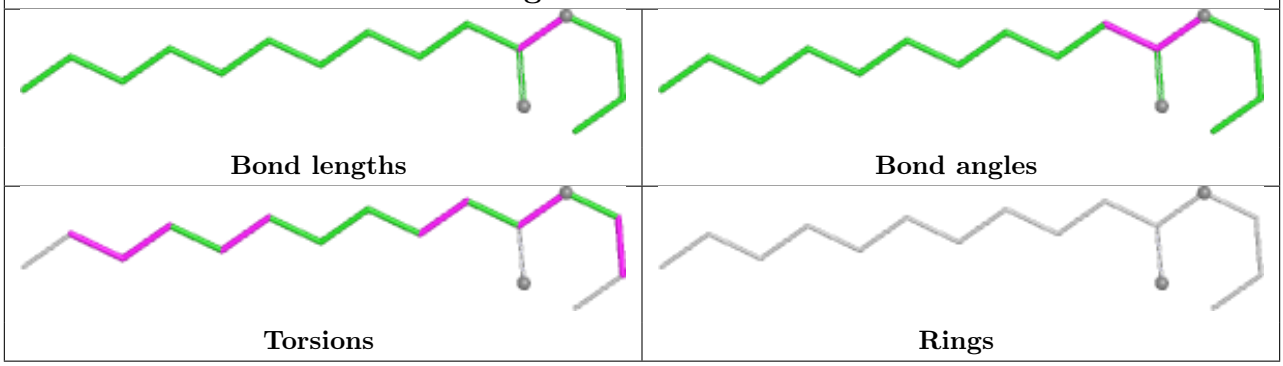
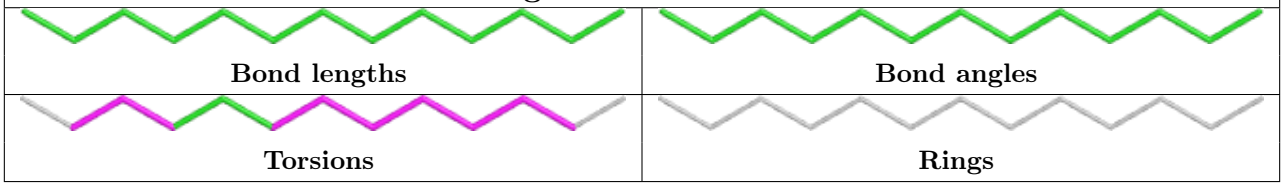
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	704	Y01	24	0
4	D	703	POV	2	0
2	A	810	Y01	7	0
2	D	706	Y01	7	0
2	B	701	Y01	7	0
4	B	702	POV	3	0
4	D	701	POV	7	0
4	D	709	POV	1	0
3	D	708	PCW	1	0
2	D	707	Y01	10	0
4	A	809	POV	2	0

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

Ligand POV B 708



Ligand POV C 706



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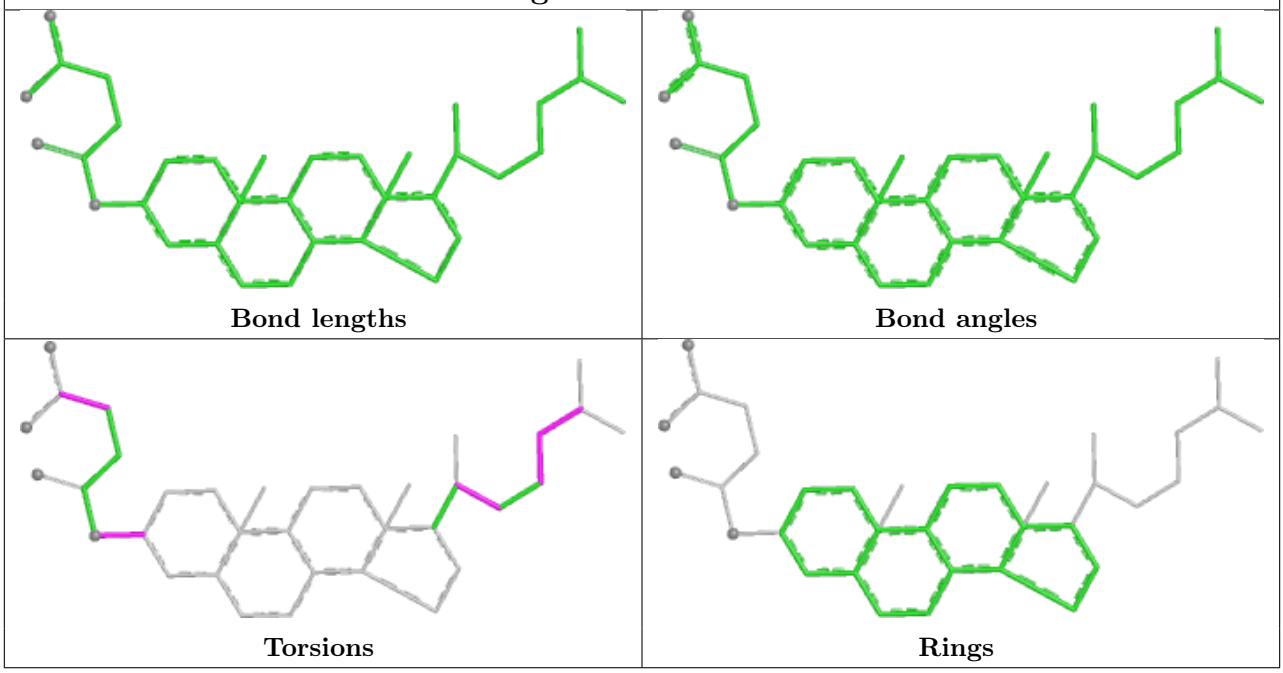

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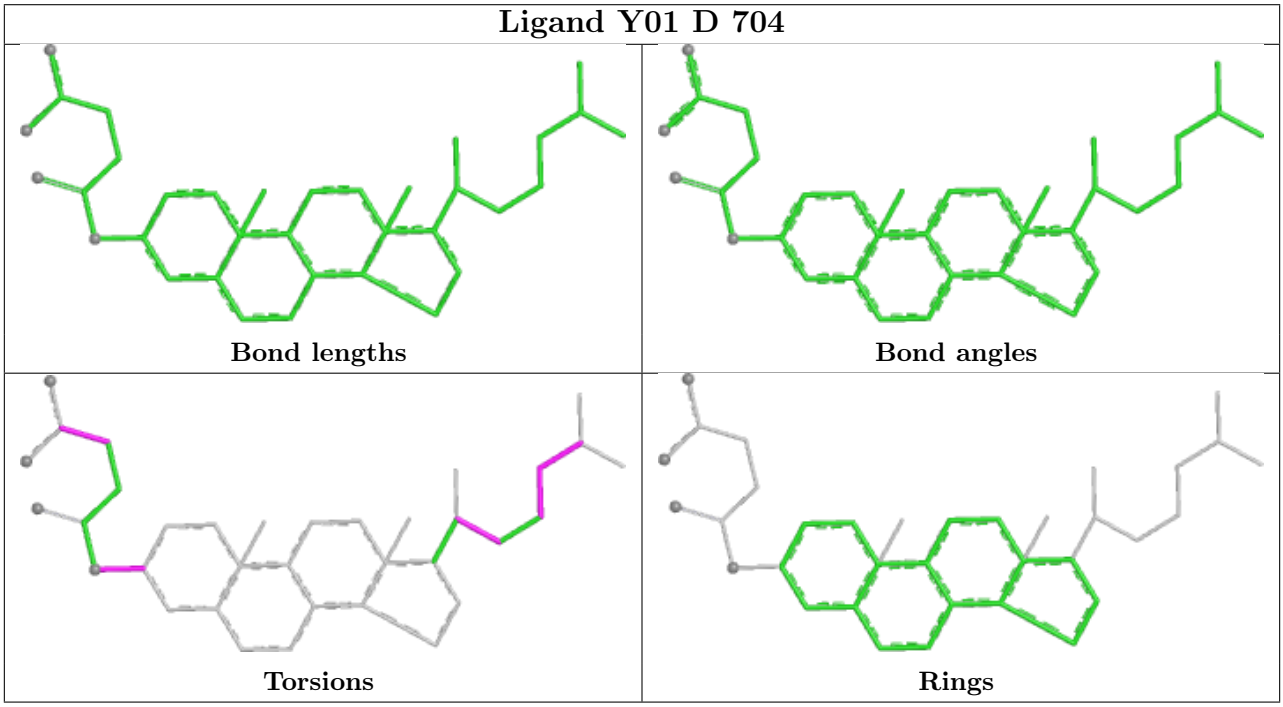

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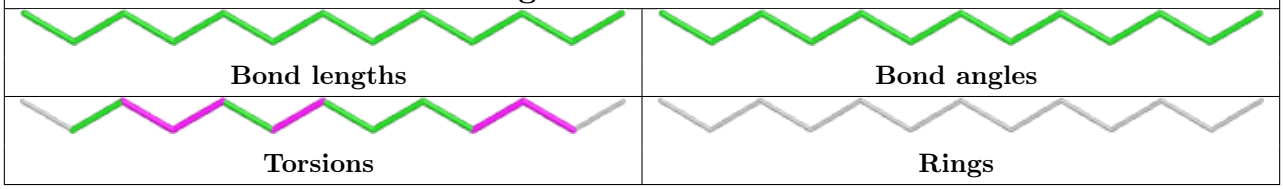
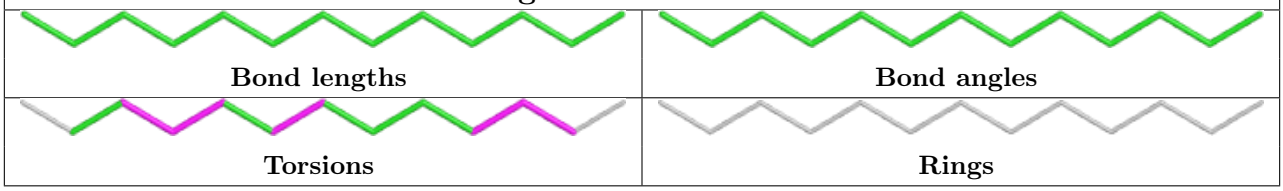


Ligand PCW A 803



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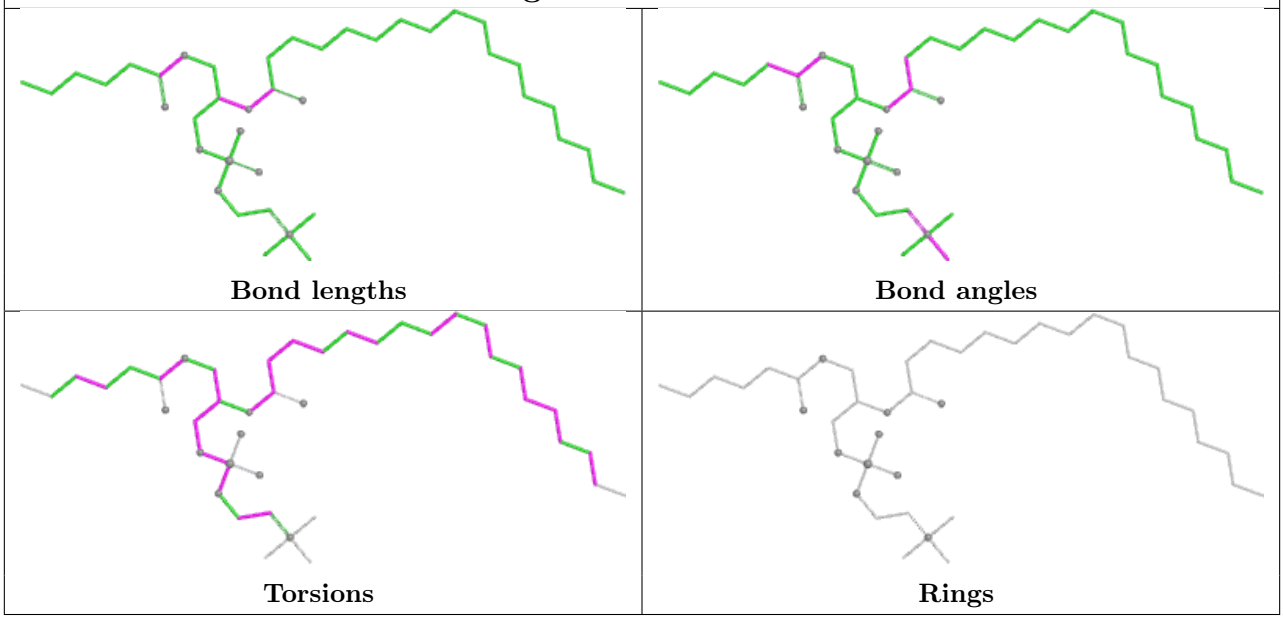

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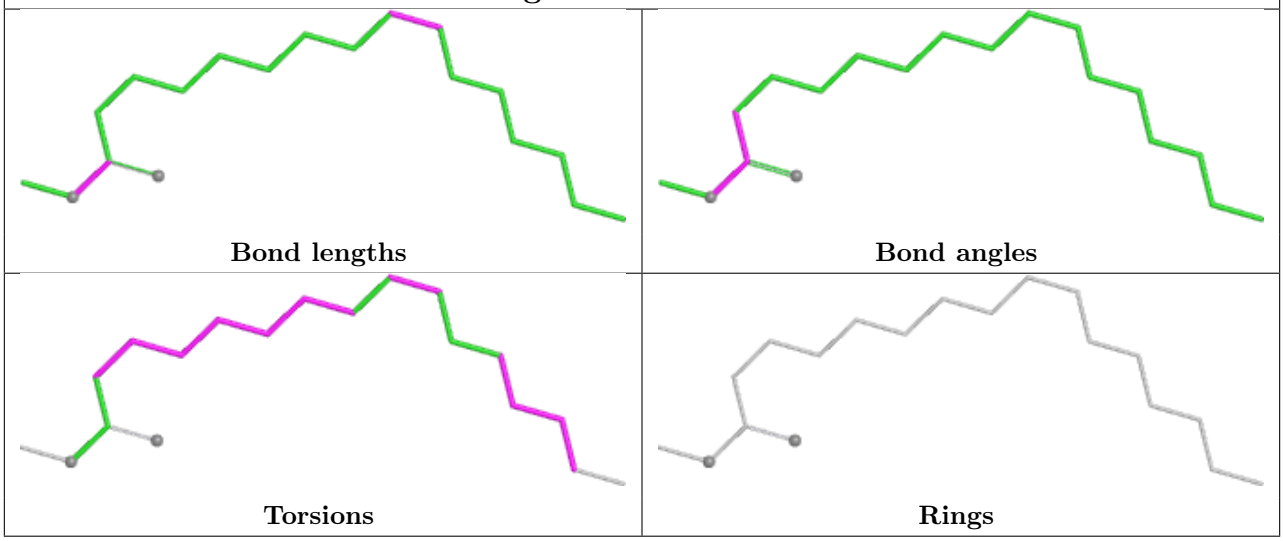

