Full wwPDB EM Validation Report ⓘ

Oct 27, 2024 – 07:35 AM EDT

PDB ID	:	7RQV
EMDB ID	:	EMD-24637
Title	:	Cryo-EM structure of the full-length TRPV1 with RTx at 4 degrees Celsius, in an intermediate-closed state, class II
Authors	:	Kwon, D.H.; Suo, Y.; Lee, S.-Y.
Deposited on	:	2021-08-08
Resolution	:	3.45 Å(reported)
Based on initial model	:	7LP9

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

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

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

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

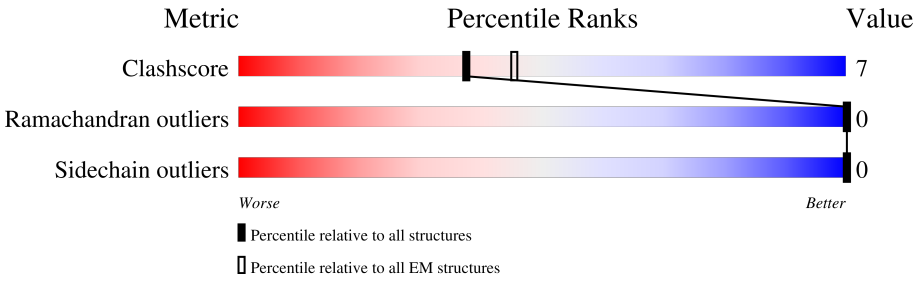
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.45 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	868	22% 58% 9% 33%
1	B	868	22% 58% 9% 33%
1	C	868	22% 58% 9% 33%
1	D	868	22% 58% 9% 33%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 35054 atoms, of which 16992 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 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	580	Total	C	H	N	O	S	0	0
			8417	2844	4059	719	772	23		
1	C	580	Total	C	H	N	O	S	0	0
			8417	2844	4059	719	772	23		
1	D	580	Total	C	H	N	O	S	0	0
			8417	2844	4059	719	772	23		
1	B	580	Total	C	H	N	O	S	0	0
			8417	2844	4059	719	772	23		

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	839	GLU	-	expression tag	UNP O35433
A	840	ASN	-	expression tag	UNP O35433
A	841	SER	-	expression tag	UNP O35433
A	842	LEU	-	expression tag	UNP O35433
A	843	GLU	-	expression tag	UNP O35433
A	844	VAL	-	expression tag	UNP O35433
A	845	LEU	-	expression tag	UNP O35433
A	846	PHE	-	expression tag	UNP O35433
A	847	GLN	-	expression tag	UNP O35433
A	848	GLY	-	expression tag	UNP O35433
A	849	PRO	-	expression tag	UNP O35433
A	850	ASP	-	expression tag	UNP O35433
A	851	TYR	-	expression tag	UNP O35433
A	852	LYS	-	expression tag	UNP O35433
A	853	ASP	-	expression tag	UNP O35433
A	854	ASP	-	expression tag	UNP O35433
A	855	ASP	-	expression tag	UNP O35433
A	856	ASP	-	expression tag	UNP O35433
A	857	LYS	-	expression tag	UNP O35433
A	858	ALA	-	expression tag	UNP O35433
A	859	HIS	-	expression tag	UNP O35433

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	860	HIS	-	expression tag	UNP O35433
A	861	HIS	-	expression tag	UNP O35433
A	862	HIS	-	expression tag	UNP O35433
A	863	HIS	-	expression tag	UNP O35433
A	864	HIS	-	expression tag	UNP O35433
A	865	HIS	-	expression tag	UNP O35433
A	866	HIS	-	expression tag	UNP O35433
A	867	HIS	-	expression tag	UNP O35433
A	868	HIS	-	expression tag	UNP O35433
C	839	GLU	-	expression tag	UNP O35433
C	840	ASN	-	expression tag	UNP O35433
C	841	SER	-	expression tag	UNP O35433
C	842	LEU	-	expression tag	UNP O35433
C	843	GLU	-	expression tag	UNP O35433
C	844	VAL	-	expression tag	UNP O35433
C	845	LEU	-	expression tag	UNP O35433
C	846	PHE	-	expression tag	UNP O35433
C	847	GLN	-	expression tag	UNP O35433
C	848	GLY	-	expression tag	UNP O35433
C	849	PRO	-	expression tag	UNP O35433
C	850	ASP	-	expression tag	UNP O35433
C	851	TYR	-	expression tag	UNP O35433
C	852	LYS	-	expression tag	UNP O35433
C	853	ASP	-	expression tag	UNP O35433
C	854	ASP	-	expression tag	UNP O35433
C	855	ASP	-	expression tag	UNP O35433
C	856	ASP	-	expression tag	UNP O35433
C	857	LYS	-	expression tag	UNP O35433
C	858	ALA	-	expression tag	UNP O35433
C	859	HIS	-	expression tag	UNP O35433
C	860	HIS	-	expression tag	UNP O35433
C	861	HIS	-	expression tag	UNP O35433
C	862	HIS	-	expression tag	UNP O35433
C	863	HIS	-	expression tag	UNP O35433
C	864	HIS	-	expression tag	UNP O35433
C	865	HIS	-	expression tag	UNP O35433
C	866	HIS	-	expression tag	UNP O35433
C	867	HIS	-	expression tag	UNP O35433
C	868	HIS	-	expression tag	UNP O35433
D	839	GLU	-	expression tag	UNP O35433
D	840	ASN	-	expression tag	UNP O35433
D	841	SER	-	expression tag	UNP O35433

Continued on next page...

Continued from previous page...

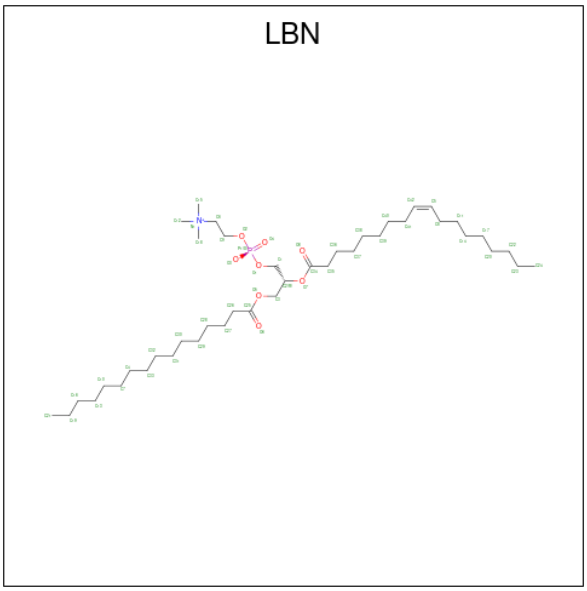
Chain	Residue	Modelled	Actual	Comment	Reference
D	842	LEU	-	expression tag	UNP O35433
D	843	GLU	-	expression tag	UNP O35433
D	844	VAL	-	expression tag	UNP O35433
D	845	LEU	-	expression tag	UNP O35433
D	846	PHE	-	expression tag	UNP O35433
D	847	GLN	-	expression tag	UNP O35433
D	848	GLY	-	expression tag	UNP O35433
D	849	PRO	-	expression tag	UNP O35433
D	850	ASP	-	expression tag	UNP O35433
D	851	TYR	-	expression tag	UNP O35433
D	852	LYS	-	expression tag	UNP O35433
D	853	ASP	-	expression tag	UNP O35433
D	854	ASP	-	expression tag	UNP O35433
D	855	ASP	-	expression tag	UNP O35433
D	856	ASP	-	expression tag	UNP O35433
D	857	LYS	-	expression tag	UNP O35433
D	858	ALA	-	expression tag	UNP O35433
D	859	HIS	-	expression tag	UNP O35433
D	860	HIS	-	expression tag	UNP O35433
D	861	HIS	-	expression tag	UNP O35433
D	862	HIS	-	expression tag	UNP O35433
D	863	HIS	-	expression tag	UNP O35433
D	864	HIS	-	expression tag	UNP O35433
D	865	HIS	-	expression tag	UNP O35433
D	866	HIS	-	expression tag	UNP O35433
D	867	HIS	-	expression tag	UNP O35433
D	868	HIS	-	expression tag	UNP O35433
B	839	GLU	-	expression tag	UNP O35433
B	840	ASN	-	expression tag	UNP O35433
B	841	SER	-	expression tag	UNP O35433
B	842	LEU	-	expression tag	UNP O35433
B	843	GLU	-	expression tag	UNP O35433
B	844	VAL	-	expression tag	UNP O35433
B	845	LEU	-	expression tag	UNP O35433
B	846	PHE	-	expression tag	UNP O35433
B	847	GLN	-	expression tag	UNP O35433
B	848	GLY	-	expression tag	UNP O35433
B	849	PRO	-	expression tag	UNP O35433
B	850	ASP	-	expression tag	UNP O35433
B	851	TYR	-	expression tag	UNP O35433
B	852	LYS	-	expression tag	UNP O35433
B	853	ASP	-	expression tag	UNP O35433

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	854	ASP	-	expression tag	UNP O35433
B	855	ASP	-	expression tag	UNP O35433
B	856	ASP	-	expression tag	UNP O35433
B	857	LYS	-	expression tag	UNP O35433
B	858	ALA	-	expression tag	UNP O35433
B	859	HIS	-	expression tag	UNP O35433
B	860	HIS	-	expression tag	UNP O35433
B	861	HIS	-	expression tag	UNP O35433
B	862	HIS	-	expression tag	UNP O35433
B	863	HIS	-	expression tag	UNP O35433
B	864	HIS	-	expression tag	UNP O35433
B	865	HIS	-	expression tag	UNP O35433
B	866	HIS	-	expression tag	UNP O35433
B	867	HIS	-	expression tag	UNP O35433
B	868	HIS	-	expression tag	UNP O35433

- Molecule 2 is 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine (three-letter code: LBN) (formula: $C_{42}H_{82}NO_8P$).



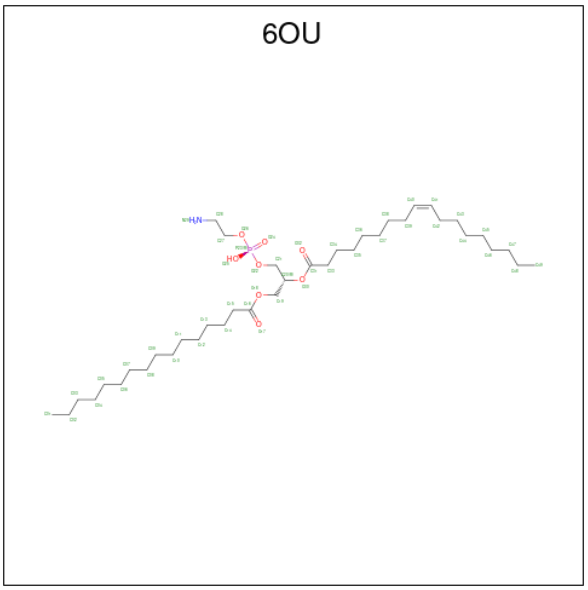
Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	H	N	O	P	0
			77	23	44	1	8	1	
2	C	1	Total	C	H	N	O	P	0
			77	23	44	1	8	1	
2	D	1	Total	C	H	N	O	P	0
			77	23	44	1	8	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						AltConf
2	B	1	Total	C	H	N	O	P	0
			77	23	44	1	8	1	

- Molecule 3 is [(2 {R})-1-[2-azanylethoxy(oxidanyl)phosphoryl]oxy-3-hexadecanoyloxy-propan-2-yl] ({Z})-octadec-9-enoate (three-letter code: 6OU) (formula: $C_{39}H_{76}NO_8P$).



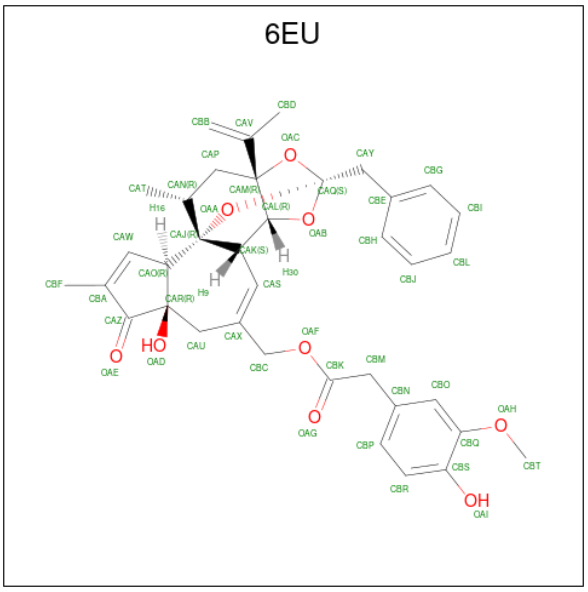
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	H	O	P	0
			80	26	45	8	1	
3	A	1	Total	C	H	O	P	0
			74	24	41	8	1	
3	A	1	Total	C	H			0
			29	10	19			
3	A	1	Total	C	H	O	P	0
			74	24	41	8	1	
3	C	1	Total	C	H	O	P	0
			80	26	45	8	1	
3	C	1	Total	C	H	O	P	0
			74	24	41	8	1	
3	C	1	Total	C	H			0
			29	10	19			
3	D	1	Total	C	H	O	P	0
			80	26	45	8	1	
3	D	1	Total	C	H			0
			29	10	19			
3	B	1	Total	C	H	O	P	0
			80	26	45	8	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
3	B	1	Total C H O P 74 24 41 8 1	0
3	B	1	Total C H 29 10 19	0

- Molecule 4 is resiniferatoxin (three-letter code: 6EU) (formula: $C_{37}H_{40}O_9$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total C H O 86 37 40 9	0
4	C	1	Total C H O 86 37 40 9	0
4	D	1	Total C H O 86 37 40 9	0
4	B	1	Total C H O 86 37 40 9	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