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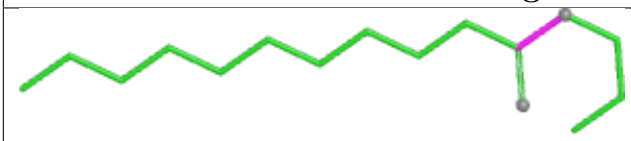
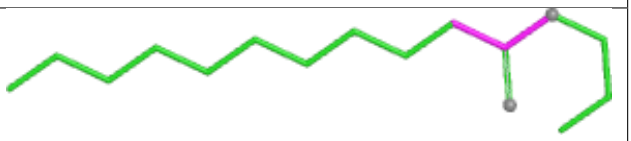
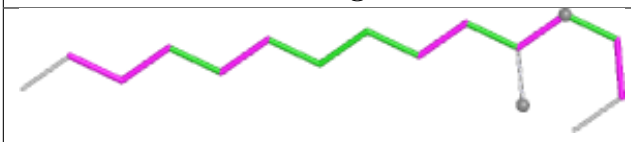


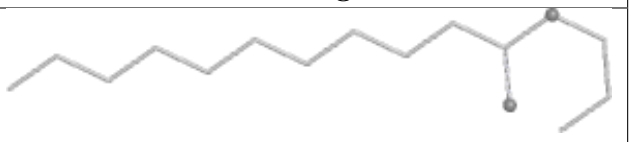
Bond lengths



Bond angles

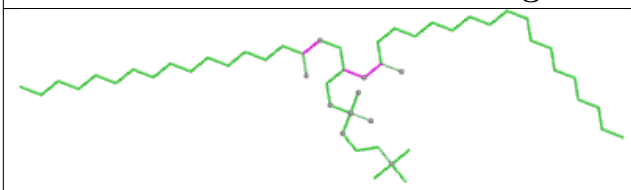


Torsions

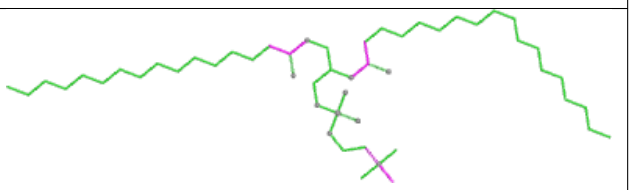


Rings

Ligand POV A 811



Bond lengths



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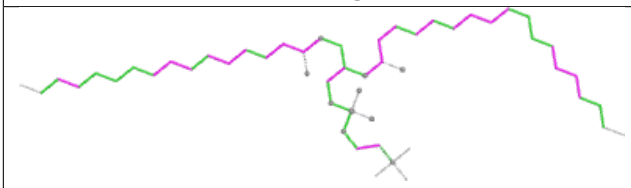
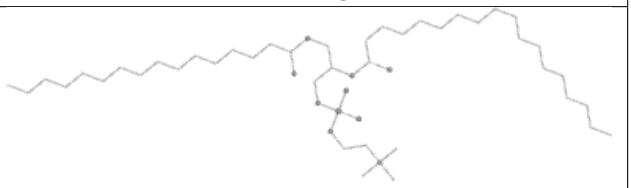
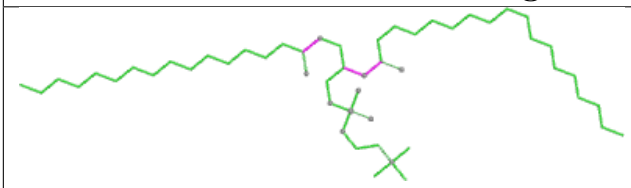


Torsions

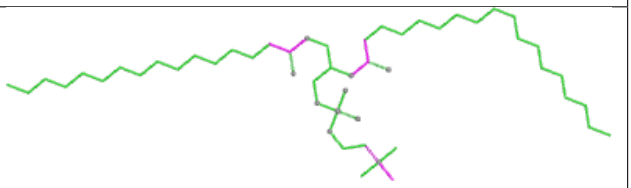


Rings

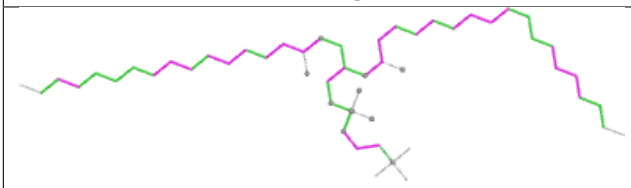
Ligand POV D 705



Bond lengths



Bond angles



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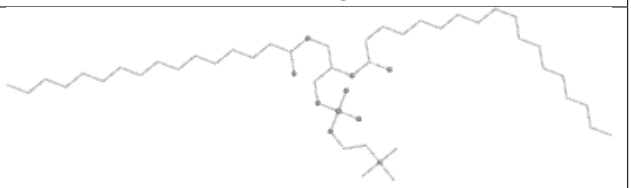
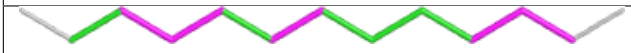


Rings

Ligand PCW B 705

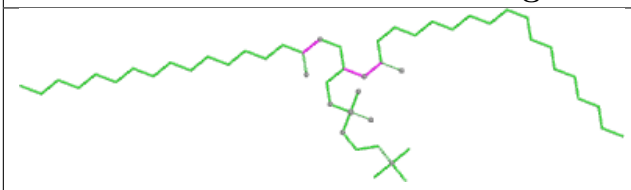
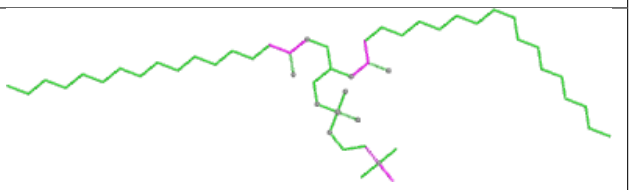
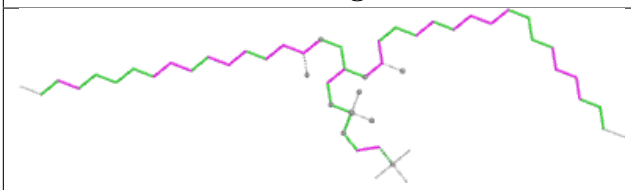
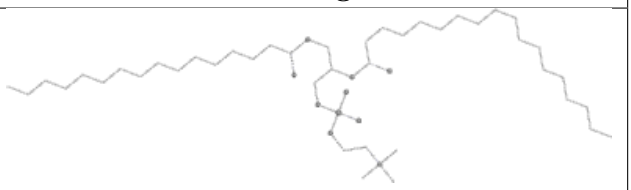
Bond lengths

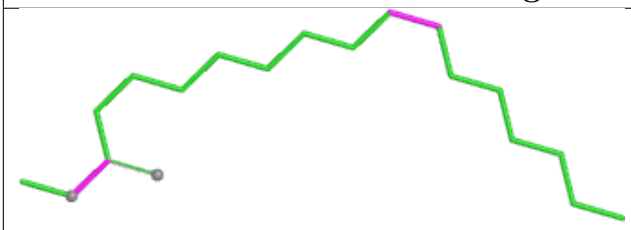
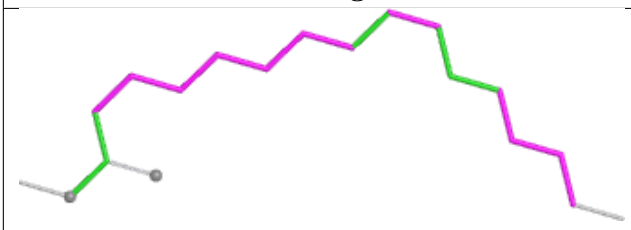
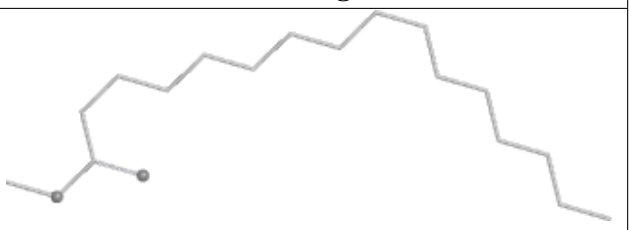
Bond angles



Torsions

Rings

Ligand POV C 702	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand POV B 707	
 Bond lengths	Bond angles
 Torsions	 Rings

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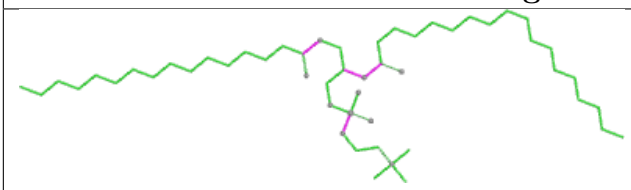
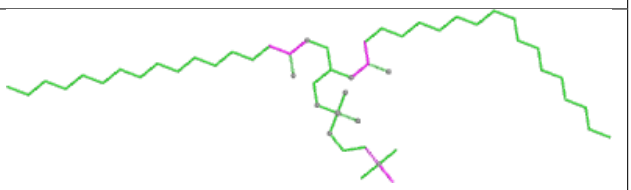
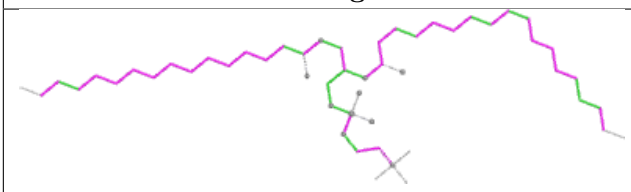
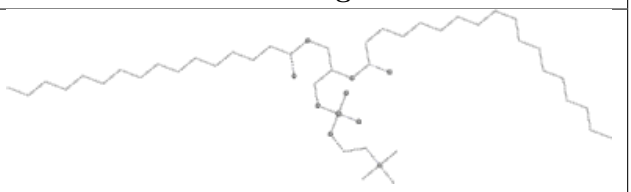
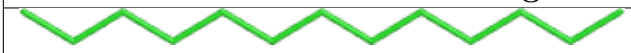
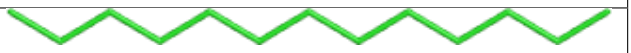
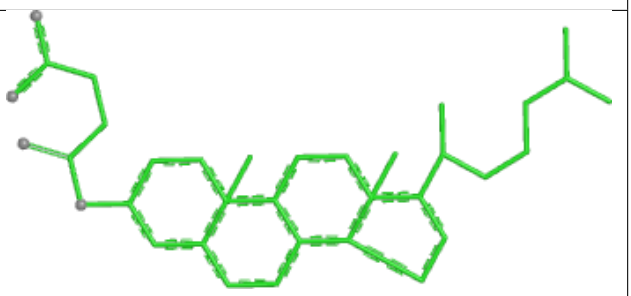
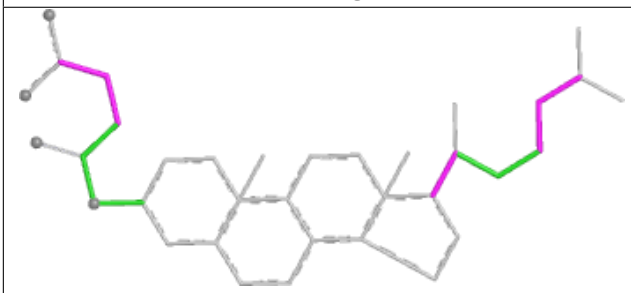
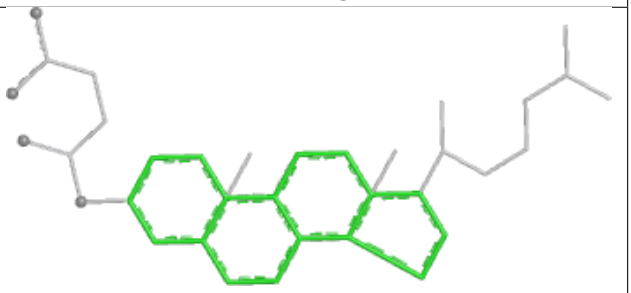
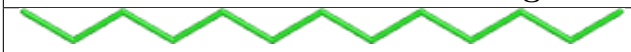
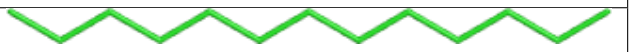
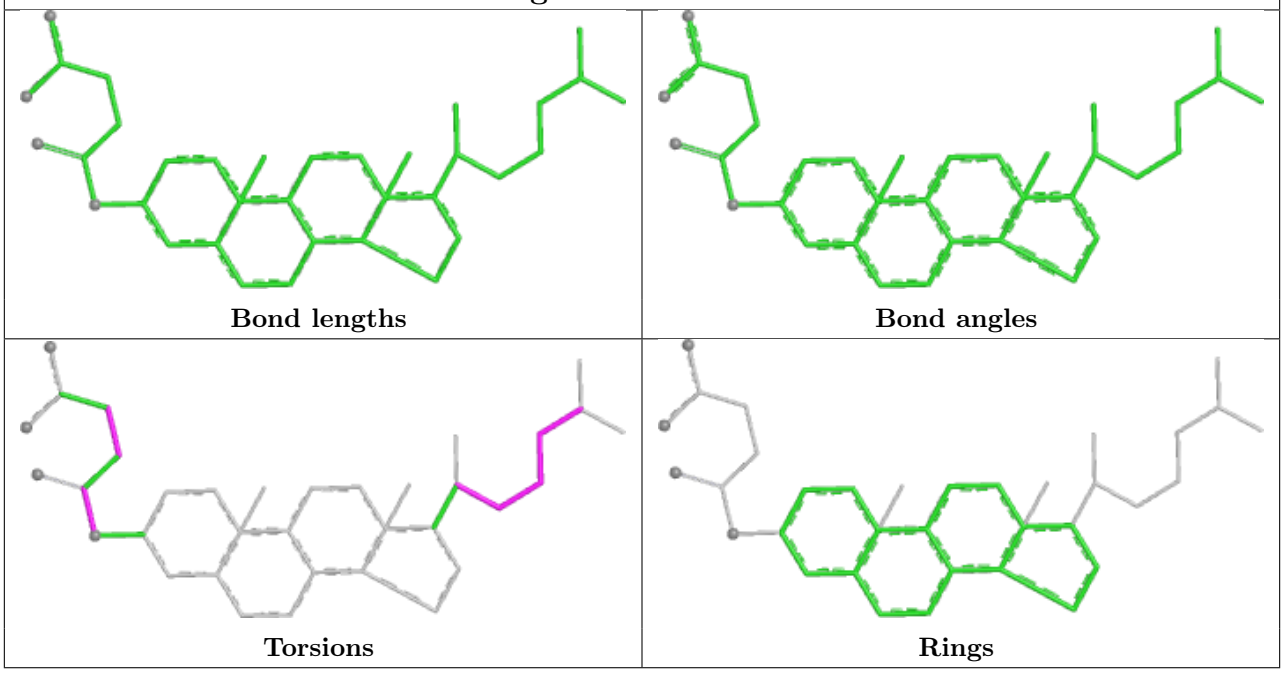
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand POV A 804	
 Bond lengths	 Bond angles
Torsions	Rings

Ligand Y01 B 703	
Bond lengths	 Bond angles
 Torsions	 Rings

Ligand POV B 706	
 Bond lengths	 Bond angles
Torsions	Rings

Ligand Y01 A 802



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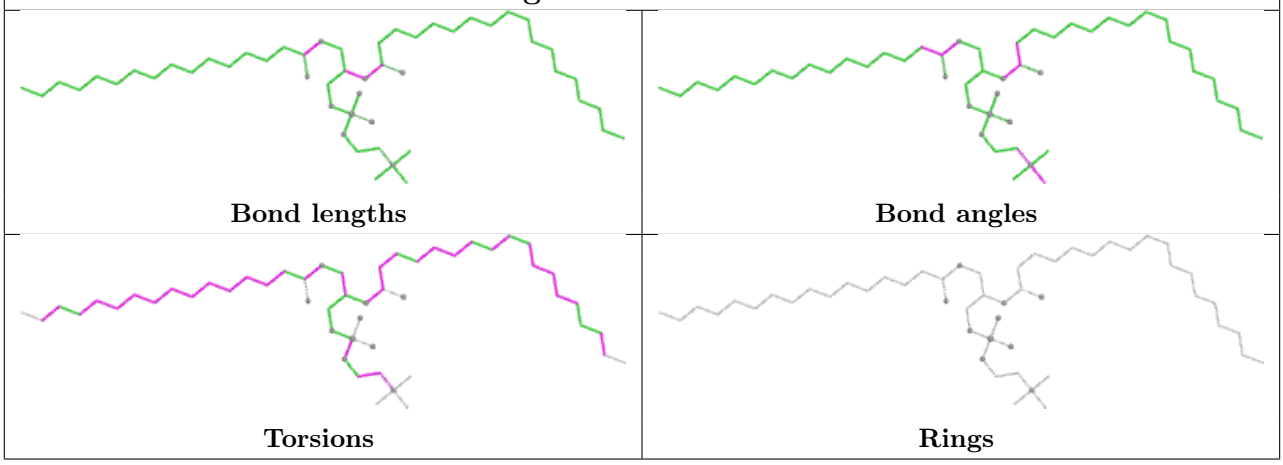
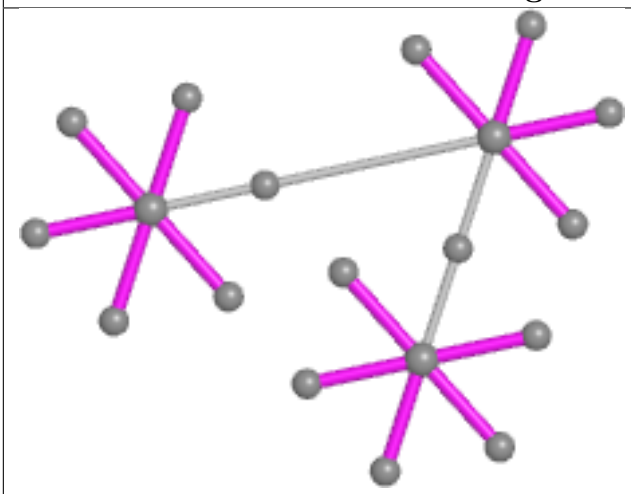
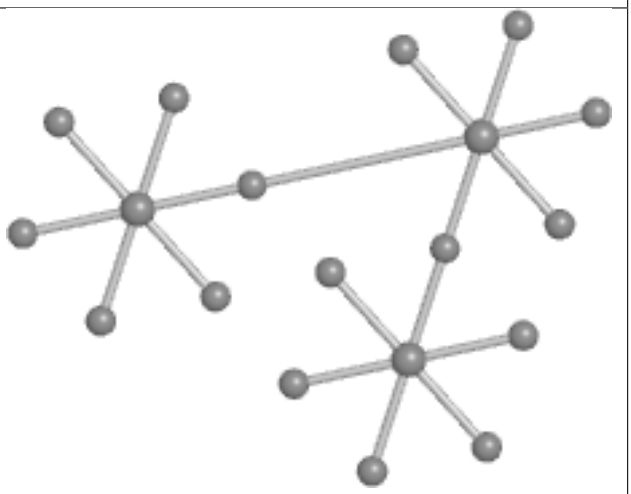


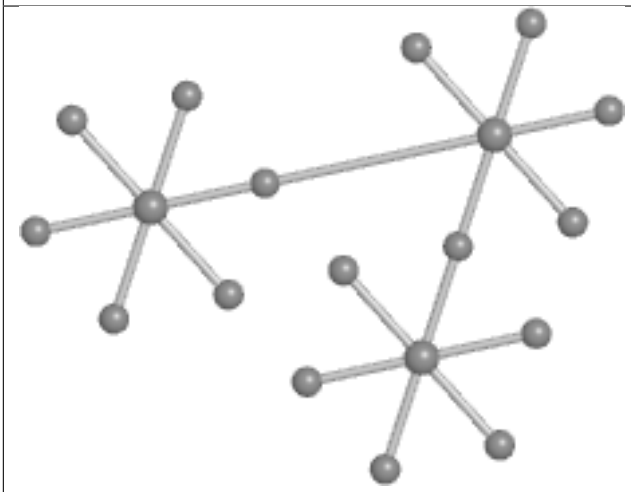
Ligand R2R A 813



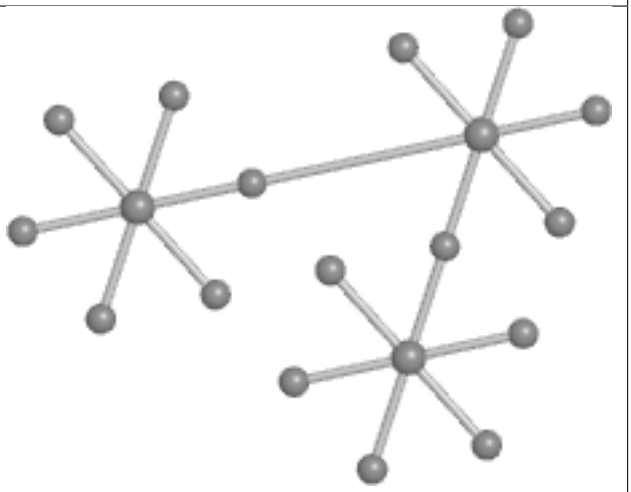
Bond lengths



Bond angles

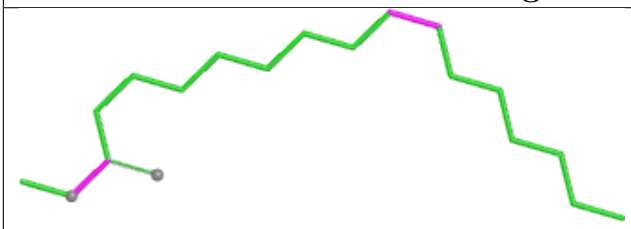


Torsions

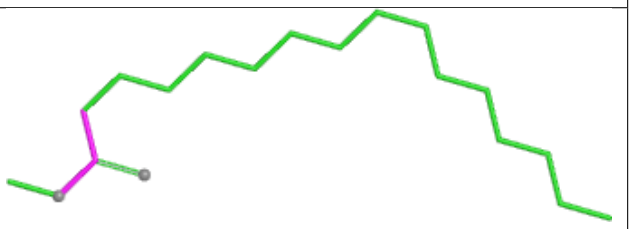


Rings

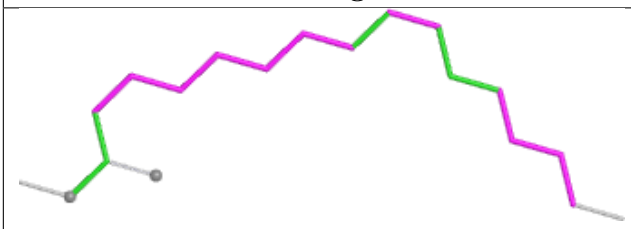
Ligand POV A 805



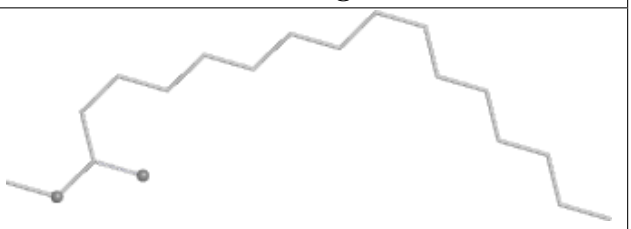
Bond lengths



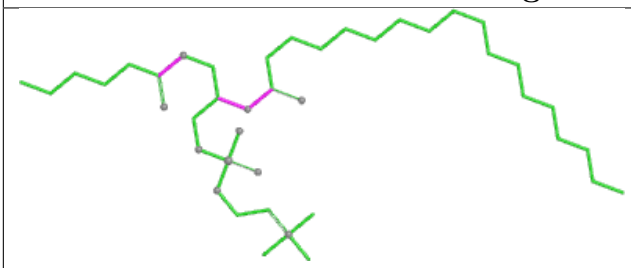
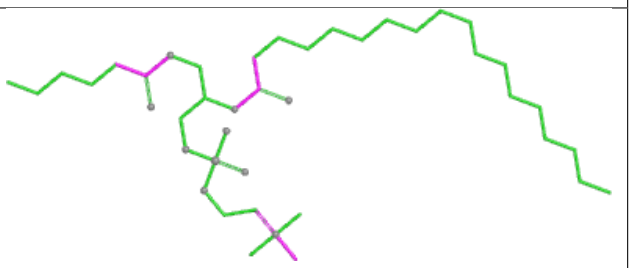
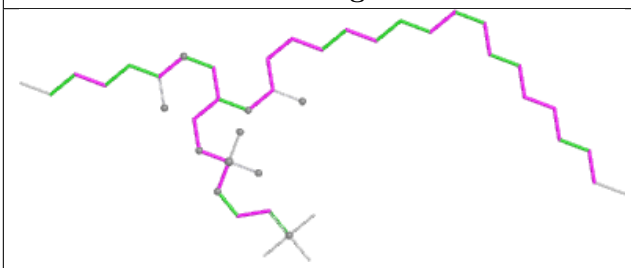
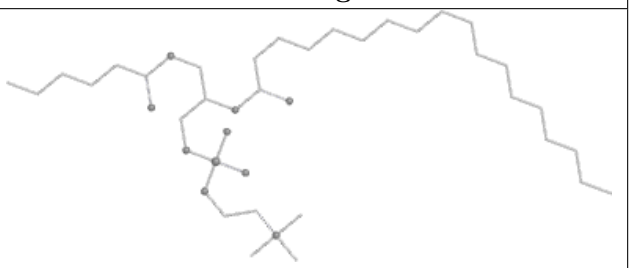
Bond angles

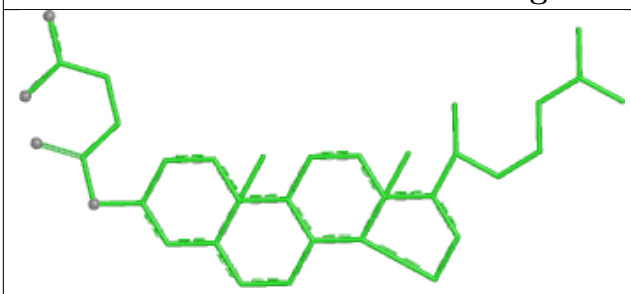
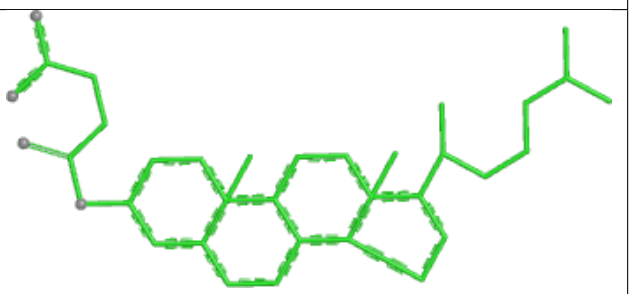
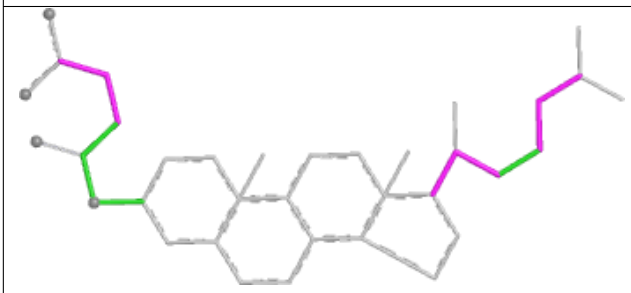
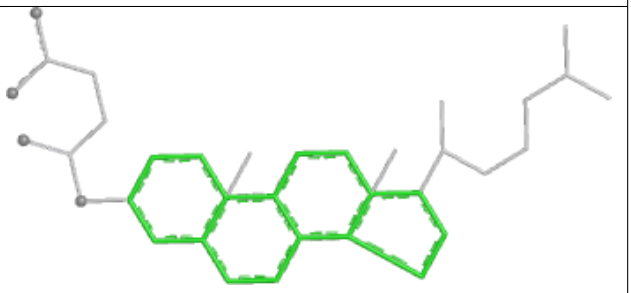