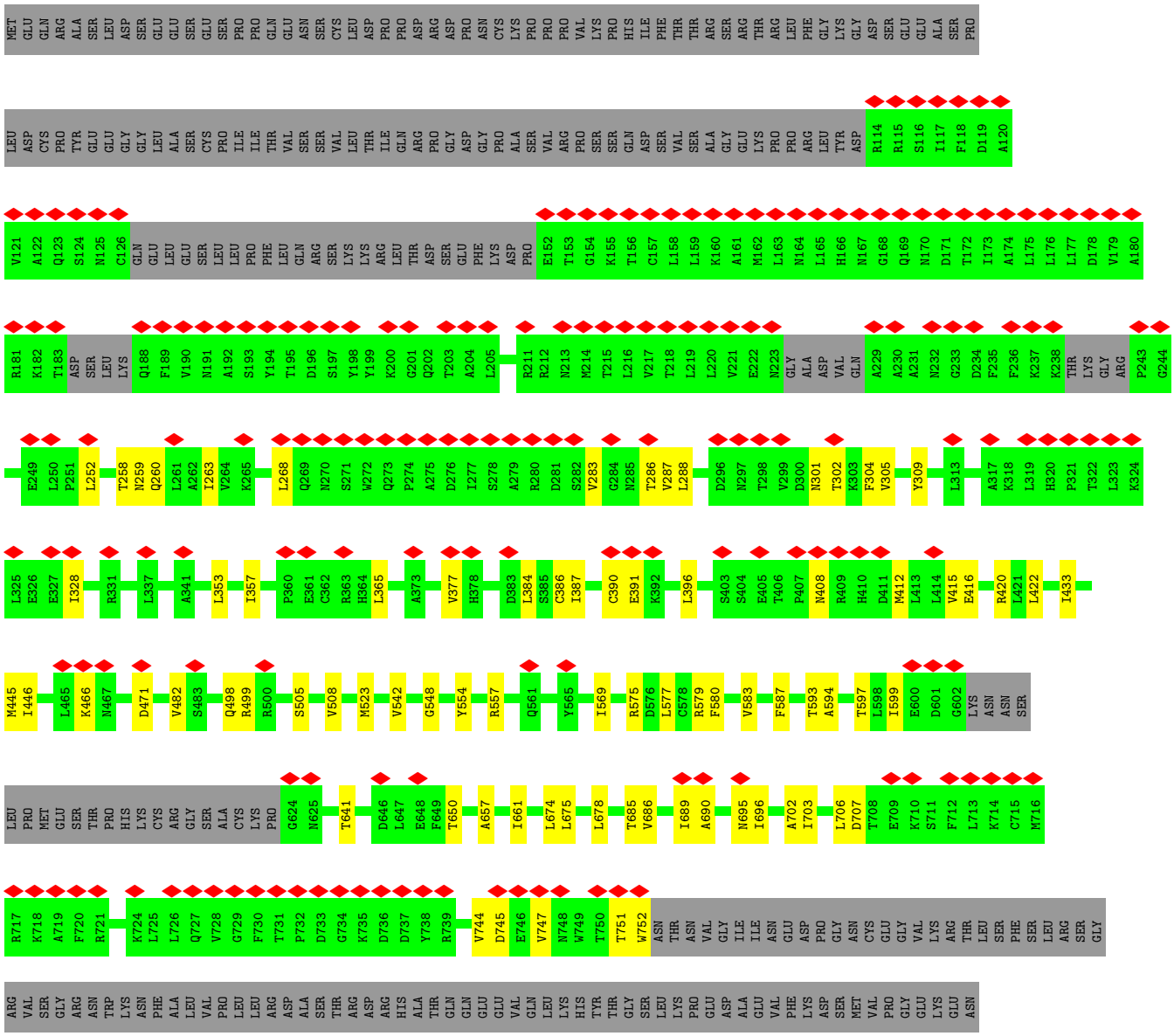
Mol	Chain	Residues	Atoms	AltConf
5	A	2	Total Na 2 2	0

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.

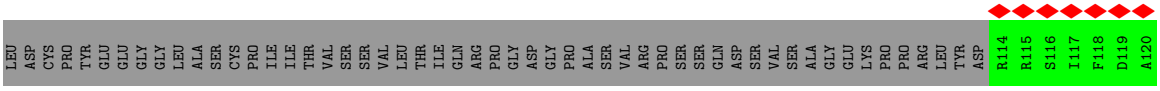
- Molecule 1: Transient receptor potential cation channel subfamily V member 1

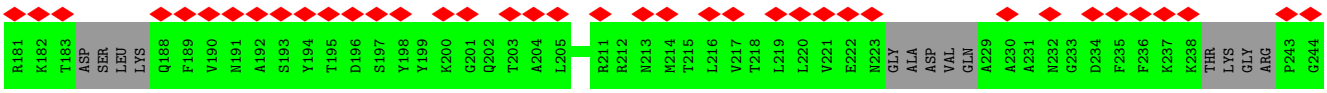
Chain A:

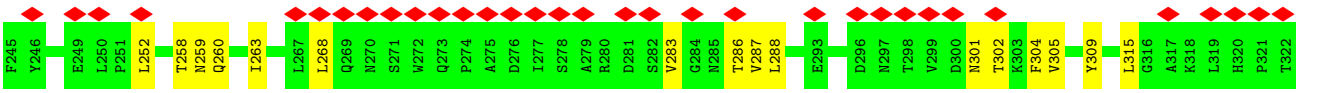


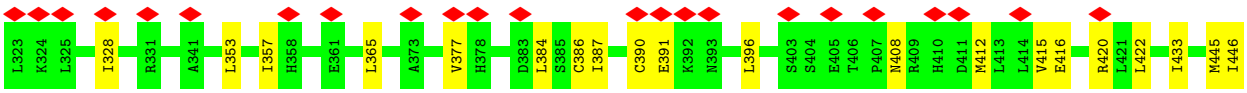
• Molecule 1: Transient receptor potential cation channel subfamily V member 1

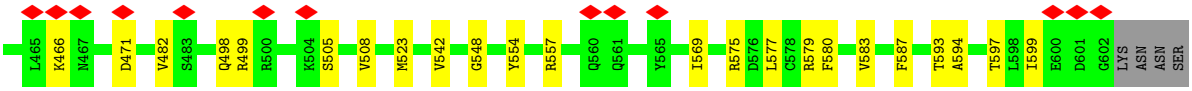
Chain C:

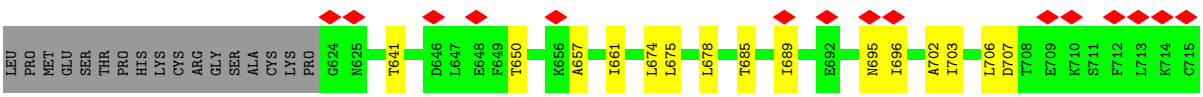


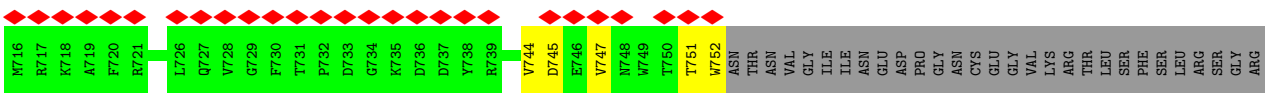


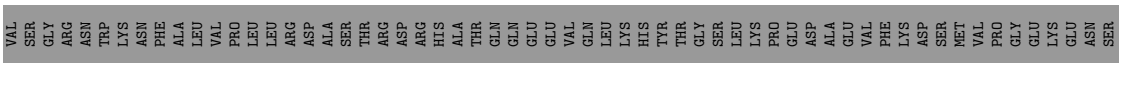






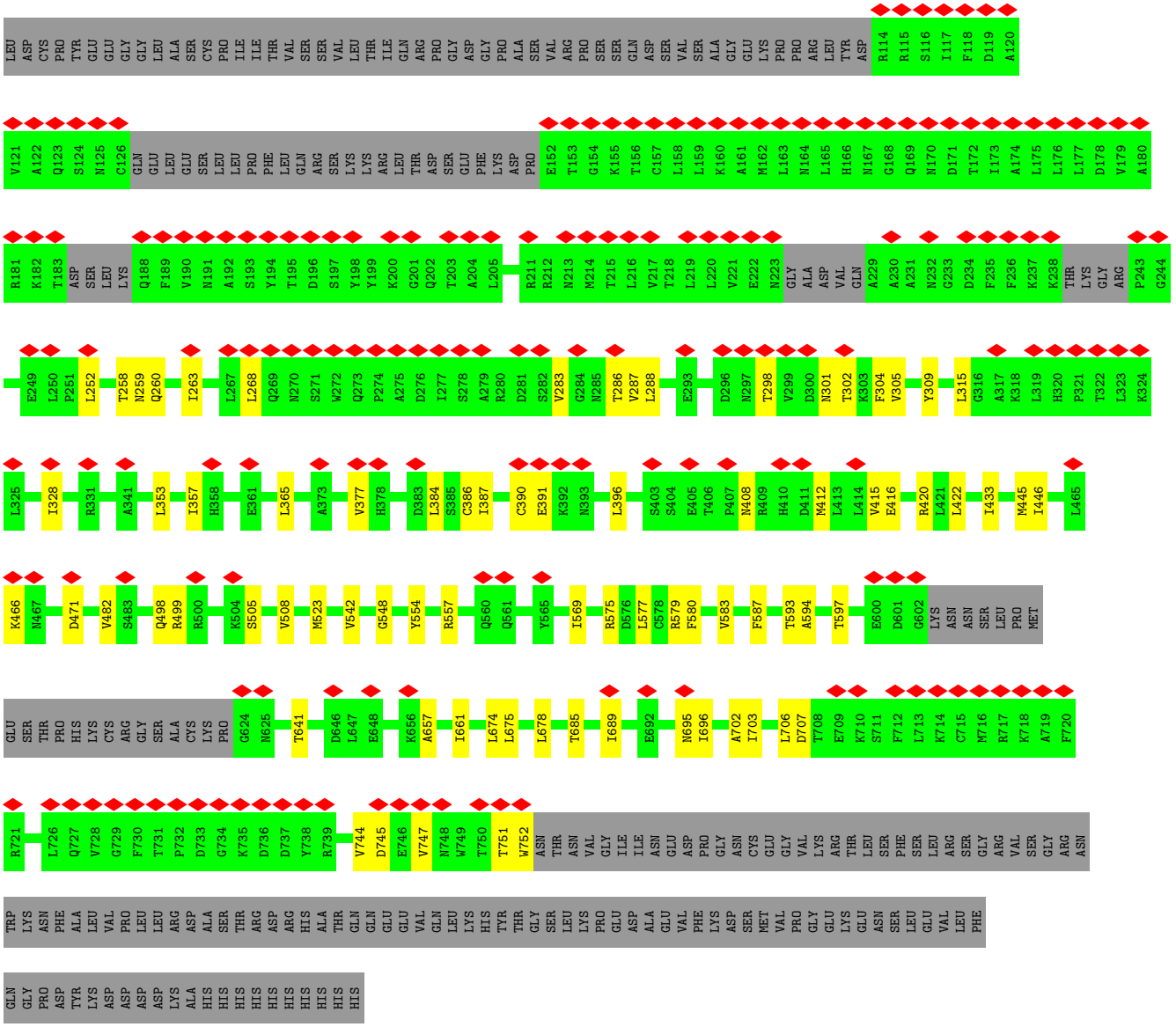






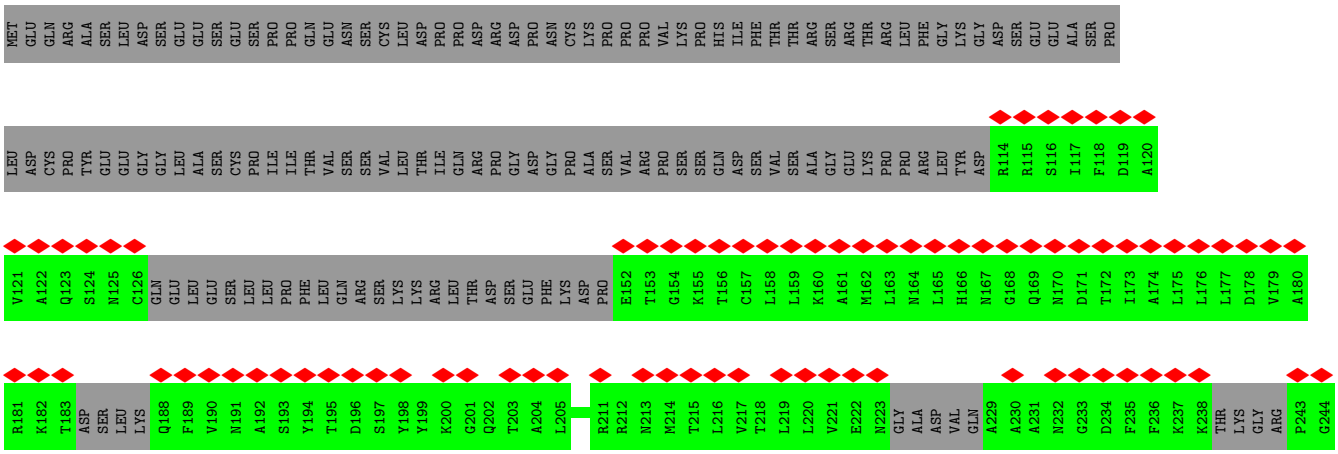
• Molecule 1: Transient receptor potential cation channel subfamily V member 1