Torsions

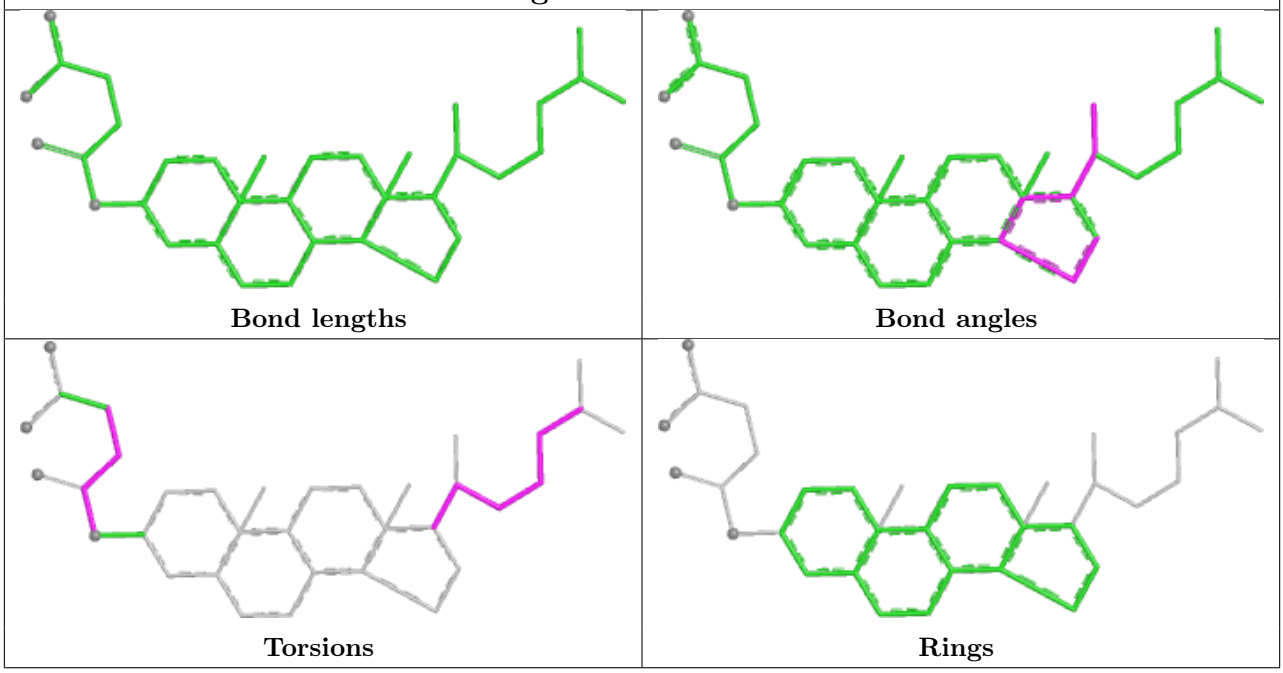


Rings

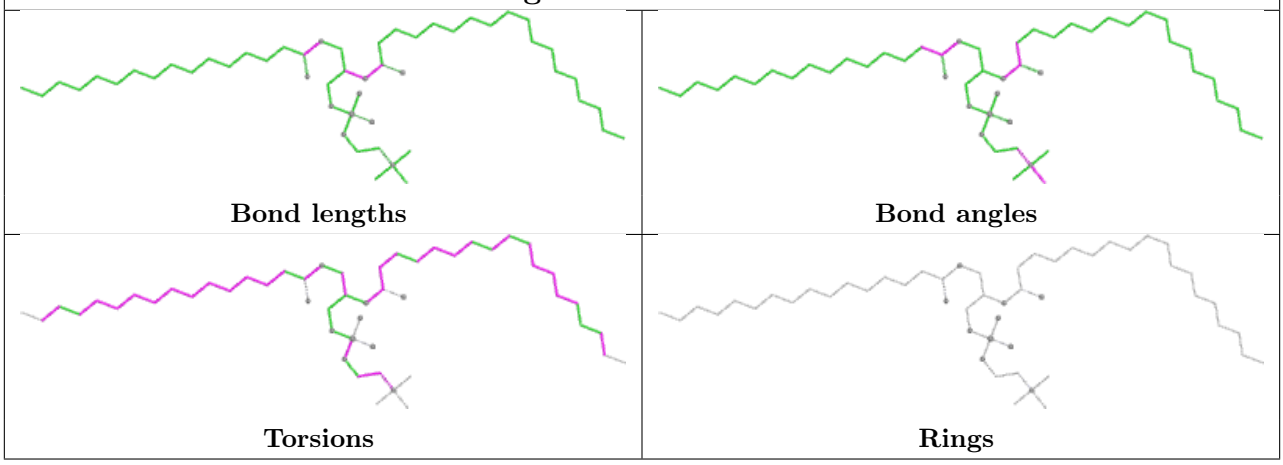
Ligand POV C 710	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand Y01 C 703	
 Bond lengths	 Bond angles
 Torsions	 Rings

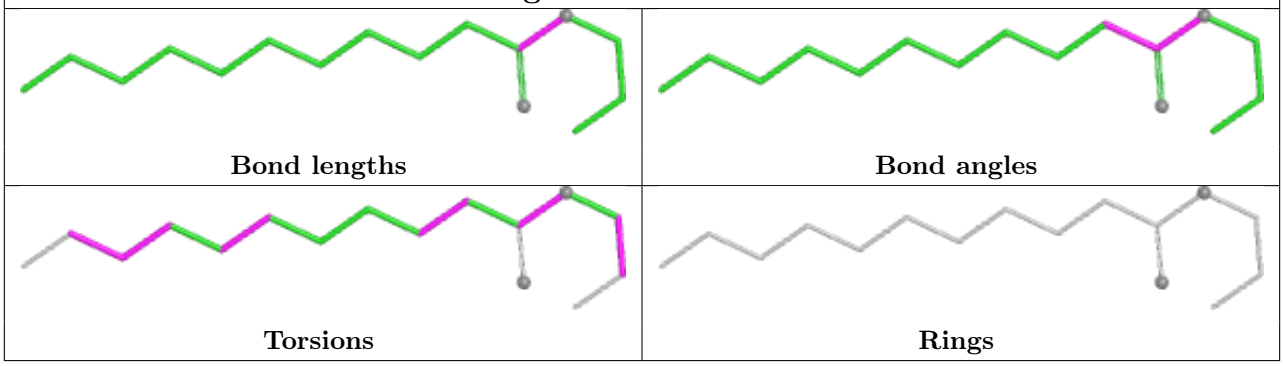
Ligand Y01 C 704



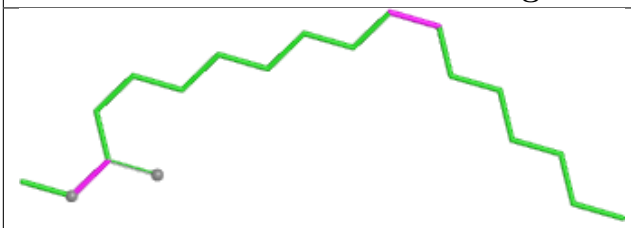
Ligand POV C 709



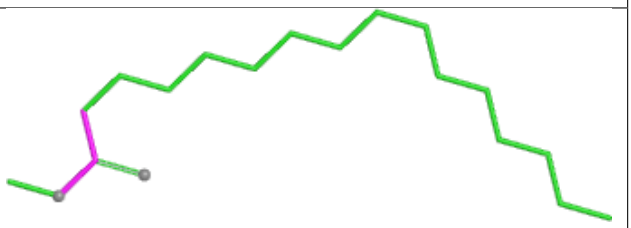
Ligand POV A 806



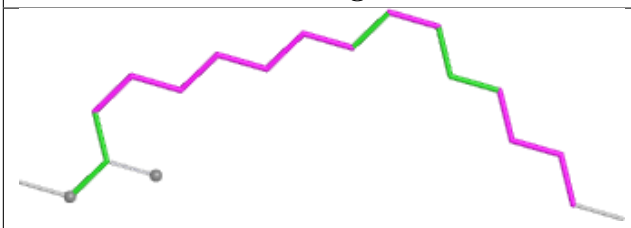
Ligand POV D 710



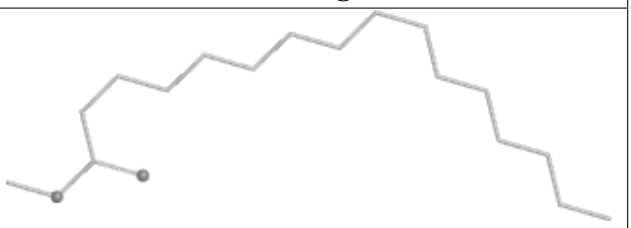
Bond lengths



Bond angles

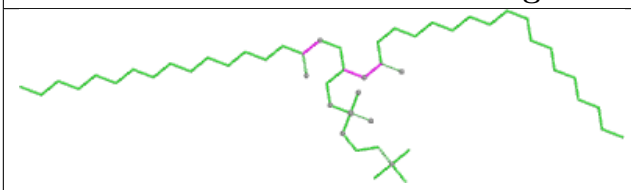


Torsions

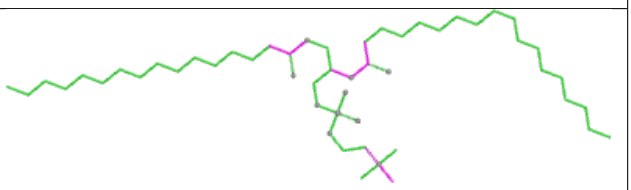


Rings

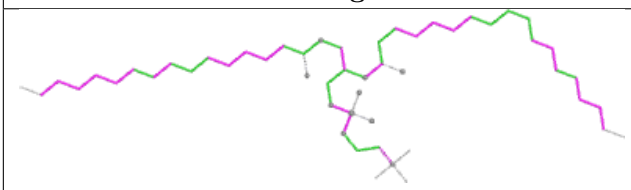
Ligand POV B 711



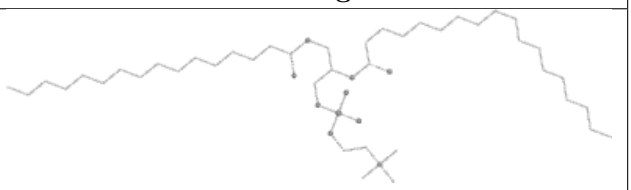
Bond lengths



Bond angles

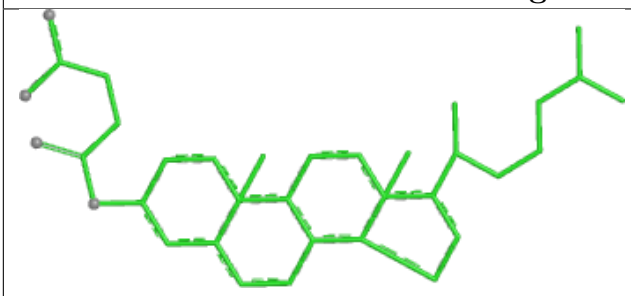


Torsions

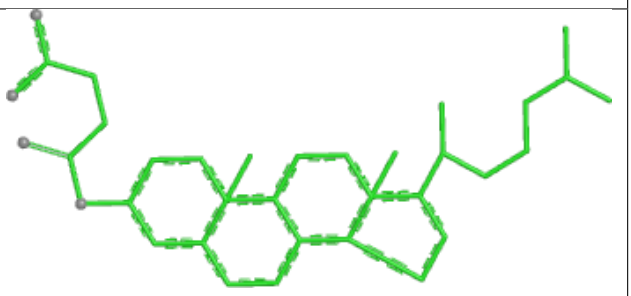


Rings

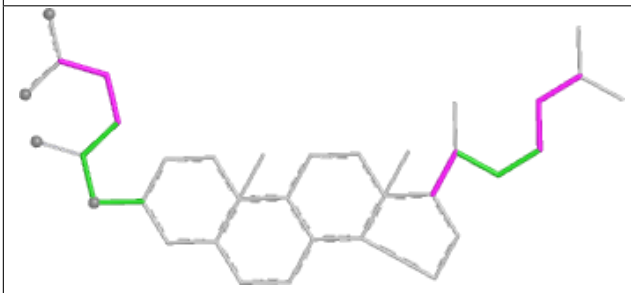
Ligand Y01 A 801



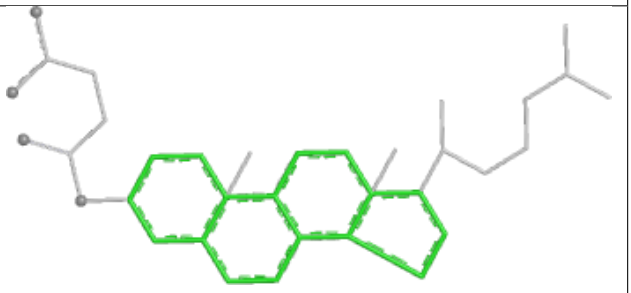
Bond lengths



Bond angles

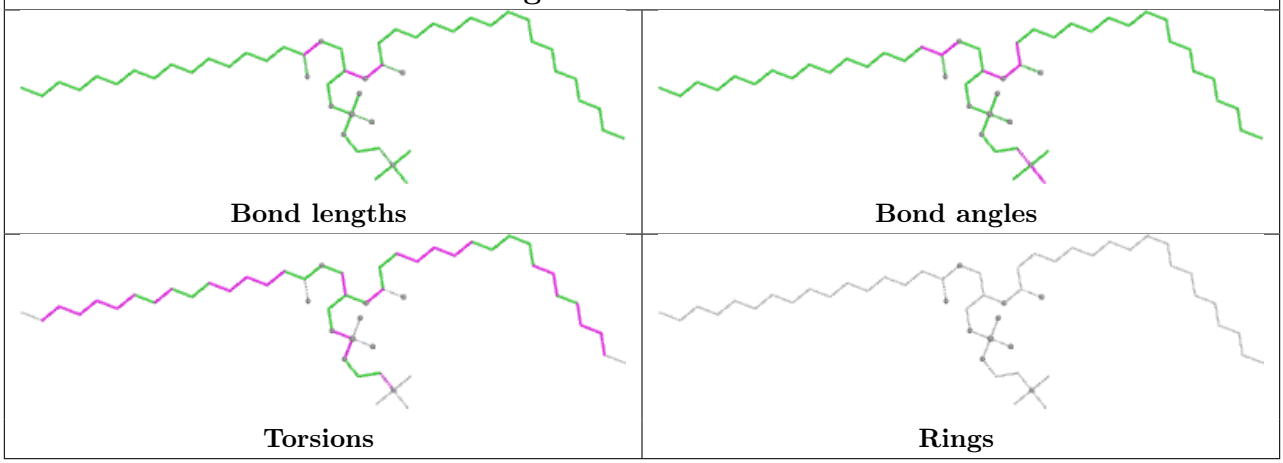


Torsions

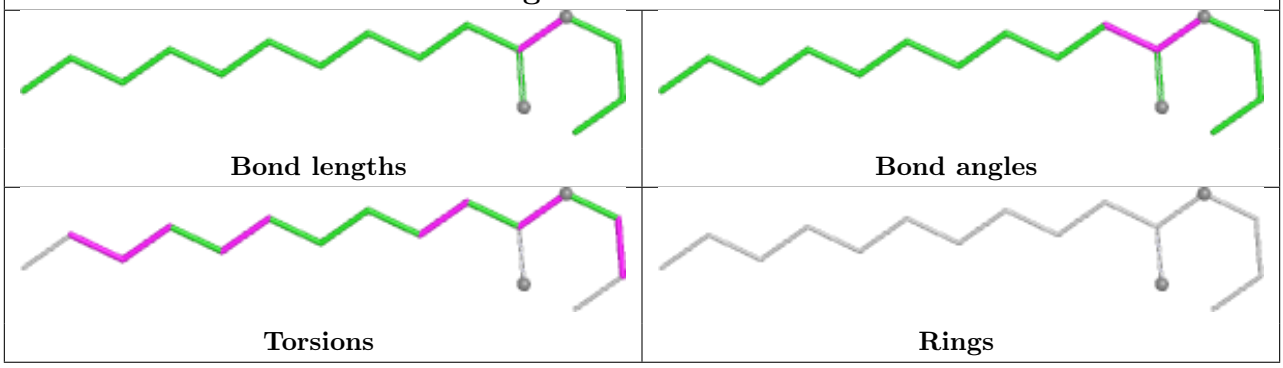


Rings

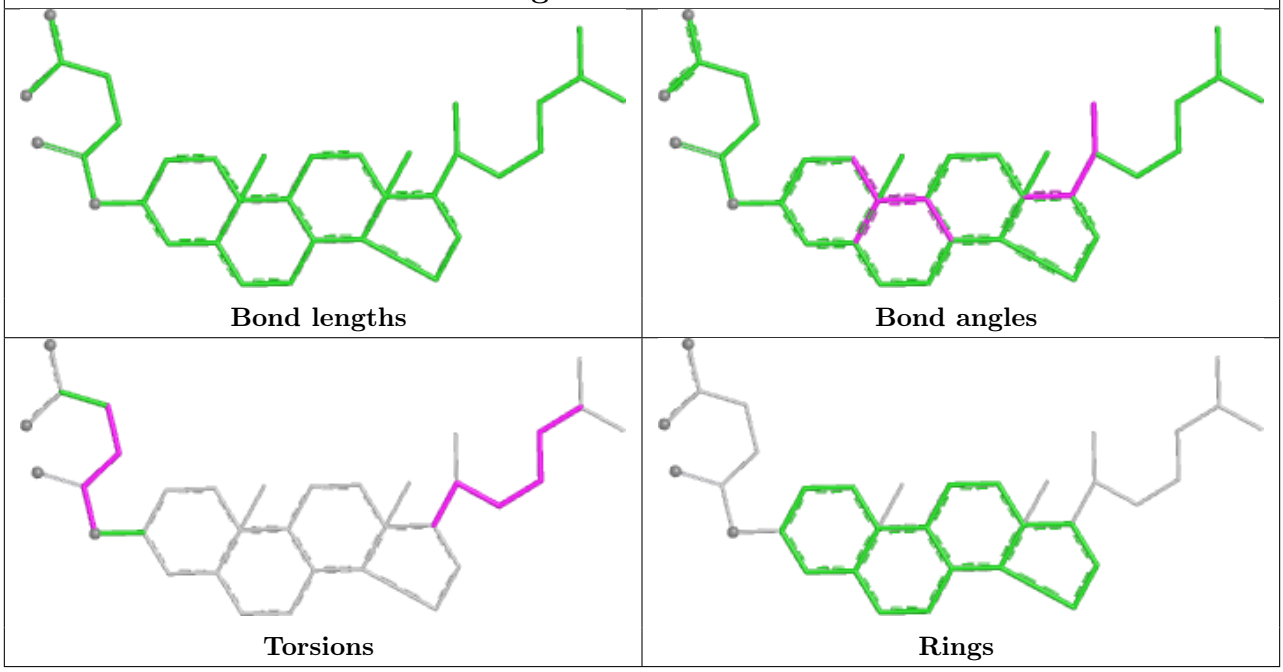
Ligand POV C 711

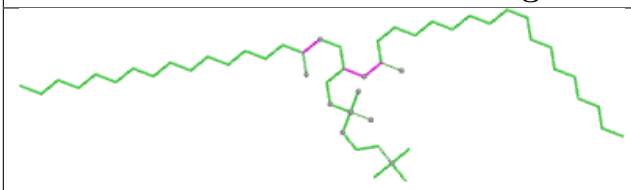
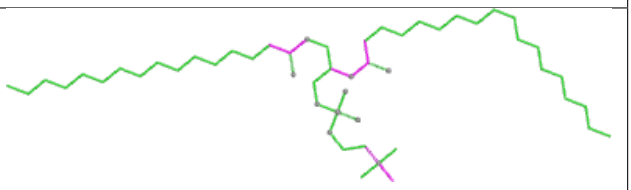
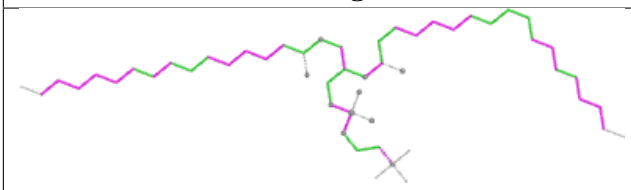
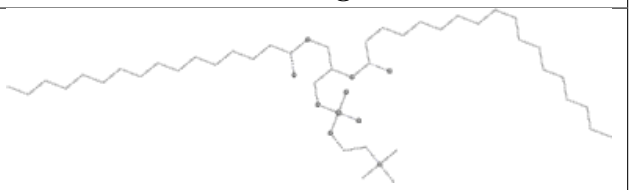


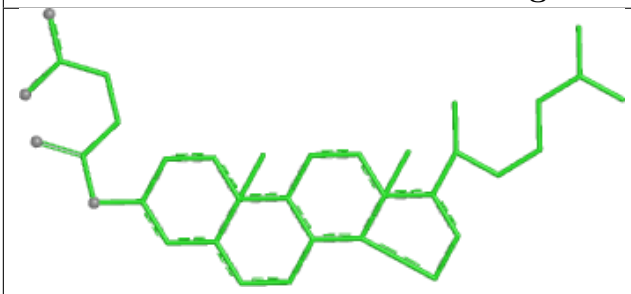
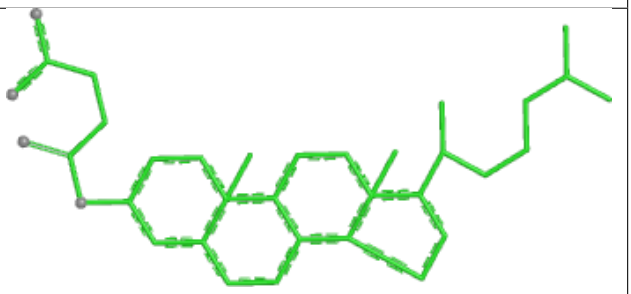
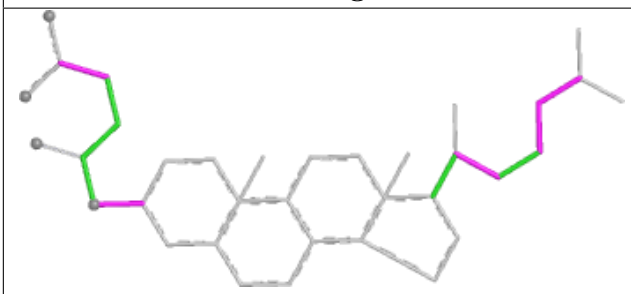
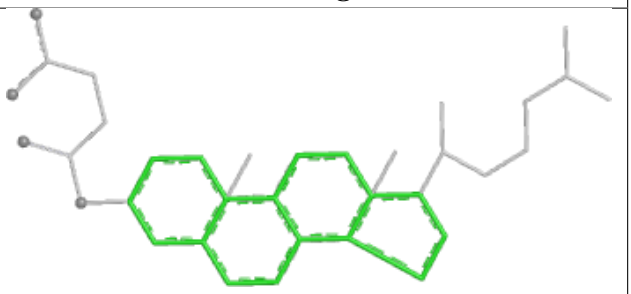
Ligand POV D 711

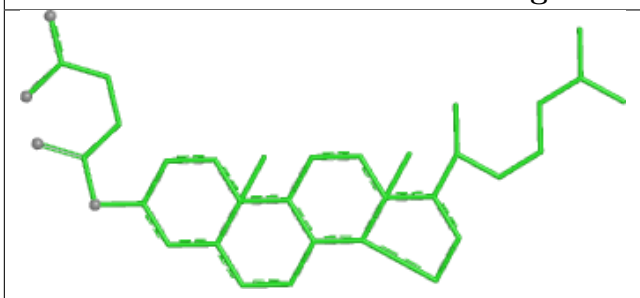
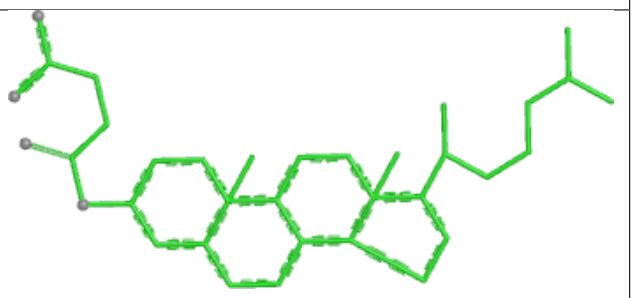
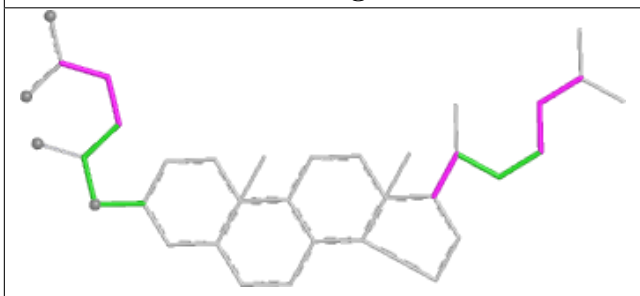
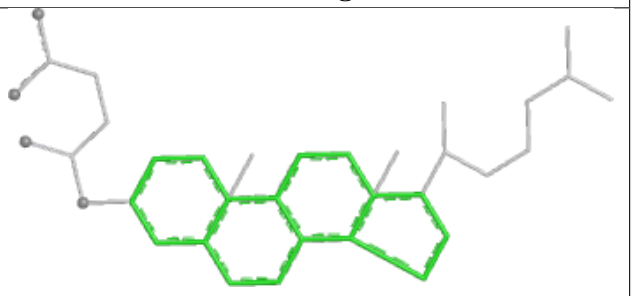