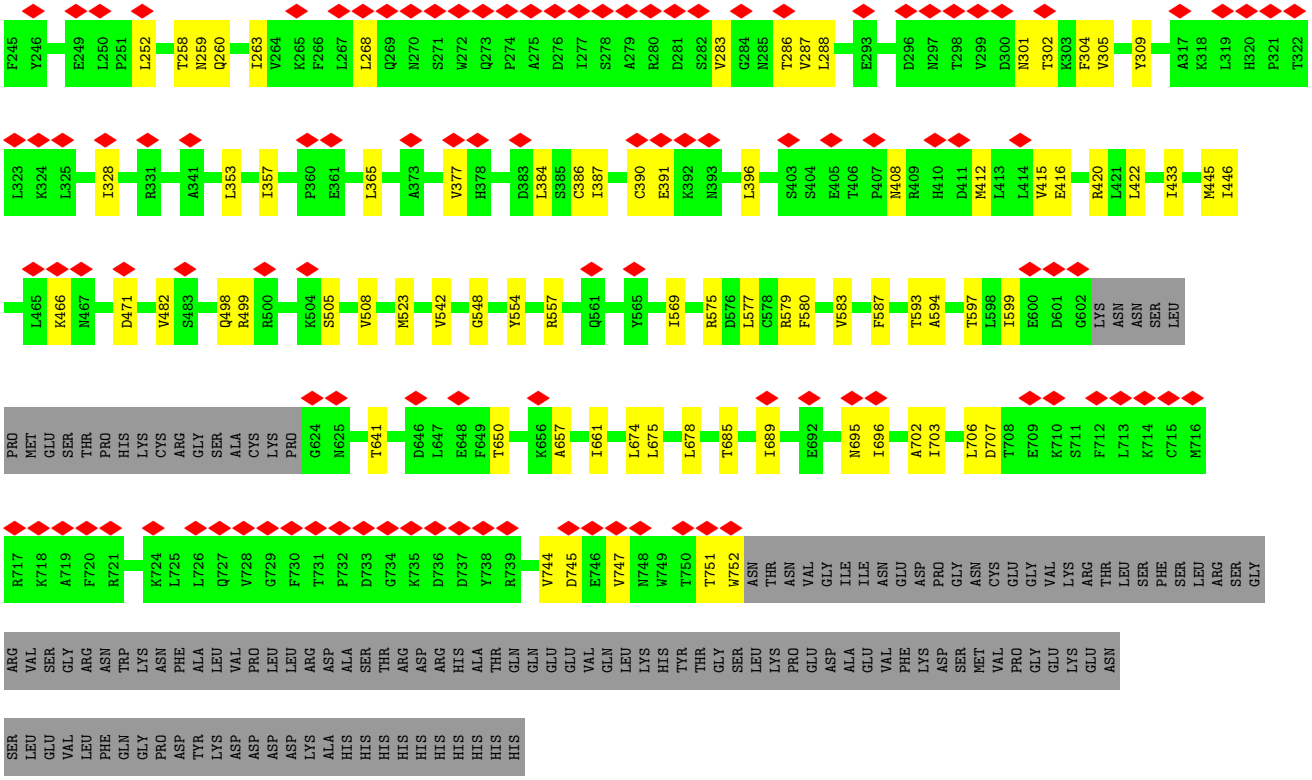
Chain D:



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

Chain B:




F245 Y246 E249 L250 P251 L252 T258 N259 Q260 I263 V264 K265 F266 L267 L268 Q269 N270 S271 W272 Q273 P274 A275 D276 I277 S278 A279 R280 D281 S282 V283 G284 N285 T286 V287 L288 E293 D296 N297 T298 V299 D300 N301 T302 K303 F304 V305 Y309 A317 K318 L319 H320 P321 T322
L323 K324 L325 I328 R331 A341 L353 I357 P360 E361 L365 A373 V377 H378 D383 L384 S385 C386 I387 C390 E391 K392 N393 L396 S403 S404 E405 T406 P407 N408 R409 H410 D411 M412 L413 L414 V415 E416 R420 L421 L422 T433 M445 I446
L465 K466 N467 D471 V482 S483 Q498 R499 R500 K504 S505 V508 M523 V542 G548 Y554 R557 Q561 Y565 I569 R575 D576 L577 C578 R579 F580 V583 F587 T593 A594 T597 L598 I599 E600 D601 G602 LYS ASN ASN SER LEU
PRO MET GLU SER THR PRO HIS LYS CYS ARG GLY SER ALA CYS LYS PRO G624 N625 T641 D646 L647 E648 F649 T650 K656 A657 I661 L674 L675 L678 T685 I689 E692 N695 I696 A702 I703 L706 D707 T708 E709 K710 S711 F712 L713 K714 C715 M716
R717 K718 A719 F720 R721 K724 L725 L726 Q727 V728 G729 F730 T731 P732 D733 G734 K735 D736 D737 Y738 R739 V744 D745 E746 V747 N748 W749 T750 T751 W752 ASN THR ASN VAL GLY ILE ILE ASN GLU ASP PRO GLY ASN CYS GLU GLY VAL LYS ARG THR LEU SER PHE SER LEU ARG SER GLY
ARG VAL SER GLY ARG ASN TRP LYS ASN PHE ALA LEU VAL PRO LEU LEU ARG ASP ALA SER THR ARG ASP ARG HIS ALA THR GLN GLU GLU VAL GLN LEU LYS HIS TYR THR GLY SER LEU LYS PRO GLU ASP ALA GLU VAL PHE LYS ASP SER MET VAL PRO GLY GLU LYS GLU ASN
SER LEU GLU VAL LEU PHE GLN GLY PRO ASP TYR LYS ASP ASP ASP ASP LYS ALA HIS HIS HIS HIS HIS HIS HIS HIS HIS HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	70786	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.142	Depositor
Minimum map value	-0.092	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0254	Depositor
Map size (Å)	276.48, 276.48, 276.48	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LBN, NA, 6EU, 6OU

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	0.29	0/4455	0.48	0/6058
1	B	0.29	0/4455	0.48	0/6058
1	C	0.28	0/4455	0.48	0/6058
1	D	0.29	0/4455	0.48	0/6058
All	All	0.28	0/17820	0.48	0/24232

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4358	4059	4074	64	0
1	B	4358	4059	4074	60	0
1	C	4358	4059	4074	61	0
1	D	4358	4059	4074	61	0
2	A	33	44	0	0	0
2	B	33	44	0	0	0
2	C	33	44	0	0	0
2	D	33	44	0	0	0
3	A	111	146	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	78	105	0	0	0
3	C	78	105	0	0	0
3	D	45	64	0	0	0
4	A	46	40	0	1	0
4	B	46	40	0	1	0
4	C	46	40	0	1	0
4	D	46	40	0	1	0
5	A	2	0	0	0	0
All	All	18062	16992	16296	246	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 7.