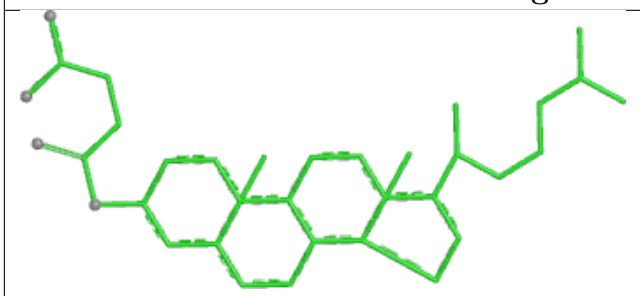
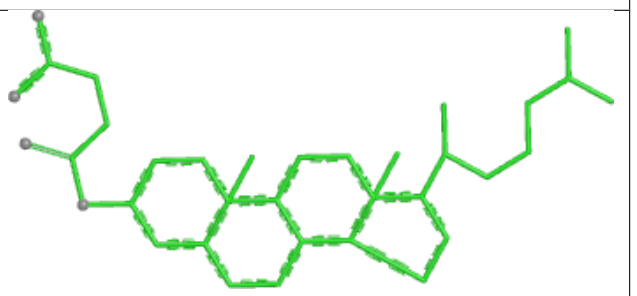
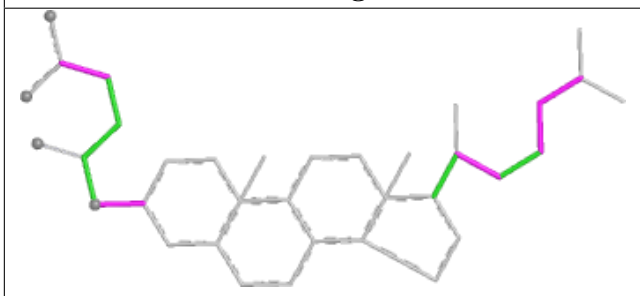
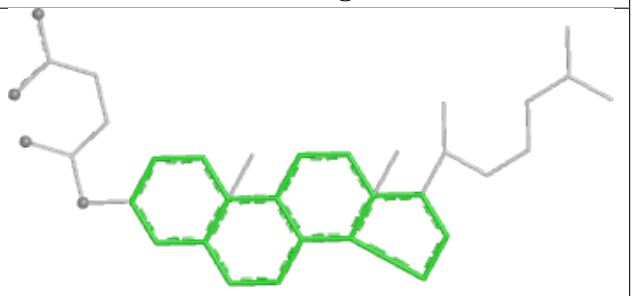
Ligand Y01 B 704

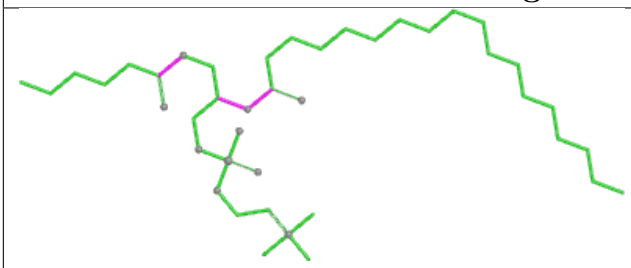
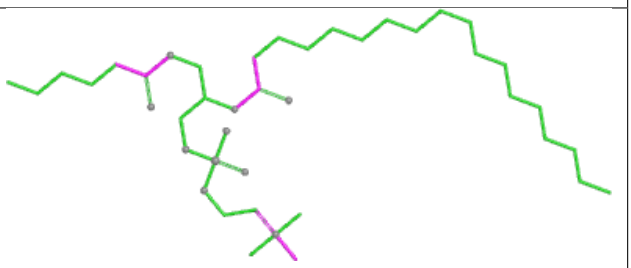
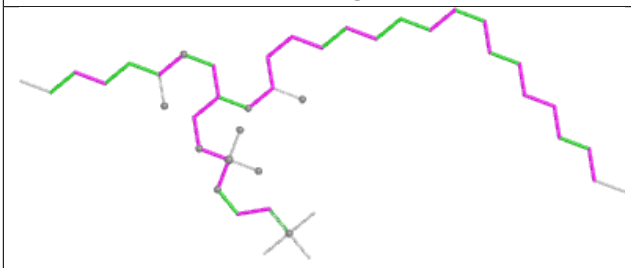
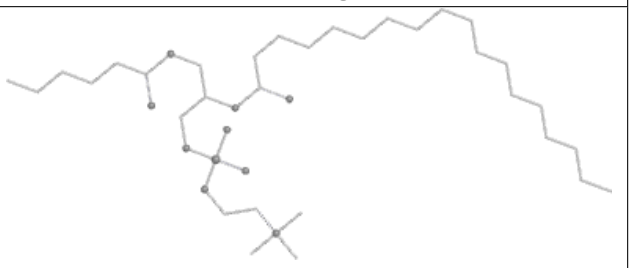


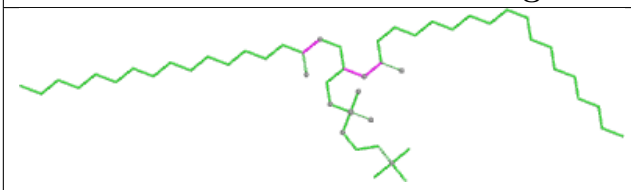
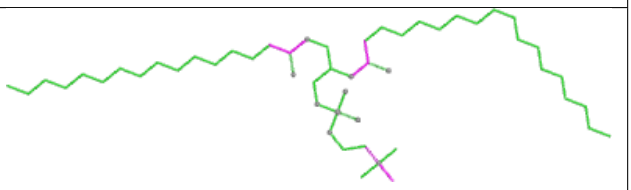
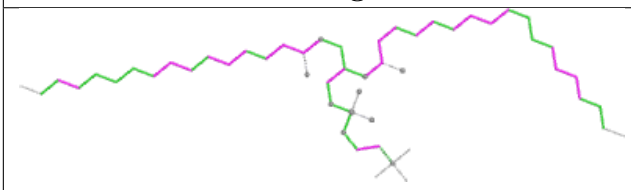
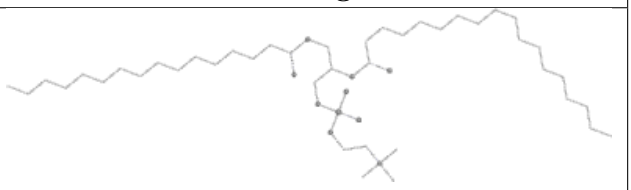
Ligand POV D 703	
 Bond lengths	 Bond angles
 Torsions	 Rings

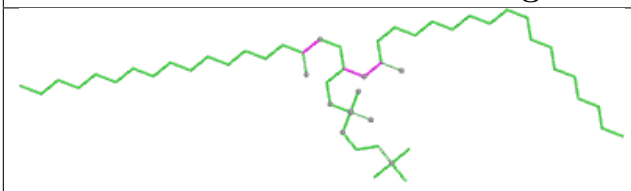
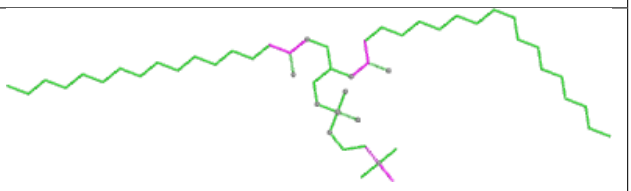
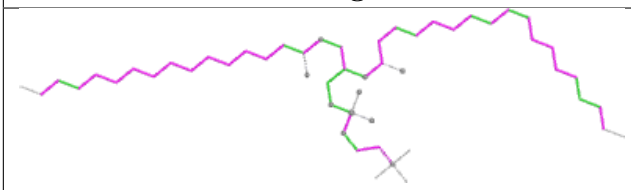
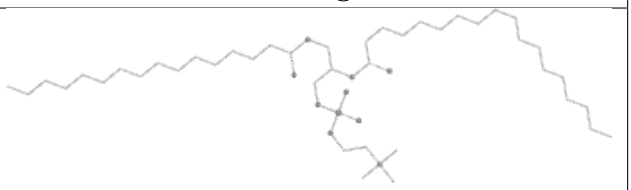
Ligand Y01 A 810	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand Y01 D 706	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand Y01 B 701	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand POV B 710	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand POV B 702	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand POV D 701	
 Bond lengths	 Bond angles
 Torsions	 Rings

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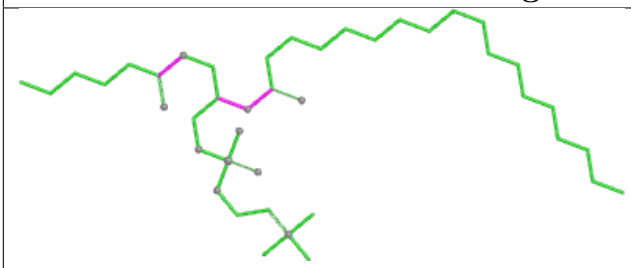
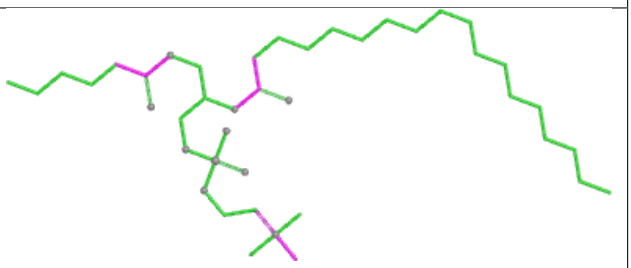
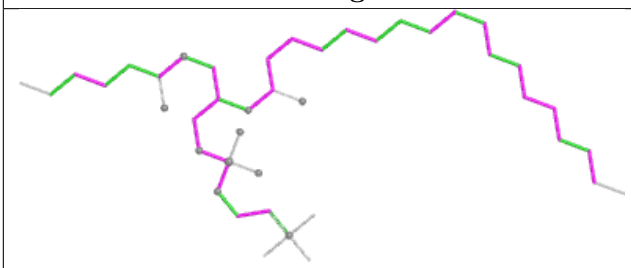
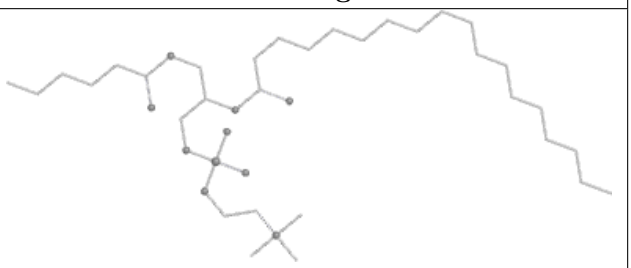
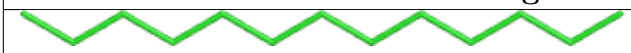
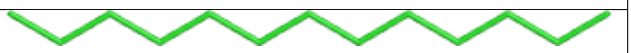
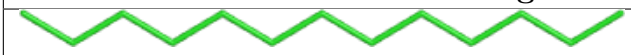
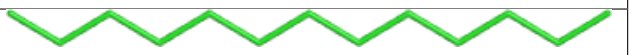
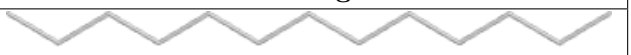
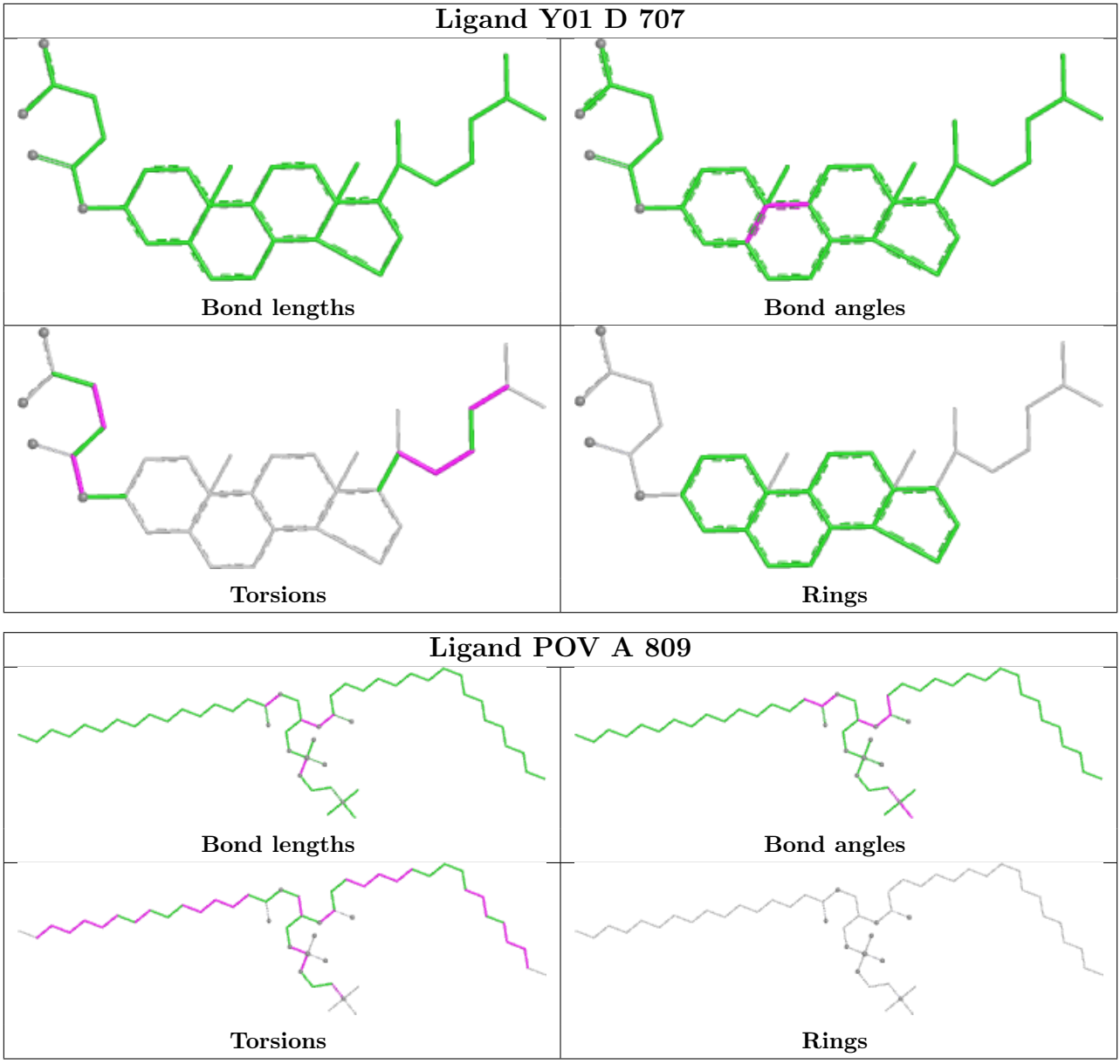
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand POV D 709	
 Bond lengths	 Bond angles
Torsions	Rings

Ligand PCW D 708	
 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.