All (246) 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:D:466:LYS:HB2	1:D:471:ASP:OD2	1.72	0.90
1:C:466:LYS:HB2	1:C:471:ASP:OD2	1.72	0.90
1:A:466:LYS:HB2	1:A:471:ASP:OD2	1.72	0.89
1:B:466:LYS:HB2	1:B:471:ASP:OD2	1.72	0.88
1:C:365:LEU:HD12	1:C:365:LEU:O	1.83	0.79
1:D:353:LEU:HD12	1:D:415:VAL:HG11	1.65	0.79
1:C:353:LEU:HD12	1:C:415:VAL:HG11	1.65	0.78
1:B:365:LEU:HD12	1:B:365:LEU:O	1.83	0.78
1:D:365:LEU:HD12	1:D:365:LEU:O	1.83	0.78
1:A:365:LEU:O	1:A:365:LEU:HD12	1.83	0.77
1:A:353:LEU:HD12	1:A:415:VAL:HG11	1.65	0.77
1:B:353:LEU:HD12	1:B:415:VAL:HG11	1.65	0.76
1:C:554:TYR:O	1:C:557:ARG:HG2	1.87	0.75
1:D:384:LEU:O	1:D:384:LEU:HD23	1.87	0.75
1:A:384:LEU:O	1:A:384:LEU:HD23	1.87	0.75
1:D:554:TYR:O	1:D:557:ARG:HG2	1.87	0.75
1:B:554:TYR:O	1:B:557:ARG:HG2	1.87	0.75
1:B:384:LEU:HD23	1:B:384:LEU:O	1.87	0.74
1:A:554:TYR:O	1:A:557:ARG:HG2	1.87	0.74
1:C:384:LEU:HD23	1:C:384:LEU:O	1.87	0.74
1:D:498:GLN:OE1	1:D:499:ARG:NH1	2.23	0.72
1:B:498:GLN:OE1	1:B:499:ARG:NH1	2.23	0.71
1:A:498:GLN:OE1	1:A:499:ARG:NH1	2.23	0.71
1:C:498:GLN:OE1	1:C:499:ARG:NH1	2.23	0.71
1:A:577:LEU:O	1:A:577:LEU:HD23	1.92	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:577:LEU:HD23	1:B:577:LEU:O	1.92	0.70
1:C:577:LEU:HD23	1:C:577:LEU:O	1.92	0.69
1:D:577:LEU:O	1:D:577:LEU:HD23	1.92	0.69
1:C:580:PHE:CD2	1:C:678:LEU:HD22	2.31	0.65
1:D:580:PHE:CD2	1:D:678:LEU:HD22	2.31	0.65
1:B:580:PHE:CD2	1:B:678:LEU:HD22	2.31	0.65
1:A:580:PHE:CD2	1:A:678:LEU:HD22	2.31	0.65
1:C:288:LEU:HD23	1:C:309:TYR:CE2	2.35	0.61
1:A:482:VAL:HA	1:A:523:MET:HE2	1.82	0.61
1:B:288:LEU:HD23	1:B:309:TYR:CE2	2.36	0.61
1:B:482:VAL:HA	1:B:523:MET:HE2	1.83	0.61
1:D:288:LEU:HD23	1:D:309:TYR:CE2	2.36	0.61
1:C:482:VAL:HA	1:C:523:MET:HE2	1.82	0.61
1:A:288:LEU:HD23	1:A:309:TYR:CE2	2.36	0.61
1:D:482:VAL:HA	1:D:523:MET:HE2	1.82	0.60
1:A:583:VAL:HG12	1:A:583:VAL:O	2.03	0.59
1:A:377:VAL:HG12	1:A:747:VAL:HG22	1.85	0.58
1:D:396:LEU:HD22	1:D:422:LEU:HD21	1.85	0.58
1:B:583:VAL:HG12	1:B:583:VAL:O	2.03	0.58
1:C:396:LEU:HD22	1:C:422:LEU:HD21	1.85	0.58
1:D:301:ASN:HA	1:D:304:PHE:CE2	2.39	0.58
1:A:396:LEU:HD22	1:A:422:LEU:HD21	1.85	0.58
1:B:301:ASN:HA	1:B:304:PHE:CE2	2.39	0.58
1:D:377:VAL:HG12	1:D:747:VAL:HG22	1.85	0.58
1:D:583:VAL:HG12	1:D:583:VAL:O	2.03	0.58
1:A:301:ASN:HA	1:A:304:PHE:CE2	2.39	0.58
1:C:301:ASN:HA	1:C:304:PHE:CE2	2.39	0.58
1:C:377:VAL:HG12	1:C:747:VAL:HG22	1.85	0.57
1:B:377:VAL:HG12	1:B:747:VAL:HG22	1.85	0.57
1:B:396:LEU:HD22	1:B:422:LEU:HD21	1.85	0.57
1:C:583:VAL:HG12	1:C:583:VAL:O	2.03	0.57
1:A:416:GLU:O	1:A:420:ARG:NH2	2.39	0.56
1:B:416:GLU:O	1:B:420:ARG:NH2	2.39	0.56
1:A:288:LEU:HD23	1:A:309:TYR:CZ	2.41	0.56
1:D:416:GLU:O	1:D:420:ARG:NH2	2.39	0.56
1:B:288:LEU:HD23	1:B:309:TYR:CZ	2.41	0.56
1:D:288:LEU:HD23	1:D:309:TYR:CZ	2.41	0.56
1:C:288:LEU:HD23	1:C:309:TYR:CZ	2.41	0.55
1:C:416:GLU:O	1:C:420:ARG:NH2	2.39	0.55
1:A:685:THR:O	1:A:689:ILE:HG12	2.07	0.55
1:D:357:ILE:HD12	1:D:365:LEU:HD12	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:685:THR:O	1:B:689:ILE:HG12	2.07	0.54
1:D:685:THR:O	1:D:689:ILE:HG12	2.07	0.54
1:B:357:ILE:HD12	1:B:365:LEU:HD12	1.89	0.54
1:B:554:TYR:O	1:B:557:ARG:CG	2.56	0.54
1:C:357:ILE:HD12	1:C:365:LEU:HD12	1.89	0.54
1:A:357:ILE:HD12	1:A:365:LEU:HD12	1.89	0.54
1:C:554:TYR:O	1:C:557:ARG:CG	2.56	0.54
1:C:593:THR:O	1:C:597:THR:HG23	2.08	0.53
1:C:685:THR:O	1:C:689:ILE:HG12	2.07	0.53
1:A:593:THR:O	1:A:597:THR:HG23	2.08	0.53
1:D:593:THR:O	1:D:597:THR:HG23	2.08	0.53
1:B:593:THR:O	1:B:597:THR:HG23	2.08	0.53
1:A:587:PHE:CD2	1:A:674:LEU:HD11	2.44	0.53
1:D:390:CYS:SG	1:D:391:GLU:N	2.82	0.53
1:A:390:CYS:SG	1:A:391:GLU:N	2.82	0.53
1:C:390:CYS:SG	1:C:391:GLU:N	2.82	0.53
1:D:587:PHE:CD2	1:D:674:LEU:HD11	2.44	0.53
1:B:390:CYS:SG	1:B:391:GLU:N	2.82	0.53
1:C:353:LEU:HD22	1:C:387:ILE:HD11	1.90	0.52
1:B:587:PHE:CD2	1:B:674:LEU:HD11	2.44	0.52
1:D:353:LEU:HD22	1:D:387:ILE:HD11	1.90	0.52
1:D:554:TYR:O	1:D:557:ARG:CG	2.56	0.52
1:A:554:TYR:O	1:A:557:ARG:CG	2.56	0.52
1:B:353:LEU:HD22	1:B:387:ILE:HD11	1.90	0.52
1:A:353:LEU:HD22	1:A:387:ILE:HD11	1.91	0.52
1:C:587:PHE:CD2	1:C:674:LEU:HD11	2.44	0.52
1:C:259:ASN:OD1	1:C:259:ASN:O	2.29	0.51
1:D:259:ASN:OD1	1:D:259:ASN:O	2.29	0.51
1:C:258:THR:HG22	1:C:258:THR:O	2.11	0.50
1:B:259:ASN:OD1	1:B:259:ASN:O	2.29	0.50
1:D:751:THR:HG23	1:D:752:TRP:N	2.27	0.50
1:B:258:THR:O	1:B:258:THR:HG22	2.12	0.50
1:B:446:ILE:HG22	1:B:446:ILE:O	2.12	0.50
1:C:751:THR:HG23	1:C:752:TRP:N	2.27	0.50
1:A:259:ASN:OD1	1:A:259:ASN:O	2.29	0.50
1:C:446:ILE:O	1:C:446:ILE:HG22	2.12	0.50
1:B:445:MET:HE1	1:B:548:GLY:HA3	1.94	0.50
1:D:258:THR:HG22	1:D:258:THR:O	2.12	0.50
1:B:751:THR:HG23	1:B:752:TRP:N	2.27	0.50
1:A:446:ILE:O	1:A:446:ILE:HG22	2.12	0.49
1:A:751:THR:HG23	1:A:752:TRP:N	2.27	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:446:ILE:HG22	1:D:446:ILE:O	2.11	0.49
1:B:641:THR:HG22	1:B:675:LEU:HD11	1.94	0.49
1:A:641:THR:HG22	1:A:675:LEU:HD11	1.95	0.49
1:C:445:MET:HE1	1:C:548:GLY:HA3	1.95	0.49
1:B:505:SER:HA	1:B:508:VAL:HG12	1.95	0.49
1:D:505:SER:HA	1:D:508:VAL:HG12	1.95	0.49
1:A:505:SER:HA	1:A:508:VAL:HG12	1.95	0.49
1:A:258:THR:HG22	1:A:258:THR:O	2.11	0.48
1:C:580:PHE:CE2	1:C:678:LEU:HD22	2.49	0.48
1:C:505:SER:HA	1:C:508:VAL:HG12	1.95	0.48
1:C:641:THR:HG22	1:C:675:LEU:HD11	1.95	0.48
1:B:580:PHE:CE2	1:B:678:LEU:HD22	2.49	0.48
1:B:587:PHE:CE2	1:B:674:LEU:HD11	2.49	0.48
1:D:641:THR:HG22	1:D:675:LEU:HD11	1.94	0.48
1:B:569:ILE:HG22	1:B:569:ILE:O	2.14	0.48
1:C:587:PHE:CE2	1:C:674:LEU:HD11	2.49	0.48
1:D:569:ILE:O	1:D:569:ILE:HG22	2.14	0.48
1:A:569:ILE:O	1:A:569:ILE:HG22	2.14	0.48
1:C:283:VAL:O	1:C:283:VAL:HG12	2.14	0.48
1:B:283:VAL:HG12	1:B:283:VAL:O	2.14	0.47
1:A:252:LEU:HD22	1:A:287:VAL:HG21	1.96	0.47
1:D:587:PHE:CE2	1:D:674:LEU:HD11	2.49	0.47
1:A:587:PHE:CE2	1:A:674:LEU:HD11	2.49	0.47
1:D:252:LEU:HD22	1:D:287:VAL:HG21	1.96	0.47
1:A:580:PHE:CE2	1:A:678:LEU:HD22	2.49	0.47
1:D:657:ALA:O	1:D:661:ILE:HD12	2.14	0.47
1:B:252:LEU:HD22	1:B:287:VAL:HG21	1.96	0.47
1:A:445:MET:CE	1:A:548:GLY:HA3	2.45	0.47
1:D:283:VAL:HG12	1:D:283:VAL:O	2.14	0.47
1:A:283:VAL:HG12	1:A:283:VAL:O	2.14	0.47
1:D:580:PHE:CE2	1:D:678:LEU:HD22	2.49	0.47
1:C:569:ILE:HG22	1:C:569:ILE:O	2.14	0.47
1:D:445:MET:CE	1:D:548:GLY:HA3	2.45	0.47
1:C:542:VAL:HG13	1:B:594:ALA:HB1	1.98	0.46
1:B:657:ALA:O	1:B:661:ILE:HD12	2.15	0.46
1:A:301:ASN:O	1:A:305:VAL:HG22	2.16	0.46
1:A:445:MET:HE1	1:A:548:GLY:HA3	1.97	0.46
1:C:252:LEU:HD22	1:C:287:VAL:HG21	1.96	0.46
1:C:445:MET:CE	1:C:548:GLY:HA3	2.45	0.46
1:C:657:ALA:O	1:C:661:ILE:HD12	2.15	0.46
1:B:445:MET:CE	1:B:548:GLY:HA3	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:657:ALA:O	1:A:661:ILE:HD12	2.15	0.46
1:A:744:VAL:HG12	1:A:745:ASP:N	2.31	0.46
1:C:702:ALA:O	1:C:706:LEU:HD23	2.16	0.46
1:C:703:ILE:O	1:C:707:ASP:OD1	2.34	0.46
1:C:744:VAL:HG12	1:C:745:ASP:N	2.31	0.46
1:D:301:ASN:O	1:D:305:VAL:HG22	2.16	0.46
1:D:702:ALA:O	1:D:706:LEU:HD23	2.16	0.46
1:B:695:ASN:OD1	1:B:696:ILE:N	2.49	0.46
1:C:695:ASN:OD1	1:C:696:ILE:N	2.49	0.46
1:D:703:ILE:O	1:D:707:ASP:OD1	2.34	0.46
1:A:260:GLN:HE21	1:A:263:ILE:HD12	1.81	0.45
1:D:260:GLN:HE21	1:D:263:ILE:HD12	1.81	0.45
1:C:301:ASN:O	1:C:305:VAL:HG22	2.16	0.45
1:B:260:GLN:HE21	1:B:263:ILE:HD12	1.81	0.45
1:B:301:ASN:O	1:B:305:VAL:HG22	2.16	0.45
1:B:744:VAL:HG12	1:B:745:ASP:N	2.31	0.45
1:A:695:ASN:OD1	1:A:696:ILE:N	2.49	0.45
1:D:695:ASN:OD1	1:D:696:ILE:N	2.49	0.45
1:A:702:ALA:O	1:A:706:LEU:HD23	2.16	0.45
1:B:702:ALA:O	1:B:706:LEU:HD23	2.16	0.45
1:A:703:ILE:O	1:A:707:ASP:OD1	2.34	0.45
1:B:302:THR:HA	1:B:305:VAL:HG22	1.99	0.45
1:A:252:LEU:HD11	1:A:268:LEU:HD21	1.99	0.45
1:D:744:VAL:HG12	1:D:745:ASP:N	2.31	0.45
4:A:905:6EU:CAT	4:A:905:6EU:CAW	2.95	0.45
4:B:905:6EU:CAW	4:B:905:6EU:CAT	2.95	0.45
1:D:252:LEU:HD11	1:D:268:LEU:HD21	1.99	0.44
1:D:302:THR:HA	1:D:305:VAL:HG22	1.99	0.44
1:B:703:ILE:O	1:B:707:ASP:OD1	2.34	0.44
1:C:594:ALA:HB1	1:D:542:VAL:HG13	1.99	0.44
1:A:594:ALA:HB1	1:B:542:VAL:HG13	2.00	0.44
1:C:302:THR:HA	1:C:305:VAL:HG22	1.99	0.44
1:C:408:ASN:O	1:C:412:MET:HB2	2.18	0.44
4:C:905:6EU:CAT	4:C:905:6EU:CAW	2.95	0.44
1:B:408:ASN:O	1:B:412:MET:HB2	2.18	0.44
1:C:260:GLN:HE21	1:C:263:ILE:HD12	1.81	0.44
1:A:302:THR:HA	1:A:305:VAL:HG22	1.99	0.44
1:D:445:MET:HE1	1:D:548:GLY:HA3	2.00	0.44
4:D:904:6EU:CAT	4:D:904:6EU:CAW	2.95	0.44
1:B:252:LEU:HD11	1:B:268:LEU:HD21	1.99	0.44
1:D:408:ASN:O	1:D:412:MET:HB2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:ILE:O	1:A:433:ILE:HG22	2.19	0.43
1:C:415:VAL:HG12	1:C:416:GLU:N	2.33	0.43
1:D:415:VAL:HG12	1:D:416:GLU:N	2.34	0.43
1:C:252:LEU:HD11	1:C:268:LEU:HD21	1.99	0.43
1:D:357:ILE:HD12	1:D:365:LEU:CD1	2.48	0.43
1:B:433:ILE:HG22	1:B:433:ILE:O	2.19	0.43
1:B:415:VAL:HG12	1:B:416:GLU:N	2.33	0.43
1:A:408:ASN:O	1:A:412:MET:HB2	2.18	0.43
1:C:433:ILE:O	1:C:433:ILE:HG22	2.19	0.42
1:A:357:ILE:HD12	1:A:365:LEU:CD1	2.48	0.42
1:C:357:ILE:HD12	1:C:365:LEU:CD1	2.48	0.42
1:D:641:THR:O	1:D:675:LEU:HD11	2.19	0.42
1:A:580:PHE:O	1:A:580:PHE:CG	2.72	0.42
1:C:641:THR:O	1:C:675:LEU:HD11	2.19	0.42
1:B:357:ILE:HD12	1:B:365:LEU:CD1	2.48	0.42
1:B:641:THR:O	1:B:675:LEU:HD11	2.19	0.42
1:A:482:VAL:CA	1:A:523:MET:HE2	2.49	0.42
1:A:641:THR:O	1:A:675:LEU:HD11	2.19	0.42
1:D:433:ILE:HG22	1:D:433:ILE:O	2.19	0.42
1:B:482:VAL:CA	1:B:523:MET:HE2	2.49	0.42
1:A:286:THR:HG21	1:A:328:ILE:HG21	2.02	0.42
1:A:415:VAL:HG12	1:A:416:GLU:N	2.33	0.42
1:C:286:THR:HG21	1:C:328:ILE:HG21	2.02	0.42
1:C:580:PHE:CG	1:C:580:PHE:O	2.72	0.42
1:B:580:PHE:O	1:B:580:PHE:CG	2.72	0.42
1:C:575:ARG:O	1:C:579:ARG:HG2	2.20	0.42
1:B:386:CYS:SG	1:B:390:CYS:CB	3.08	0.42
1:D:286:THR:HG21	1:D:328:ILE:HG21	2.02	0.41
1:D:580:PHE:O	1:D:580:PHE:CG	2.72	0.41
1:B:575:ARG:O	1:B:579:ARG:HG2	2.20	0.41
1:A:542:VAL:HG13	1:D:594:ALA:HB1	2.02	0.41
1:C:482:VAL:CA	1:C:523:MET:HE2	2.49	0.41
1:D:575:ARG:O	1:D:579:ARG:HG2	2.20	0.41
1:C:268:LEU:HD13	1:C:315:LEU:HD13	2.03	0.41
1:A:386:CYS:SG	1:A:390:CYS:CB	3.08	0.41
1:D:482:VAL:CA	1:D:523:MET:HE2	2.50	0.41
1:A:575:ARG:HB3	1:A:575:ARG:NH1	2.36	0.41
1:D:268:LEU:HD13	1:D:315:LEU:HD13	2.03	0.41
1:D:298:THR:O	1:D:302:THR:N	2.42	0.41
1:B:286:THR:HG21	1:B:328:ILE:HG21	2.02	0.41
1:A:260:GLN:NE2	1:A:263:ILE:HD12	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:575:ARG:O	1:A:579:ARG:HG2	2.20	0.41
1:A:599:ILE:HD11	1:A:650:THR:HG21	2.03	0.41
1:A:641:THR:CG2	1:A:675:LEU:HD11	2.51	0.41
1:C:386:CYS:SG	1:C:390:CYS:CB	3.08	0.41
1:D:260:GLN:NE2	1:D:263:ILE:HD12	2.36	0.41
1:D:386:CYS:SG	1:D:390:CYS:CB	3.08	0.41
1:D:575:ARG:HB3	1:D:575:ARG:NH1	2.36	0.41
1:B:575:ARG:NH1	1:B:575:ARG:HB3	2.36	0.41
1:B:599:ILE:HD11	1:B:650:THR:HG21	2.03	0.41
1:B:641:THR:CG2	1:B:675:LEU:HD11	2.51	0.40
1:A:288:LEU:H	1:A:288:LEU:HD12	1.87	0.40
1:A:686:VAL:O	1:A:690:ALA:CB	2.70	0.40
1:A:686:VAL:O	1:A:690:ALA:HB2	2.22	0.40
1:C:583:VAL:O	1:C:583:VAL:CG1	2.70	0.40
1:C:599:ILE:HD11	1:C:650:THR:HG21	2.03	0.40
1:C:641:THR:CG2	1:C:675:LEU:HD11	2.51	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	568/868 (65%)	543 (96%)	25 (4%)	0	100	100
1	B	568/868 (65%)	543 (96%)	25 (4%)	0	100	100
1	C	568/868 (65%)	543 (96%)	25 (4%)	0	100	100
1	D	568/868 (65%)	543 (96%)	25 (4%)	0	100	100
All	All	2272/3472 (65%)	2172 (96%)	100 (4%)	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	414/770 (54%)	414 (100%)	0	100	100
1	B	414/770 (54%)	414 (100%)	0	100	100
1	C	414/770 (54%)	414 (100%)	0	100	100
1	D	414/770 (54%)	414 (100%)	0	100	100
All	All	1656/3080 (54%)	1656 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
1	A	260	GLN
1	A	687	ASN
1	C	260	GLN
1	C	687	ASN
1	D	260	GLN
1	D	687	ASN
1	B	260	GLN
1	B	687	ASN

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 22 ligands modelled in this entry, 2 are monoatomic - leaving 20 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	6EU	A	905	-	45,52,52	4.45	16 (35%)	44,83,83	2.01	10 (22%)
4	6EU	D	904	-	45,52,52	4.45	16 (35%)	44,83,83	2.01	10 (22%)
2	LBN	A	901	-	32,32,51	1.38	3 (9%)	38,40,59	0.98	1 (2%)
3	6OU	D	902	-	34,34,48	1.69	4 (11%)	37,39,53	0.92	2 (5%)
4	6EU	C	905	-	45,52,52	4.44	16 (35%)	44,83,83	2.01	10 (22%)
3	6OU	C	903	-	32,32,48	1.54	3 (9%)	35,37,53	0.81	2 (5%)
3	6OU	D	903	-	9,9,48	0.73	0	8,8,53	0.36	0
3	6OU	C	904	-	9,9,48	0.74	0	8,8,53	0.36	0
3	6OU	A	906	-	32,32,48	1.54	3 (9%)	35,37,53	0.81	2 (5%)
4	6EU	B	905	-	45,52,52	4.44	16 (35%)	44,83,83	2.00	10 (22%)
2	LBN	B	901	-	32,32,51	1.37	3 (9%)	38,40,59	0.98	1 (2%)
2	LBN	C	901	-	32,32,51	1.38	3 (9%)	38,40,59	0.98	1 (2%)
3	6OU	B	902	-	34,34,48	1.69	5 (14%)	37,39,53	0.92	2 (5%)
2	LBN	D	901	-	32,32,51	1.38	3 (9%)	38,40,59	0.98	1 (2%)
3	6OU	A	902	-	34,34,48	1.69	4 (11%)	37,39,53	0.92	2 (5%)
3	6OU	A	903	-	32,32,48	1.54	3 (9%)	35,37,53	0.81	2 (5%)
3	6OU	B	904	-	9,9,48	0.74	0	8,8,53	0.36	0
3	6OU	C	902	-	34,34,48	1.69	4 (11%)	37,39,53	0.92	2 (5%)
3	6OU	A	904	-	9,9,48	0.74	0	8,8,53	0.36	0
3	6OU	B	903	-	32,32,48	1.54	3 (9%)	35,37,53	0.81	2 (5%)

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	6EU	A	905	-	-	7/20/101/101	0/8/7/7

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	6EU	D	904	-	-	7/20/101/101	0/8/7/7
2	LBN	A	901	-	-	20/36/36/55	-
3	6OU	D	902	-	-	16/36/36/52	-
4	6EU	C	905	-	-	7/20/101/101	0/8/7/7
3	6OU	C	903	-	-	18/36/36/52	-
3	6OU	D	903	-	-	5/7/7/52	-
3	6OU	C	904	-	-	5/7/7/52	-
3	6OU	A	906	-	-	18/36/36/52	-
4	6EU	B	905	-	-	7/20/101/101	0/8/7/7
2	LBN	B	901	-	-	20/36/36/55	-
2	LBN	C	901	-	-	20/36/36/55	-
3	6OU	B	902	-	-	16/36/36/52	-
2	LBN	D	901	-	-	20/36/36/55	-
3	6OU	A	902	-	-	16/36/36/52	-
3	6OU	A	903	-	-	18/36/36/52	-
3	6OU	B	904	-	-	5/7/7/52	-
3	6OU	C	902	-	-	16/36/36/52	-
3	6OU	A	904	-	-	5/7/7/52	-
3	6OU	B	903	-	-	18/36/36/52	-

All (105) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	904	6EU	CAS-CAX	17.73	1.61	1.33
4	A	905	6EU	CAS-CAX	17.71	1.61	1.33
4	C	905	6EU	CAS-CAX	17.71	1.61	1.33
4	B	905	6EU	CAS-CAX	17.69	1.61	1.33
4	D	904	6EU	OAB-CAL	-11.00	1.27	1.43
4	A	905	6EU	OAB-CAL	-10.99	1.27	1.43
4	C	905	6EU	OAB-CAL	-10.99	1.27	1.43
4	B	905	6EU	OAB-CAL	-10.92	1.27	1.43
4	A	905	6EU	CAW-CBA	9.34	1.52	1.33
4	C	905	6EU	CAW-CBA	9.29	1.52	1.33
4	B	905	6EU	CAW-CBA	9.29	1.52	1.33
4	D	904	6EU	CAW-CBA	9.28	1.52	1.33
4	A	905	6EU	CAM-CAL	7.71	1.66	1.54
4	B	905	6EU	CAM-CAL	7.71	1.66	1.54
4	D	904	6EU	CAM-CAL	7.70	1.66	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	905	6EU	CAM-CAL	7.68	1.66	1.54
4	B	905	6EU	CAK-CAS	7.50	1.67	1.50
4	D	904	6EU	CAK-CAS	7.49	1.67	1.50
4	A	905	6EU	CAK-CAS	7.48	1.67	1.50
4	C	905	6EU	CAK-CAS	7.46	1.67	1.50
4	D	904	6EU	CAP-CAM	7.21	1.67	1.53
4	C	905	6EU	CAP-CAM	7.19	1.67	1.53
4	A	905	6EU	CAP-CAM	7.15	1.67	1.53
4	B	905	6EU	CAP-CAM	7.14	1.67	1.53
4	D	904	6EU	OAA-CAJ	6.46	1.58	1.44
4	B	905	6EU	OAA-CAJ	6.44	1.58	1.44
4	C	905	6EU	OAA-CAJ	6.42	1.58	1.44
4	A	905	6EU	OAA-CAJ	6.39	1.58	1.44
4	A	905	6EU	OAA-CAQ	6.10	1.50	1.42
4	B	905	6EU	OAA-CAQ	6.08	1.50	1.42
4	C	905	6EU	OAA-CAQ	6.06	1.50	1.42
4	D	904	6EU	OAA-CAQ	6.04	1.50	1.42
3	D	902	6OU	P23-O22	5.46	1.77	1.60
3	B	902	6OU	P23-O22	5.46	1.77	1.60
3	C	902	6OU	P23-O22	5.45	1.77	1.60
3	A	902	6OU	P23-O22	5.44	1.77	1.60
3	C	902	6OU	P23-O26	4.91	1.73	1.54
3	D	902	6OU	P23-O26	4.91	1.73	1.54
3	A	902	6OU	P23-O26	4.91	1.73	1.54
3	B	902	6OU	P23-O26	4.91	1.73	1.54
4	C	905	6EU	CAJ-CAO	4.77	1.62	1.54
4	B	905	6EU	CAJ-CAO	4.77	1.62	1.54
4	A	905	6EU	CAJ-CAO	4.76	1.62	1.54
4	D	904	6EU	CAJ-CAO	4.75	1.62	1.54
2	A	901	LBN	P1-O2	4.69	1.77	1.59
2	C	901	LBN	P1-O2	4.68	1.77	1.59
2	D	901	LBN	P1-O2	4.68	1.77	1.59
2	B	901	LBN	P1-O2	4.66	1.77	1.59
3	C	903	6OU	P23-O22	4.65	1.77	1.59
3	B	903	6OU	P23-O22	4.65	1.77	1.59
3	A	906	6OU	P23-O22	4.64	1.77	1.59
3	A	903	6OU	P23-O22	4.64	1.77	1.59
4	D	904	6EU	OAC-CAM	-4.31	1.37	1.44
4	A	905	6EU	OAC-CAM	-4.29	1.37	1.44
4	B	905	6EU	OAC-CAM	-4.28	1.37	1.44
4	C	905	6EU	OAC-CAM	-4.27	1.37	1.44
4	B	905	6EU	OAB-CAQ	-4.06	1.34	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	905	6EU	OAB-CAQ	-4.06	1.34	1.41
4	C	905	6EU	OAB-CAQ	-4.02	1.34	1.41
4	D	904	6EU	OAB-CAQ	-3.97	1.34	1.41
3	A	906	6OU	P23-O26	3.66	1.73	1.59
3	A	903	6OU	P23-O26	3.65	1.73	1.59
3	C	903	6OU	P23-O26	3.65	1.73	1.59
3	B	903	6OU	P23-O26	3.65	1.73	1.59
4	A	905	6EU	CAY-CBE	2.85	1.56	1.51
4	C	905	6EU	OAF-CBK	2.83	1.41	1.33
4	D	904	6EU	OAF-CBK	2.83	1.41	1.33
4	B	905	6EU	OAF-CBK	2.83	1.41	1.33
4	C	905	6EU	CAY-CBE	2.82	1.55	1.51
4	B	905	6EU	CAY-CBE	2.82	1.55	1.51
4	A	905	6EU	OAF-CBK	2.82	1.41	1.33
4	D	904	6EU	CAY-CBE	2.82	1.55	1.51
4	D	904	6EU	OAH-CBQ	2.73	1.41	1.37
4	B	905	6EU	OAH-CBQ	2.73	1.41	1.37
4	C	905	6EU	OAH-CBQ	2.73	1.41	1.37
4	A	905	6EU	OAH-CBQ	2.73	1.41	1.37
2	A	901	LBN	O2-C9	-2.49	1.34	1.44
2	C	901	LBN	O2-C9	-2.49	1.34	1.44
2	B	901	LBN	O2-C9	-2.49	1.34	1.44
2	D	901	LBN	O2-C9	-2.48	1.34	1.44
3	A	903	6OU	C21-C20	2.40	1.58	1.50
3	B	903	6OU	C21-C20	2.39	1.58	1.50
3	C	903	6OU	C21-C20	2.39	1.58	1.50
3	A	906	6OU	C21-C20	2.38	1.58	1.50
3	D	902	6OU	C21-C20	2.37	1.58	1.50
3	B	902	6OU	C21-C20	2.37	1.58	1.50
3	C	902	6OU	C21-C20	2.36	1.58	1.50
3	A	902	6OU	C21-C20	2.35	1.58	1.50
4	D	904	6EU	OAI-CBS	2.22	1.40	1.36
4	A	905	6EU	OAI-CBS	2.20	1.40	1.36
4	C	905	6EU	OAI-CBS	2.18	1.40	1.36
4	B	905	6EU	OAI-CBS	2.18	1.40	1.36
3	D	902	6OU	C19-C20	2.07	1.57	1.50
3	B	902	6OU	C19-C20	2.07	1.57	1.50
2	A	901	LBN	P1-O1	2.07	1.67	1.59
2	C	901	LBN	P1-O1	2.07	1.67	1.59
2	B	901	LBN	P1-O1	2.07	1.67	1.59
2	D	901	LBN	P1-O1	2.06	1.67	1.59
3	C	902	6OU	C19-C20	2.06	1.57	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	902	6OU	C19-C20	2.05	1.57	1.50
4	B	905	6EU	CAP-CAN	2.04	1.63	1.52
4	C	905	6EU	CAP-CAN	2.03	1.63	1.52
4	A	905	6EU	CAP-CAN	2.02	1.63	1.52
4	D	904	6EU	CAP-CAN	2.02	1.63	1.52
3	B	902	6OU	C33-C31	2.00	1.56	1.50