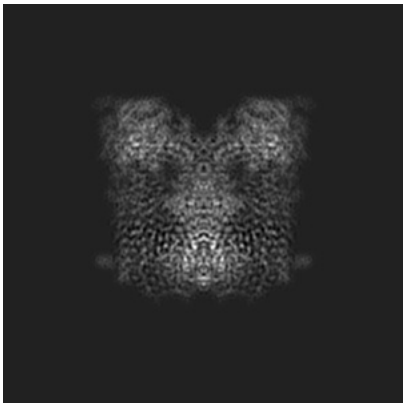
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-24892. These allow visual inspection of the internal detail of the map and identification of artifacts.

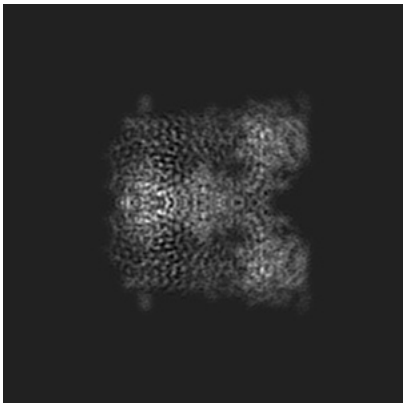
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

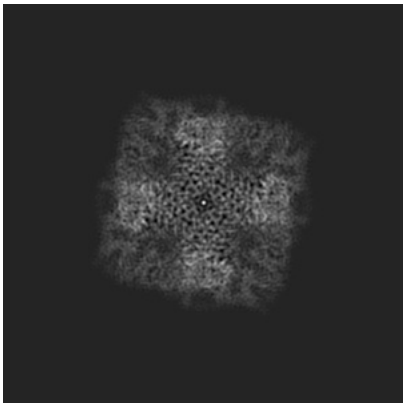
6.1.1 Primary map



X



Y



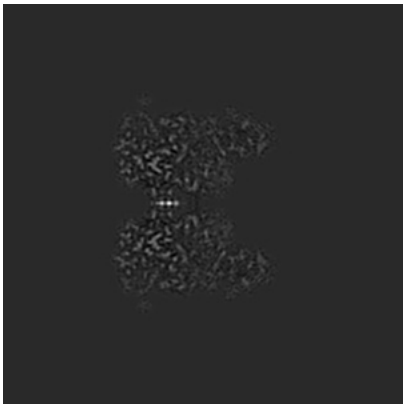
Z

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

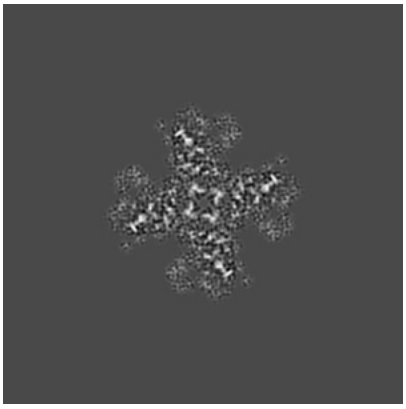
6.2 Central slices (i)

6.2.1 Primary map

X Index: 128



Y Index: 128



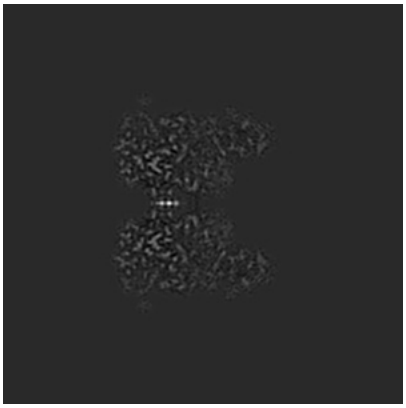
Z Index: 128

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

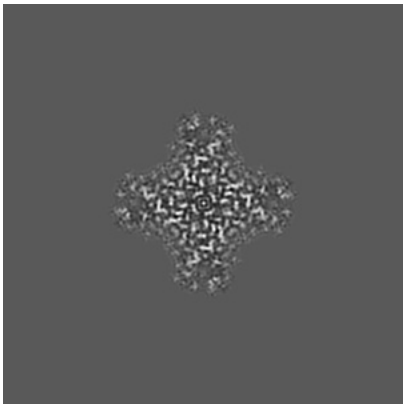
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 128



Y Index: 128

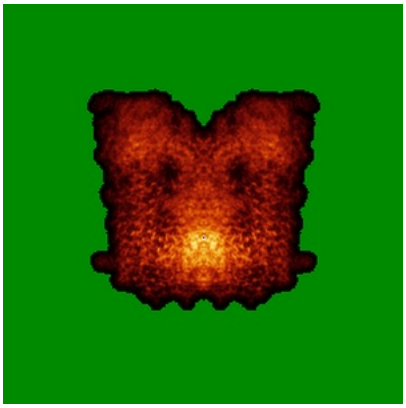


Z Index: 99

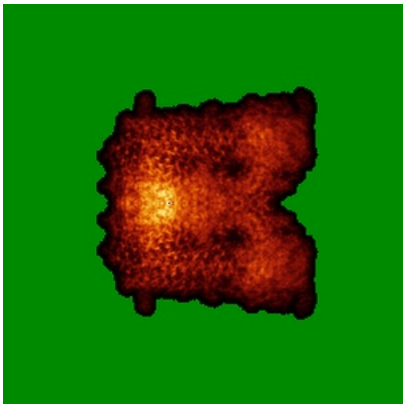
The images above show the largest variance slices of the map in three orthogonal directions.

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

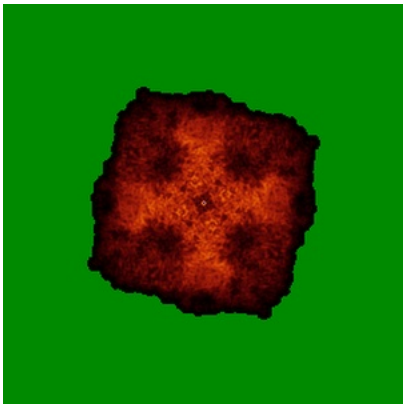
6.4.1 Primary map



X



Y

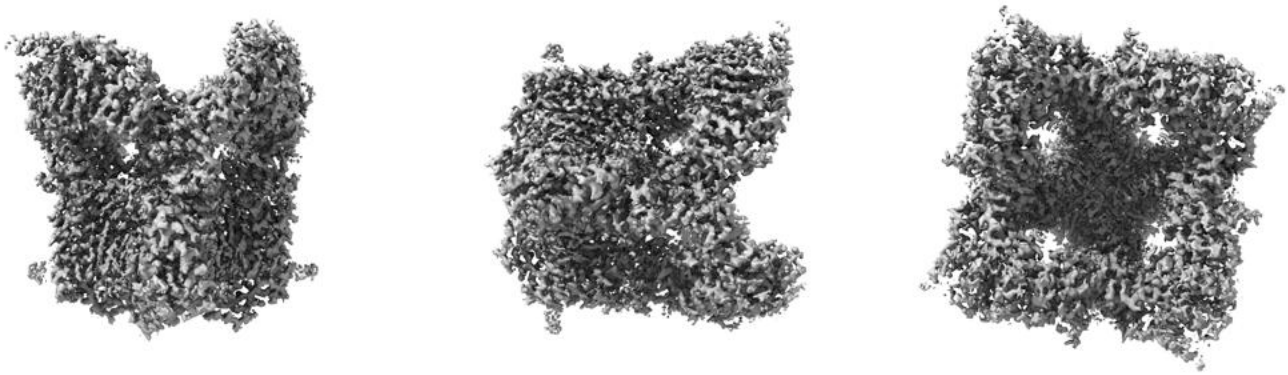


Z

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 0.0219. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

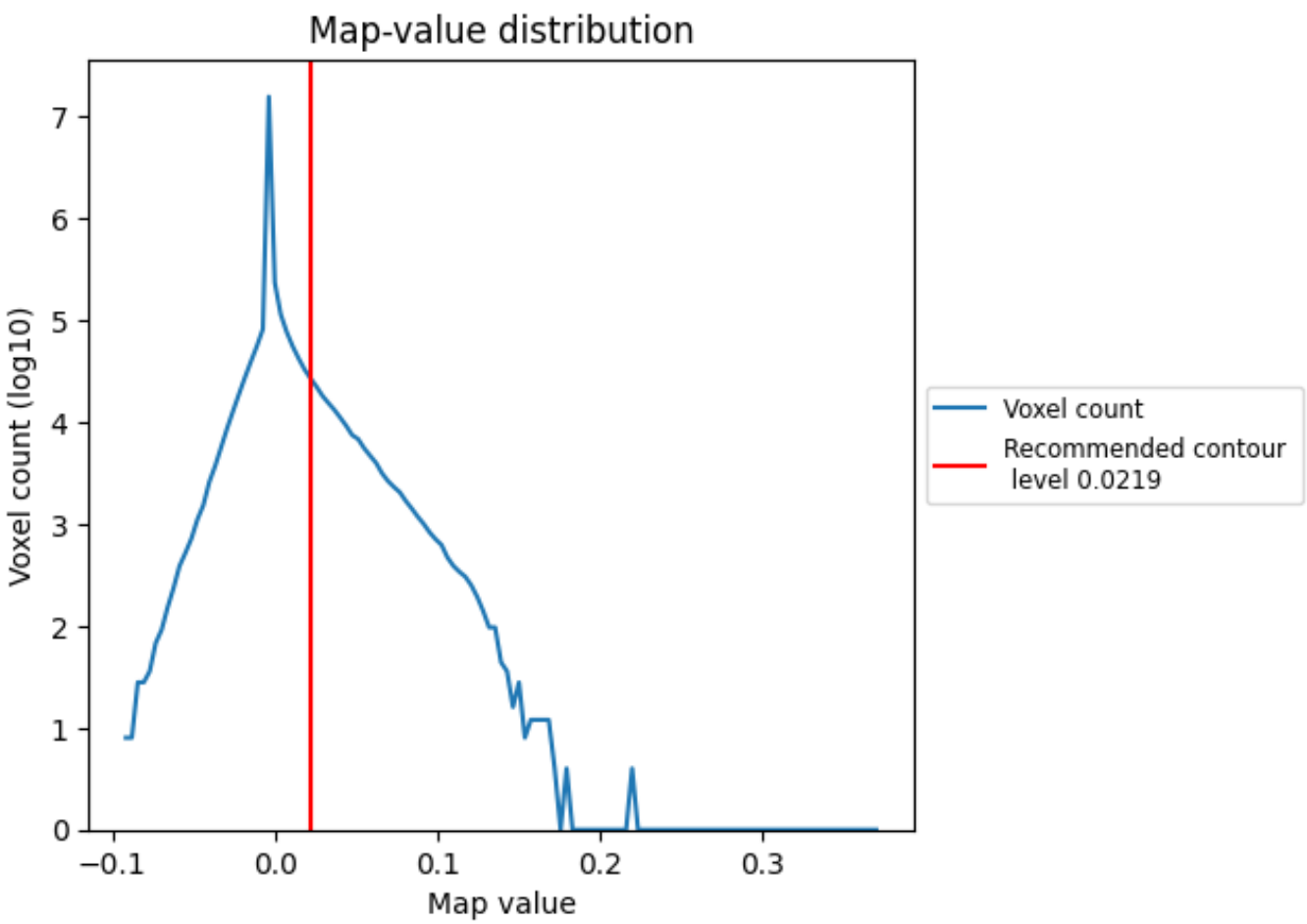
6.6 Mask visualisation (i)

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

7 Map analysis (i)

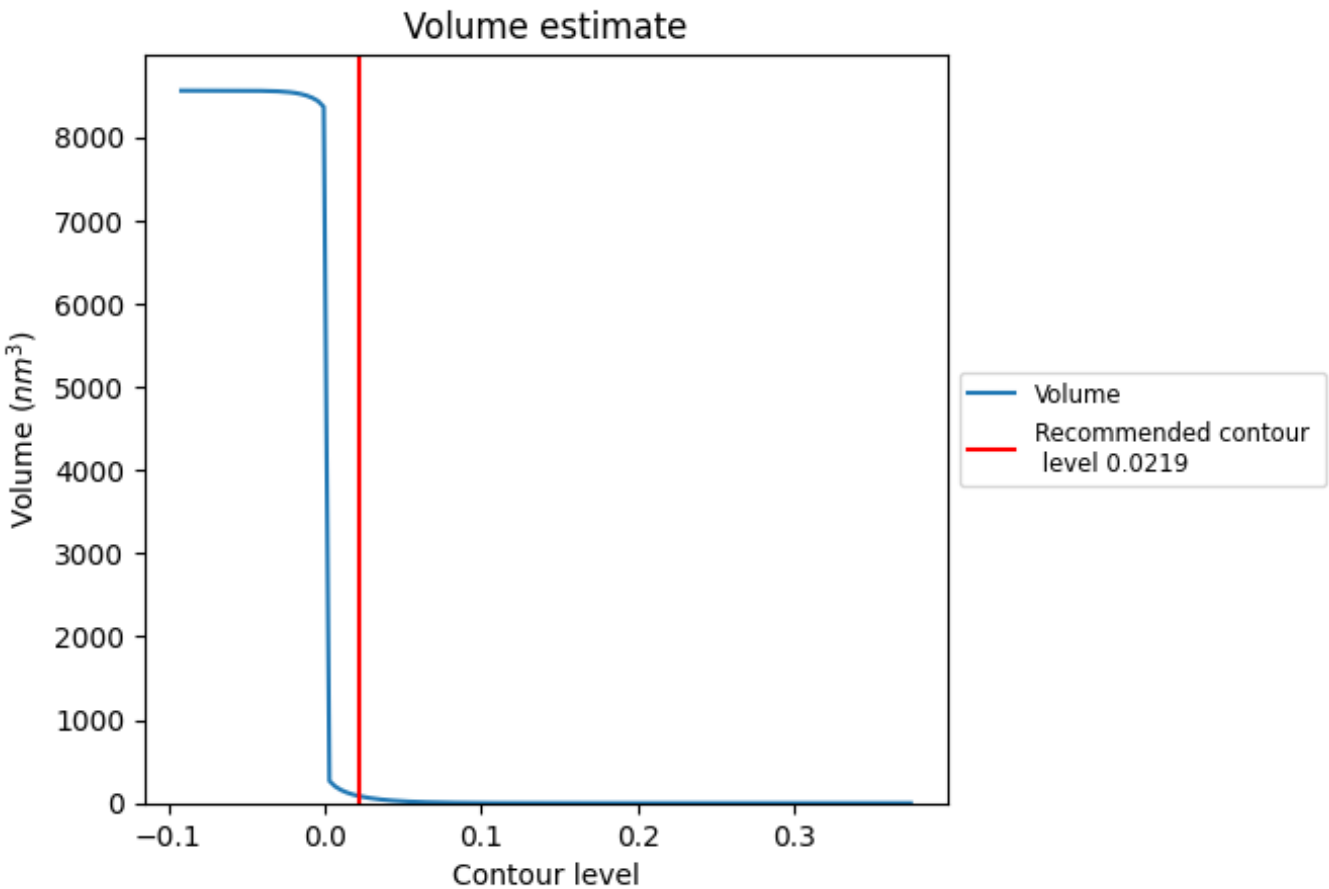
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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.