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	905	6EU	OAF-CBK-CBM	6.60	121.53	111.21
4	C	905	6EU	OAF-CBK-CBM	6.60	121.52	111.21
4	A	905	6EU	OAF-CBK-CBM	6.60	121.52	111.21
4	D	904	6EU	OAF-CBK-CBM	6.59	121.50	111.21
4	A	905	6EU	CBD-CAV-CAM	-6.55	100.79	116.79
4	D	904	6EU	CBD-CAV-CAM	-6.53	100.82	116.79
4	C	905	6EU	CBD-CAV-CAM	-6.53	100.82	116.79
4	B	905	6EU	CBD-CAV-CAM	-6.53	100.83	116.79
4	D	904	6EU	CAQ-CAY-CBE	-4.35	108.49	113.60
4	C	905	6EU	CAQ-CAY-CBE	-4.35	108.50	113.60
4	B	905	6EU	CAQ-CAY-CBE	-4.33	108.52	113.60
4	A	905	6EU	CAQ-CAY-CBE	-4.33	108.52	113.60
4	D	904	6EU	OAH-CBQ-CBS	3.63	119.99	114.55
4	B	905	6EU	OAH-CBQ-CBS	3.59	119.94	114.55
4	C	905	6EU	OAH-CBQ-CBS	3.59	119.93	114.55
4	A	905	6EU	OAH-CBQ-CBS	3.56	119.89	114.55
2	A	901	LBN	O3-P1-O4	3.47	128.60	112.44
2	C	901	LBN	O3-P1-O4	3.47	128.60	112.44
2	D	901	LBN	O3-P1-O4	3.47	128.59	112.44
2	B	901	LBN	O3-P1-O4	3.47	128.58	112.44
3	B	902	6OU	O25-P23-O24	3.46	124.31	110.83
3	C	902	6OU	O25-P23-O24	3.45	124.29	110.83
3	A	902	6OU	O25-P23-O24	3.45	124.27	110.83
3	D	902	6OU	O25-P23-O24	3.45	124.26	110.83
4	A	905	6EU	CAJ-OAA-CAQ	3.14	118.75	113.53
4	D	904	6EU	CAJ-OAA-CAQ	3.13	118.74	113.53
4	C	905	6EU	CAJ-OAA-CAQ	3.13	118.73	113.53
4	B	905	6EU	CAJ-OAA-CAQ	3.10	118.69	113.53
4	D	904	6EU	CAM-CAV-CBB	2.94	129.81	121.88
4	B	905	6EU	CAM-CAV-CBB	2.94	129.79	121.88
4	C	905	6EU	CAM-CAV-CBB	2.93	129.79	121.88
4	A	905	6EU	CAM-CAV-CBB	2.93	129.77	121.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	906	6OU	O25-P23-O24	2.50	124.09	112.44
3	C	903	6OU	O25-P23-O24	2.50	124.09	112.44
3	B	903	6OU	O25-P23-O24	2.50	124.09	112.44
3	A	903	6OU	O25-P23-O24	2.50	124.08	112.44
3	A	903	6OU	O30-C31-C33	2.41	116.68	111.48
3	C	903	6OU	O30-C31-C33	2.40	116.67	111.48
3	B	903	6OU	O30-C31-C33	2.40	116.67	111.48
3	A	906	6OU	O30-C31-C33	2.39	116.64	111.48
4	A	905	6EU	CBF-CBA-CAW	-2.35	125.91	130.40
4	C	905	6EU	CBF-CBA-CAW	-2.34	125.92	130.40
4	D	904	6EU	CBF-CBA-CAW	-2.33	125.93	130.40
4	B	905	6EU	CBF-CBA-CAW	-2.33	125.94	130.40
3	A	902	6OU	O30-C31-C33	2.30	116.45	111.48
3	D	902	6OU	O30-C31-C33	2.28	116.42	111.48
3	C	902	6OU	O30-C31-C33	2.28	116.41	111.48
3	B	902	6OU	O30-C31-C33	2.27	116.38	111.48
4	A	905	6EU	CBD-CAV-CBB	2.19	129.03	121.12
4	C	905	6EU	CBD-CAV-CBB	2.18	128.98	121.12
4	D	904	6EU	CBD-CAV-CBB	2.17	128.97	121.12
4	B	905	6EU	CBD-CAV-CBB	2.17	128.96	121.12
4	B	905	6EU	OAH-CBQ-CBO	-2.15	120.38	124.08
4	D	904	6EU	OAH-CBQ-CBO	-2.14	120.39	124.08
4	D	904	6EU	OAC-CAQ-CAY	2.13	114.25	111.18
4	C	905	6EU	OAH-CBQ-CBO	-2.13	120.42	124.08
4	B	905	6EU	OAC-CAQ-CAY	2.13	114.23	111.18
4	A	905	6EU	OAC-CAQ-CAY	2.12	114.23	111.18
4	A	905	6EU	OAH-CBQ-CBO	-2.12	120.43	124.08
4	C	905	6EU	OAC-CAQ-CAY	2.11	114.21	111.18

There are no chirality outliers.

All (264) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	LBN	C1-O1-P1-O2
2	A	901	LBN	C1-O1-P1-O3
2	A	901	LBN	N1-C6-C9-O2
2	C	901	LBN	C1-O1-P1-O2
2	C	901	LBN	C1-O1-P1-O3
2	C	901	LBN	N1-C6-C9-O2
2	D	901	LBN	C1-O1-P1-O2
2	D	901	LBN	C1-O1-P1-O3
2	D	901	LBN	N1-C6-C9-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	901	LBN	C1-O1-P1-O2
2	B	901	LBN	C1-O1-P1-O3
2	B	901	LBN	N1-C6-C9-O2
3	A	902	6OU	C21-O22-P23-O24
3	A	902	6OU	C21-O22-P23-O25
3	A	902	6OU	C21-O22-P23-O26
3	A	903	6OU	C21-O22-P23-O24
3	A	903	6OU	C21-O22-P23-O26
3	A	906	6OU	C21-O22-P23-O24
3	A	906	6OU	C21-O22-P23-O26
3	C	902	6OU	C21-O22-P23-O24
3	C	902	6OU	C21-O22-P23-O25
3	C	902	6OU	C21-O22-P23-O26
3	C	903	6OU	C21-O22-P23-O24
3	C	903	6OU	C21-O22-P23-O26
3	D	902	6OU	C21-O22-P23-O24
3	D	902	6OU	C21-O22-P23-O25
3	D	902	6OU	C21-O22-P23-O26
3	B	902	6OU	C21-O22-P23-O24
3	B	902	6OU	C21-O22-P23-O25
3	B	902	6OU	C21-O22-P23-O26
3	B	903	6OU	C21-O22-P23-O24
3	B	903	6OU	C21-O22-P23-O26
4	A	905	6EU	OAC-CAM-CAV-CBB
4	A	905	6EU	OAC-CAM-CAV-CBD
4	A	905	6EU	OAA-CAQ-CAY-CBE
4	A	905	6EU	OAC-CAQ-CAY-CBE
4	A	905	6EU	OAB-CAQ-CAY-CBE
4	C	905	6EU	OAC-CAM-CAV-CBB
4	C	905	6EU	OAC-CAM-CAV-CBD
4	C	905	6EU	OAA-CAQ-CAY-CBE
4	C	905	6EU	OAC-CAQ-CAY-CBE
4	C	905	6EU	OAB-CAQ-CAY-CBE
4	D	904	6EU	OAC-CAM-CAV-CBB
4	D	904	6EU	OAC-CAM-CAV-CBD
4	D	904	6EU	OAA-CAQ-CAY-CBE
4	D	904	6EU	OAC-CAQ-CAY-CBE
4	D	904	6EU	OAB-CAQ-CAY-CBE
4	B	905	6EU	OAC-CAM-CAV-CBB
4	B	905	6EU	OAC-CAM-CAV-CBD
4	B	905	6EU	OAA-CAQ-CAY-CBE
4	B	905	6EU	OAC-CAQ-CAY-CBE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	905	6EU	OAB-CAQ-CAY-CBE
4	A	905	6EU	OAG-CBK-OAF-CBC
4	C	905	6EU	OAG-CBK-OAF-CBC
4	D	904	6EU	OAG-CBK-OAF-CBC
4	B	905	6EU	OAG-CBK-OAF-CBC
4	A	905	6EU	CBM-CBK-OAF-CBC
4	C	905	6EU	CBM-CBK-OAF-CBC
4	D	904	6EU	CBM-CBK-OAF-CBC
4	B	905	6EU	CBM-CBK-OAF-CBC
3	A	903	6OU	O17-C16-O18-C19
3	A	906	6OU	O17-C16-O18-C19
3	C	903	6OU	O17-C16-O18-C19
3	B	903	6OU	O17-C16-O18-C19
3	A	903	6OU	C15-C16-O18-C19
3	A	906	6OU	C15-C16-O18-C19
3	C	903	6OU	C15-C16-O18-C19
3	B	903	6OU	C15-C16-O18-C19
2	A	901	LBN	C34-C35-C36-C37
2	C	901	LBN	C34-C35-C36-C37
2	D	901	LBN	C34-C35-C36-C37
2	B	901	LBN	C34-C35-C36-C37
3	A	902	6OU	C31-C33-C34-C35
3	C	902	6OU	C31-C33-C34-C35
3	D	902	6OU	C31-C33-C34-C35
3	B	902	6OU	C31-C33-C34-C35
3	A	902	6OU	C36-C37-C38-C39
3	A	904	6OU	C44-C45-C46-C47
3	C	902	6OU	C36-C37-C38-C39
3	C	904	6OU	C44-C45-C46-C47
3	D	902	6OU	C36-C37-C38-C39
3	D	903	6OU	C44-C45-C46-C47
3	B	902	6OU	C36-C37-C38-C39
3	B	904	6OU	C44-C45-C46-C47
3	A	903	6OU	C33-C34-C35-C36
3	C	903	6OU	C33-C34-C35-C36
3	B	903	6OU	C33-C34-C35-C36
3	A	906	6OU	C33-C34-C35-C36
3	A	902	6OU	C35-C36-C37-C38
3	C	902	6OU	C35-C36-C37-C38
3	D	902	6OU	C35-C36-C37-C38
3	B	902	6OU	C35-C36-C37-C38
3	A	906	6OU	C12-C13-C14-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	903	6OU	C12-C13-C14-C15
3	A	903	6OU	C12-C13-C14-C15
3	B	903	6OU	C12-C13-C14-C15
3	A	902	6OU	C09-C10-C11-C12
3	C	902	6OU	C09-C10-C11-C12
3	B	902	6OU	C09-C10-C11-C12
3	D	902	6OU	C09-C10-C11-C12
3	A	902	6OU	C40-C41-C42-C43
3	A	903	6OU	C40-C41-C42-C43
3	A	906	6OU	C40-C41-C42-C43
3	C	902	6OU	C40-C41-C42-C43
3	C	903	6OU	C40-C41-C42-C43
3	D	902	6OU	C40-C41-C42-C43
3	B	902	6OU	C40-C41-C42-C43
3	B	903	6OU	C40-C41-C42-C43
2	A	901	LBN	C2-C1-O1-P1
2	C	901	LBN	C2-C1-O1-P1
2	D	901	LBN	C2-C1-O1-P1
2	B	901	LBN	C2-C1-O1-P1
3	A	902	6OU	C10-C11-C12-C13
3	C	902	6OU	C10-C11-C12-C13
3	D	902	6OU	C10-C11-C12-C13
3	B	902	6OU	C10-C11-C12-C13
3	A	902	6OU	C11-C12-C13-C14
3	C	902	6OU	C11-C12-C13-C14
3	D	902	6OU	C11-C12-C13-C14
3	B	902	6OU	C11-C12-C13-C14
3	D	902	6OU	C07-C08-C09-C10
3	A	902	6OU	C07-C08-C09-C10
3	C	902	6OU	C07-C08-C09-C10
3	B	902	6OU	C07-C08-C09-C10
3	A	903	6OU	C33-C31-O30-C20
3	A	906	6OU	C33-C31-O30-C20
3	C	903	6OU	C33-C31-O30-C20
3	B	903	6OU	C33-C31-O30-C20
3	A	903	6OU	C36-C37-C38-C39
3	B	903	6OU	C36-C37-C38-C39
3	A	906	6OU	C36-C37-C38-C39
3	C	903	6OU	C36-C37-C38-C39
3	A	902	6OU	C12-C13-C14-C15
3	C	902	6OU	C12-C13-C14-C15
3	D	902	6OU	C12-C13-C14-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	902	6OU	C12-C13-C14-C15
2	A	901	LBN	C28-C29-C30-C31
2	C	901	LBN	C28-C29-C30-C31
2	D	901	LBN	C28-C29-C30-C31
2	B	901	LBN	C28-C29-C30-C31
3	A	904	6OU	C45-C46-C47-C48
3	C	904	6OU	C45-C46-C47-C48
3	D	903	6OU	C45-C46-C47-C48
3	B	904	6OU	C45-C46-C47-C48
2	A	901	LBN	C26-C25-O5-C3
2	C	901	LBN	C26-C25-O5-C3
2	D	901	LBN	C26-C25-O5-C3
2	B	901	LBN	C26-C25-O5-C3
2	A	901	LBN	C27-C28-C29-C30
2	C	901	LBN	C27-C28-C29-C30
2	D	901	LBN	C27-C28-C29-C30
2	B	901	LBN	C27-C28-C29-C30
2	A	901	LBN	C35-C36-C37-C38
2	C	901	LBN	C35-C36-C37-C38
2	D	901	LBN	C35-C36-C37-C38
2	B	901	LBN	C35-C36-C37-C38
3	D	903	6OU	C42-C43-C44-C45
3	A	904	6OU	C42-C43-C44-C45
3	C	904	6OU	C42-C43-C44-C45
3	B	904	6OU	C42-C43-C44-C45
3	A	904	6OU	C40-C41-C42-C43
3	C	904	6OU	C40-C41-C42-C43
3	D	903	6OU	C40-C41-C42-C43
3	B	904	6OU	C40-C41-C42-C43
3	A	906	6OU	O32-C31-O30-C20
3	A	903	6OU	O32-C31-O30-C20
3	C	903	6OU	O32-C31-O30-C20
3	B	903	6OU	O32-C31-O30-C20
2	A	901	LBN	O6-C25-O5-C3
2	C	901	LBN	O6-C25-O5-C3
2	D	901	LBN	O6-C25-O5-C3
2	B	901	LBN	O6-C25-O5-C3
3	A	903	6OU	O30-C20-C21-O22
3	A	906	6OU	O30-C20-C21-O22
3	C	903	6OU	O30-C20-C21-O22
3	B	903	6OU	O30-C20-C21-O22
3	A	902	6OU	C34-C35-C36-C37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	902	6OU	C34-C35-C36-C37
3	C	902	6OU	C34-C35-C36-C37
3	D	902	6OU	C34-C35-C36-C37
3	A	903	6OU	C10-C11-C12-C13
3	A	906	6OU	C10-C11-C12-C13
3	C	903	6OU	C10-C11-C12-C13
3	B	903	6OU	C10-C11-C12-C13
3	A	903	6OU	C19-C20-C21-O22
3	A	906	6OU	C19-C20-C21-O22
3	C	903	6OU	C19-C20-C21-O22
3	B	903	6OU	C19-C20-C21-O22
3	A	903	6OU	C21-O22-P23-O25
3	A	906	6OU	C21-O22-P23-O25
3	C	903	6OU	C21-O22-P23-O25
3	B	903	6OU	C21-O22-P23-O25
3	A	902	6OU	C20-C21-O22-P23
3	C	902	6OU	C20-C21-O22-P23
3	D	902	6OU	C20-C21-O22-P23
3	B	902	6OU	C20-C21-O22-P23
3	C	904	6OU	C43-C44-C45-C46
3	A	904	6OU	C43-C44-C45-C46
3	D	903	6OU	C43-C44-C45-C46
3	B	904	6OU	C43-C44-C45-C46
3	A	902	6OU	C08-C09-C10-C11
3	D	902	6OU	C08-C09-C10-C11
3	C	902	6OU	C08-C09-C10-C11
3	B	902	6OU	C08-C09-C10-C11
3	A	903	6OU	C20-C21-O22-P23
3	A	906	6OU	C20-C21-O22-P23
3	C	903	6OU	C20-C21-O22-P23
3	B	903	6OU	C20-C21-O22-P23
2	A	901	LBN	O7-C2-C3-O5
2	C	901	LBN	O7-C2-C3-O5
2	D	901	LBN	O7-C2-C3-O5
2	B	901	LBN	O7-C2-C3-O5
2	A	901	LBN	C1-C2-C3-O5
2	C	901	LBN	C1-C2-C3-O5
2	D	901	LBN	C1-C2-C3-O5
2	B	901	LBN	C1-C2-C3-O5
2	A	901	LBN	C9-C6-N1-C12
2	C	901	LBN	C9-C6-N1-C12
2	D	901	LBN	C9-C6-N1-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	901	LBN	C9-C6-N1-C12
2	A	901	LBN	C9-C6-N1-C15
2	A	901	LBN	C9-C6-N1-C18
2	C	901	LBN	C9-C6-N1-C15
2	C	901	LBN	C9-C6-N1-C18
2	D	901	LBN	C9-C6-N1-C15
2	D	901	LBN	C9-C6-N1-C18
2	B	901	LBN	C9-C6-N1-C15
2	B	901	LBN	C9-C6-N1-C18
2	D	901	LBN	O7-C34-C35-C36
2	B	901	LBN	O7-C34-C35-C36
2	A	901	LBN	O7-C34-C35-C36
2	C	901	LBN	O7-C34-C35-C36
3	A	903	6OU	O30-C31-C33-C34
3	A	906	6OU	O30-C31-C33-C34
3	C	903	6OU	O30-C31-C33-C34
3	B	903	6OU	O30-C31-C33-C34
2	A	901	LBN	O5-C25-C26-C27
2	C	901	LBN	O5-C25-C26-C27
2	D	901	LBN	O5-C25-C26-C27
2	B	901	LBN	O5-C25-C26-C27
3	A	903	6OU	O32-C31-C33-C34
3	A	906	6OU	O32-C31-C33-C34
3	C	903	6OU	O32-C31-C33-C34
3	B	903	6OU	O32-C31-C33-C34
3	A	903	6OU	C38-C39-C40-C41
3	C	903	6OU	C38-C39-C40-C41
2	A	901	LBN	O8-C34-C35-C36
2	C	901	LBN	O8-C34-C35-C36
2	D	901	LBN	O8-C34-C35-C36
2	B	901	LBN	O8-C34-C35-C36
2	D	901	LBN	C30-C31-C32-C33
2	A	901	LBN	C30-C31-C32-C33
2	C	901	LBN	C30-C31-C32-C33
2	B	901	LBN	C30-C31-C32-C33
3	A	906	6OU	C38-C39-C40-C41
3	B	903	6OU	C38-C39-C40-C41
2	C	901	LBN	O6-C25-C26-C27
3	A	902	6OU	C14-C15-C16-O18
3	B	902	6OU	C14-C15-C16-O18
2	A	901	LBN	O6-C25-C26-C27
2	D	901	LBN	O6-C25-C26-C27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	901	LBN	O6-C25-C26-C27
3	C	902	6OU	C14-C15-C16-O18
3	D	902	6OU	C14-C15-C16-O18