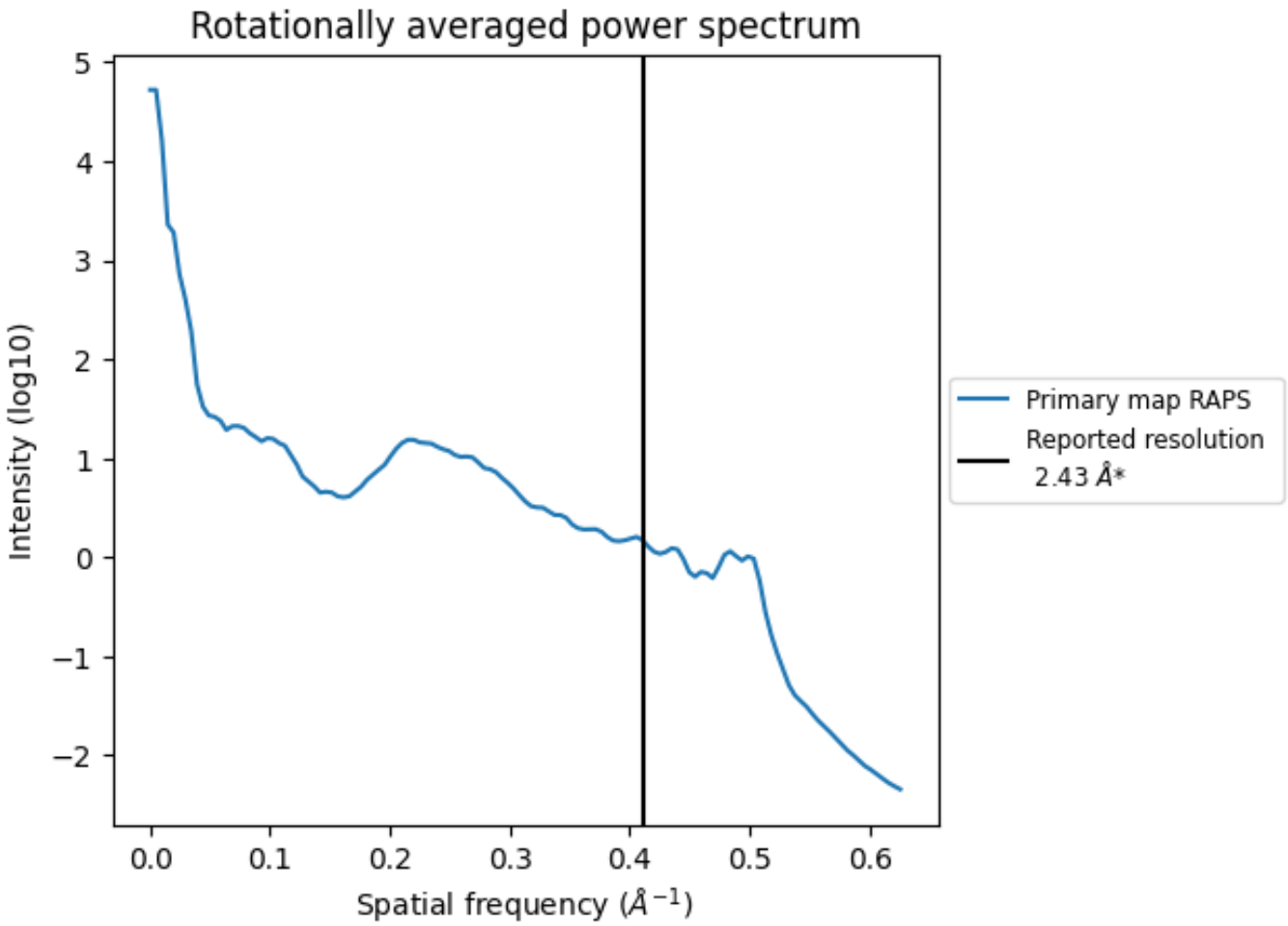
7.2 Volume estimate (i)



The volume at the recommended contour level is 86 nm^3; this corresponds to an approximate mass of 77 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 0.412 Å^{-1}

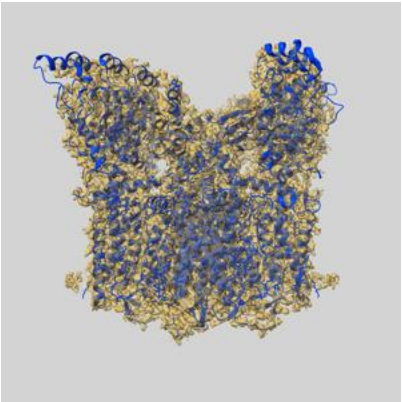
8 Fourier-Shell correlation (i)

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

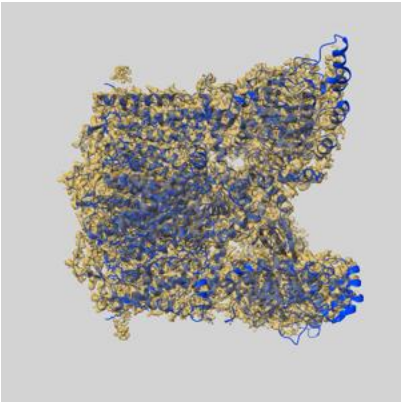
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-24892 and PDB model 7S8B. Per-residue inclusion information can be found in section 3 on page 11.

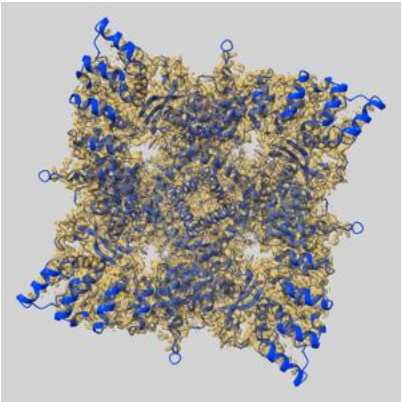
9.1 Map-model overlay (i)



X



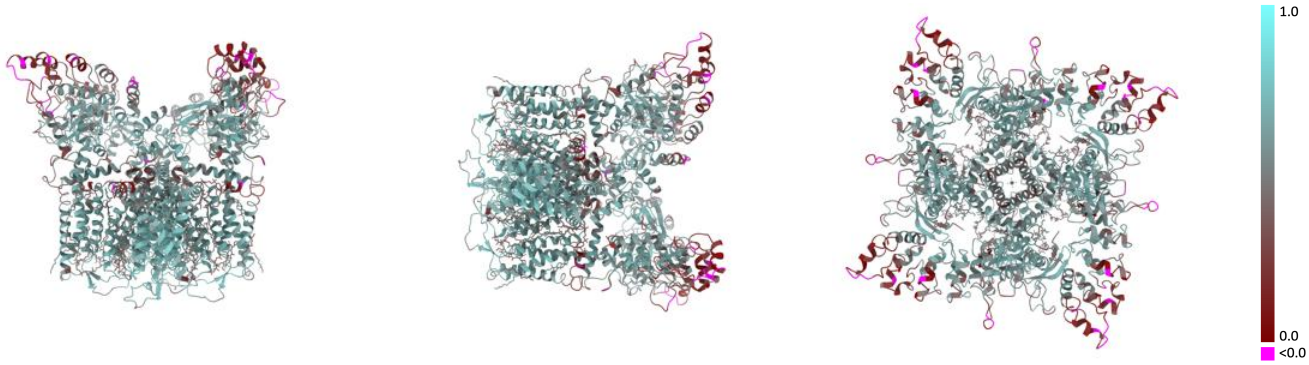
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0219 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.

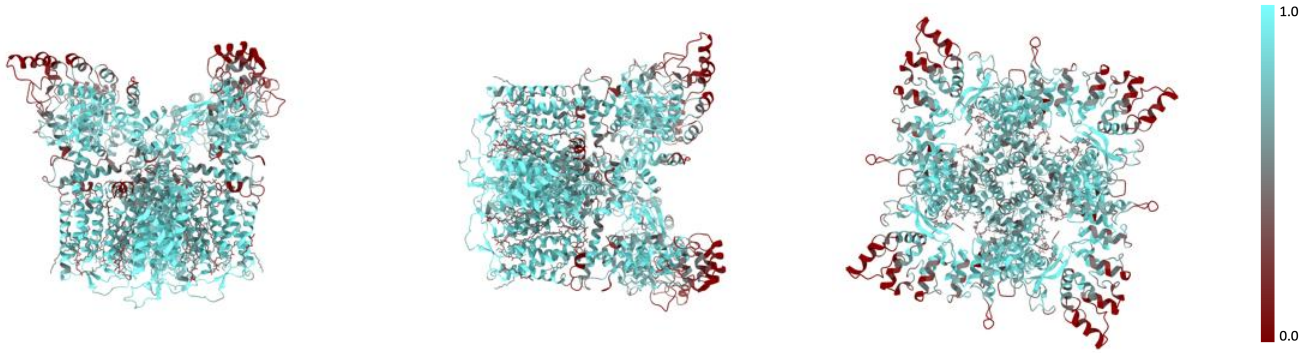
9.2 Q-score mapped to coordinate model (i)



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.

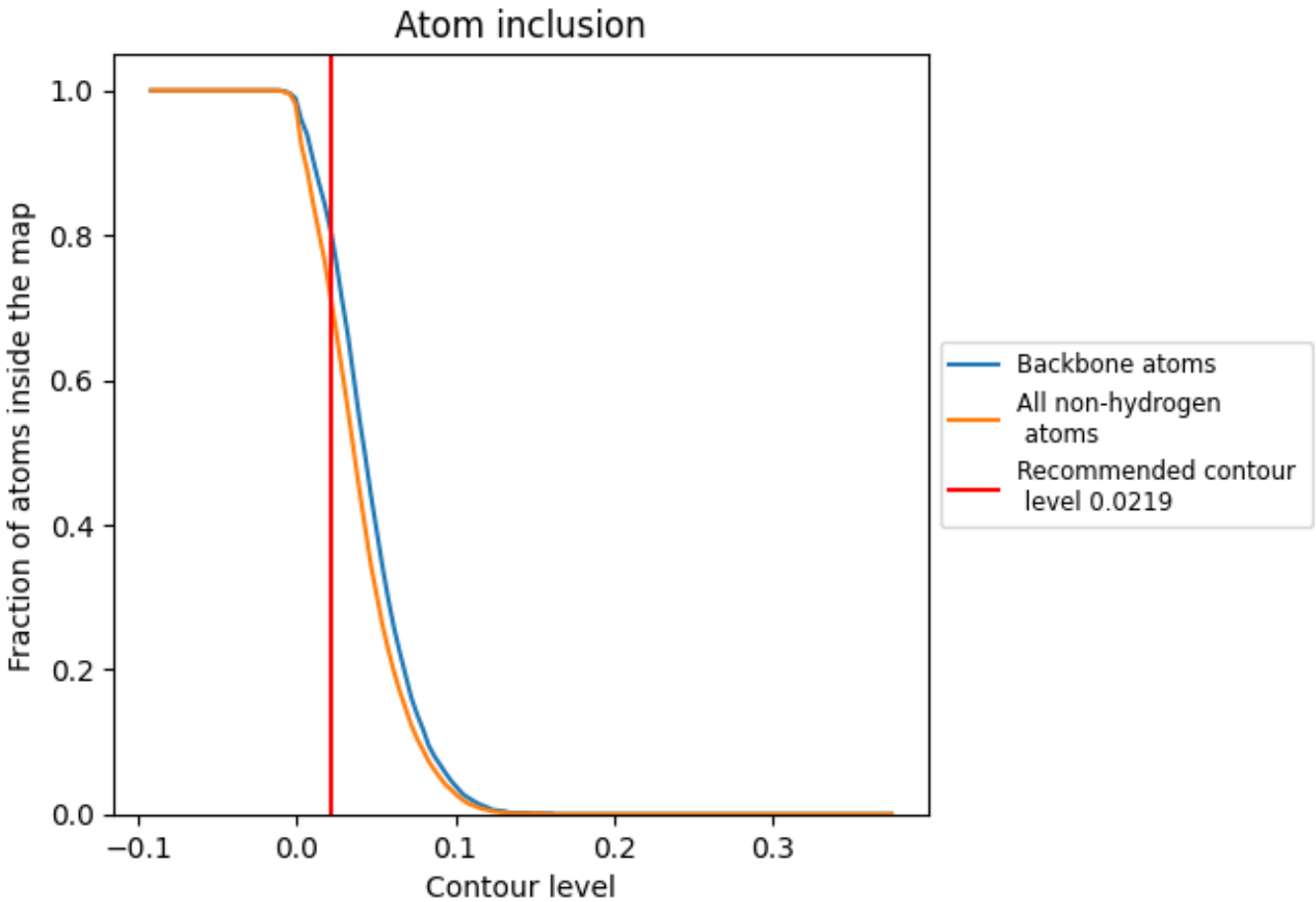
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0219).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 71% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0219) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7080	0.5320
A	0.7080	0.5320
B	0.7080	0.5320
C	0.7060	0.5310
D	0.7090	0.5320