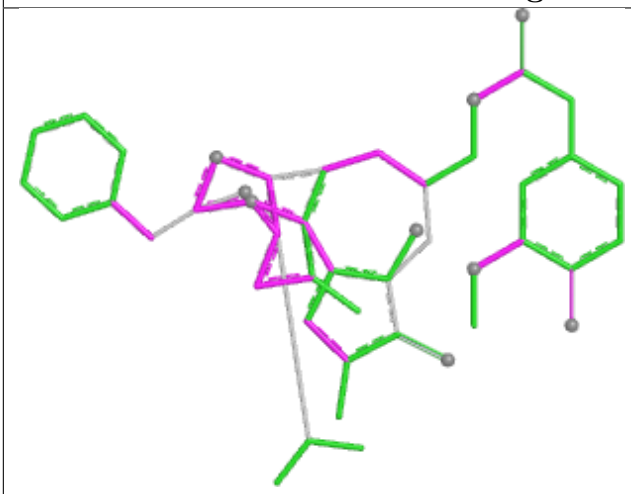
There are no ring outliers.

4 monomers are involved in 4 short contacts:

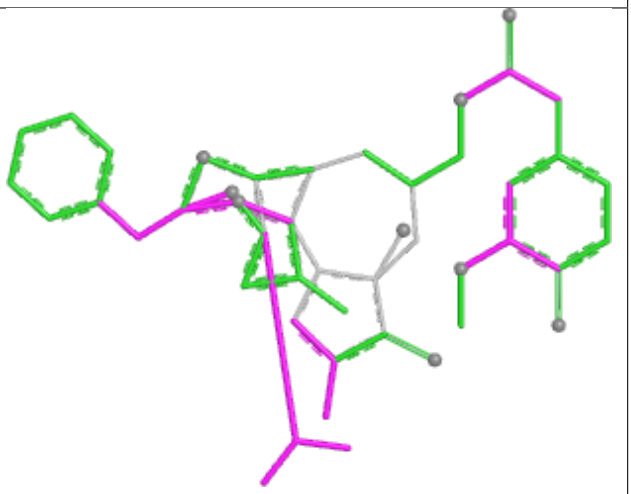
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	905	6EU	1	0
4	D	904	6EU	1	0
4	C	905	6EU	1	0
4	B	905	6EU	1	0

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

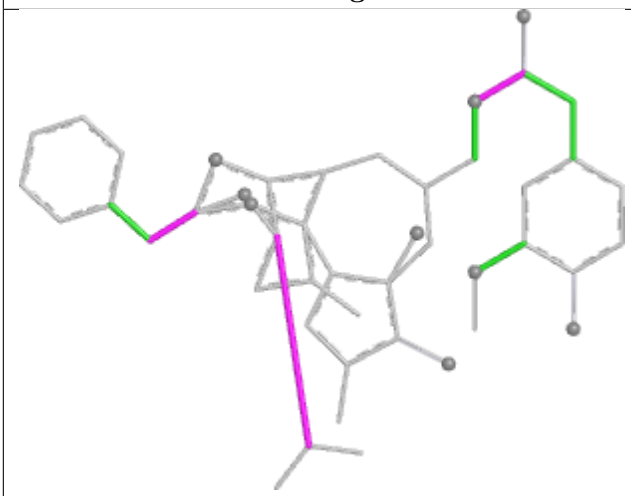
Ligand 6EU A 905



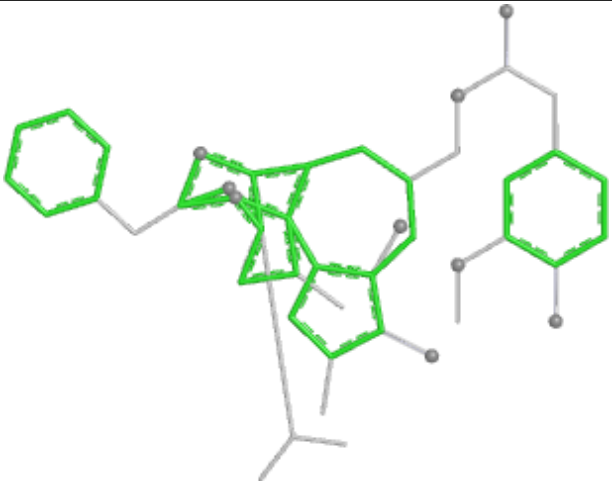
Bond lengths



Bond angles

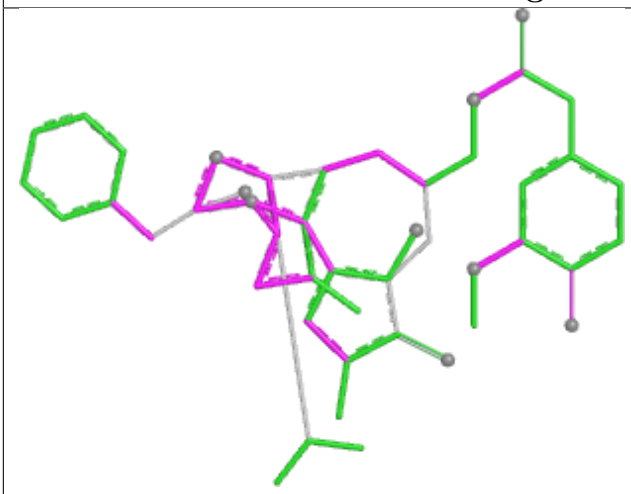


Torsions

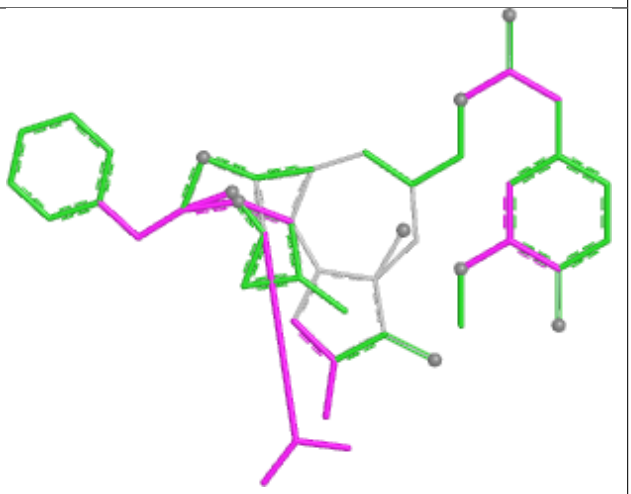


Rings

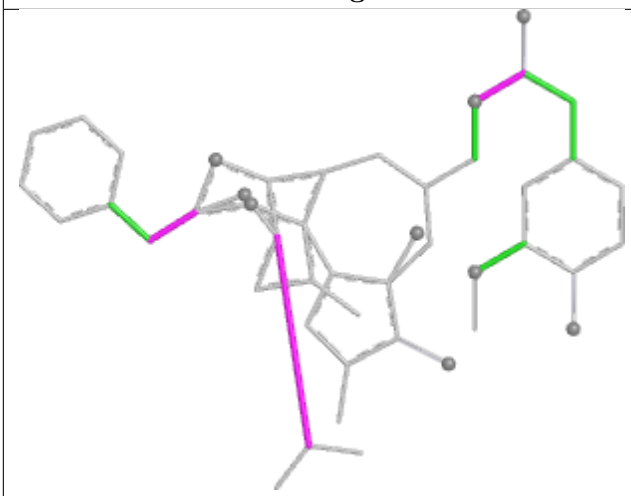
Ligand 6EU D 904



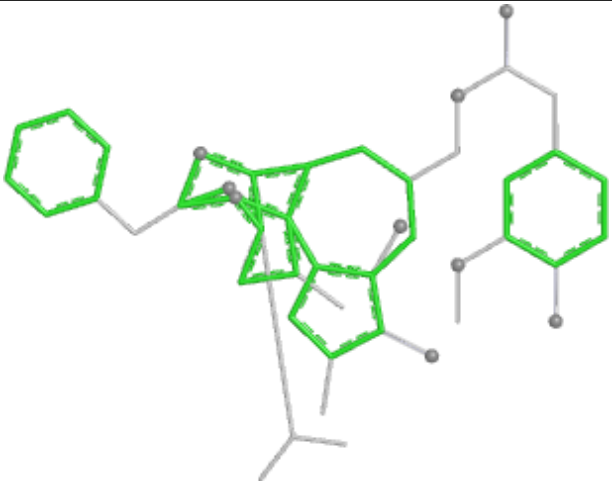
Bond lengths



Bond angles

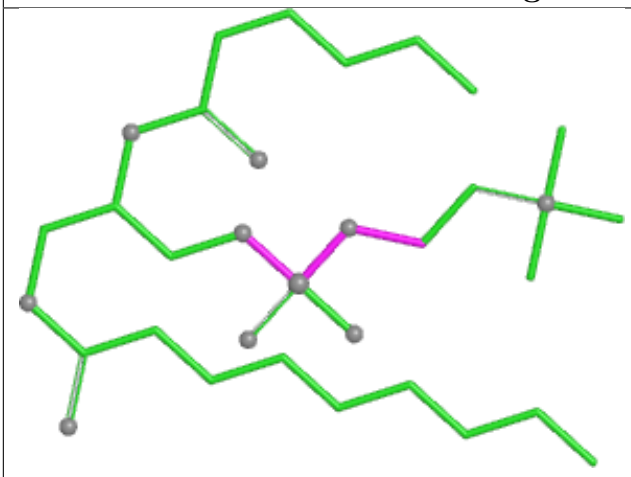


Torsions

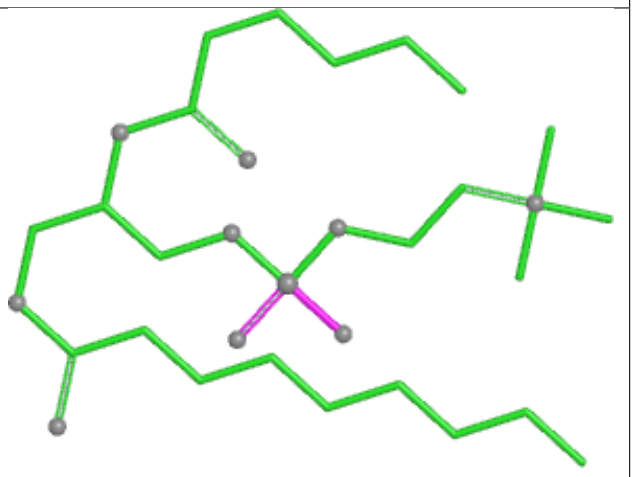


Rings

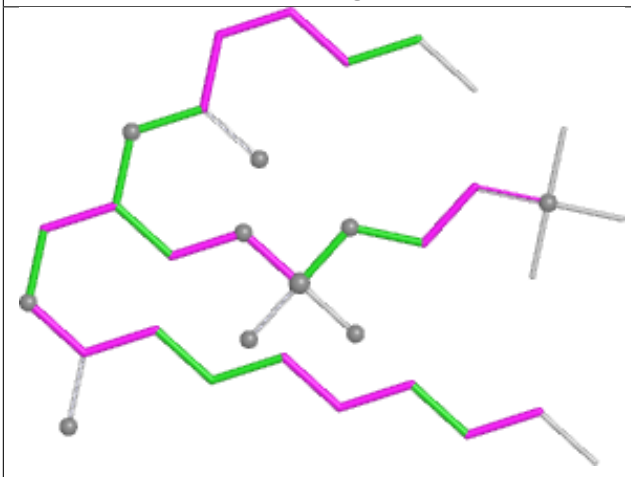
Ligand LBN A 901



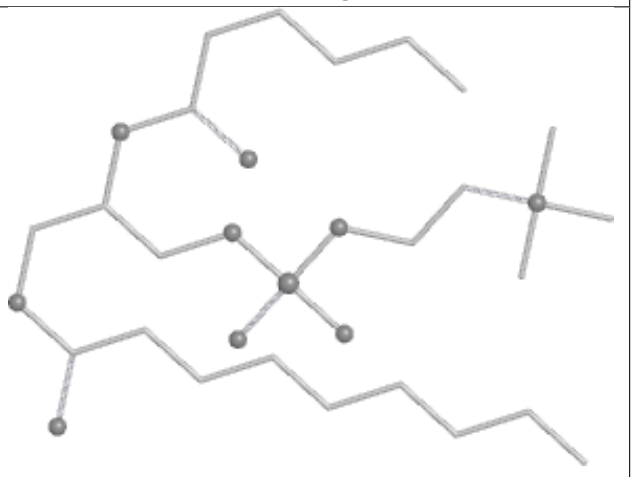
Bond lengths



Bond angles

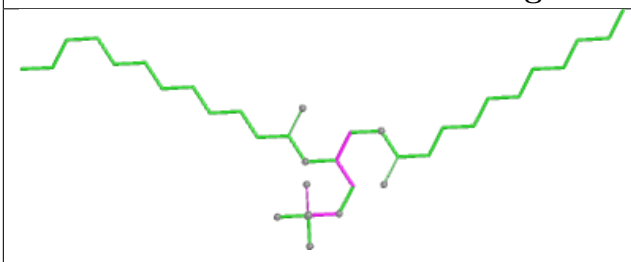


Torsions

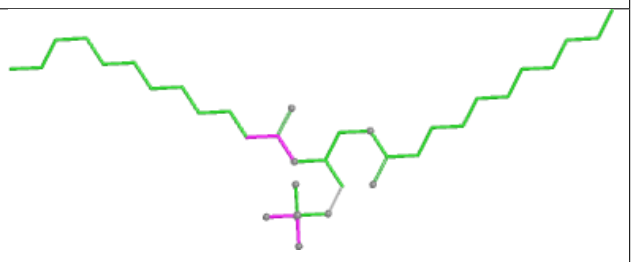


Rings

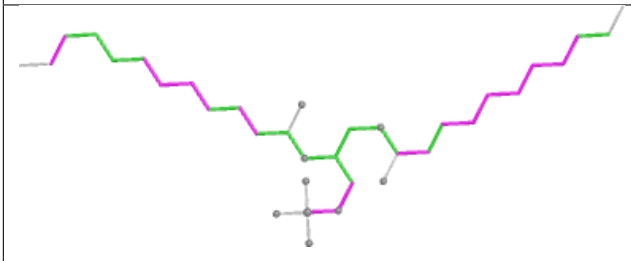
Ligand 6OU D 902



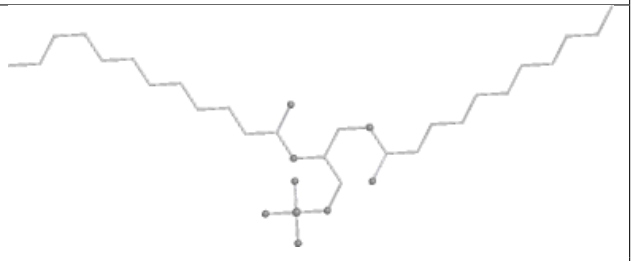
Bond lengths



Bond angles

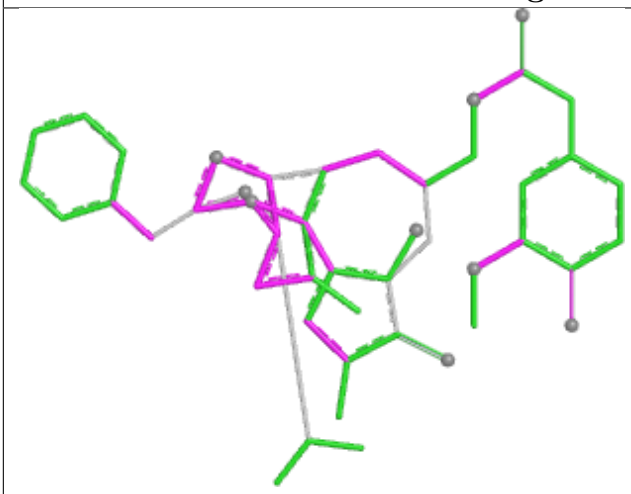


Torsions

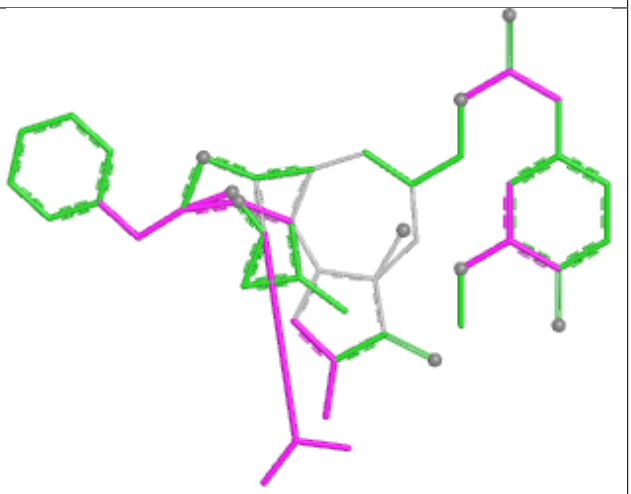


Rings

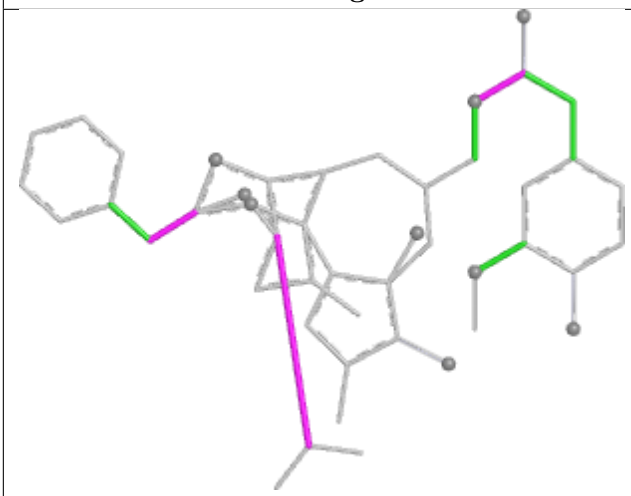
Ligand 6EU C 905



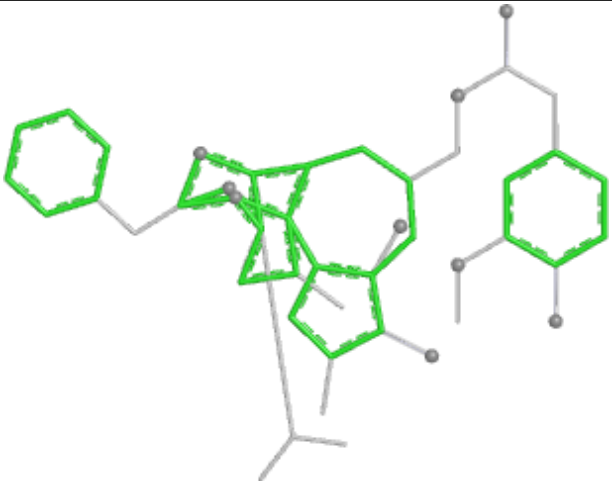
Bond lengths



Bond angles

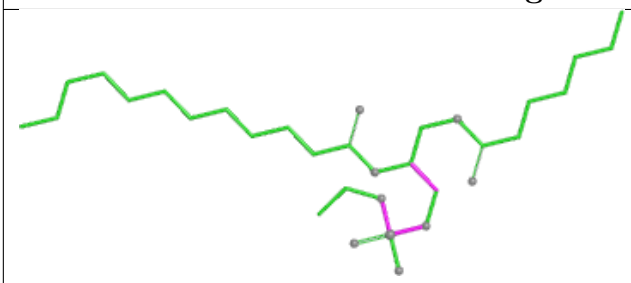


Torsions

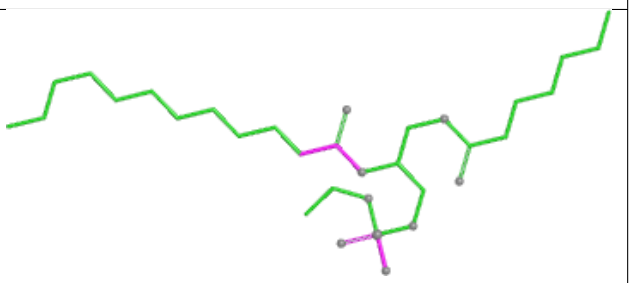


Rings

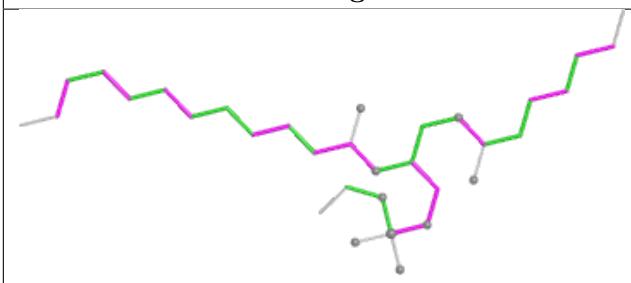
Ligand 6OU C 903



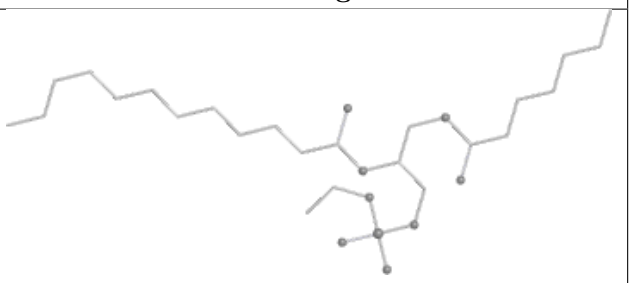
Bond lengths



Bond angles

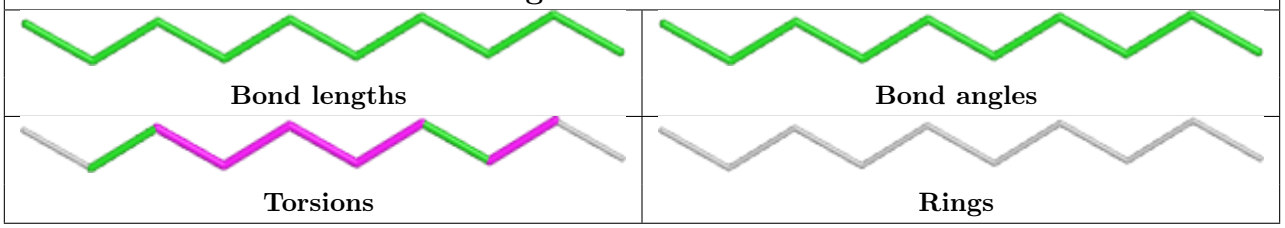


Torsions

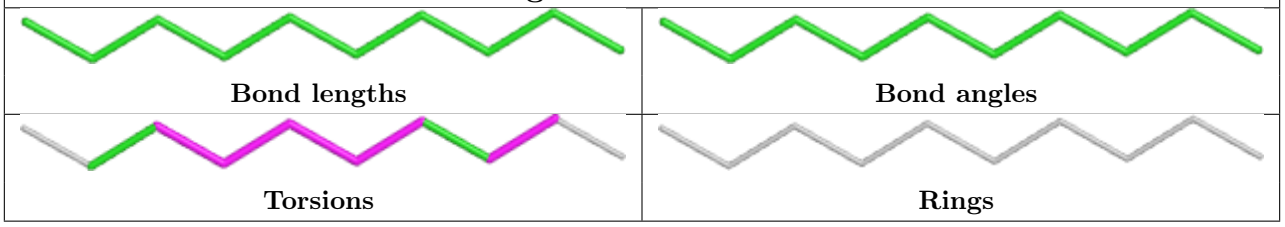


Rings

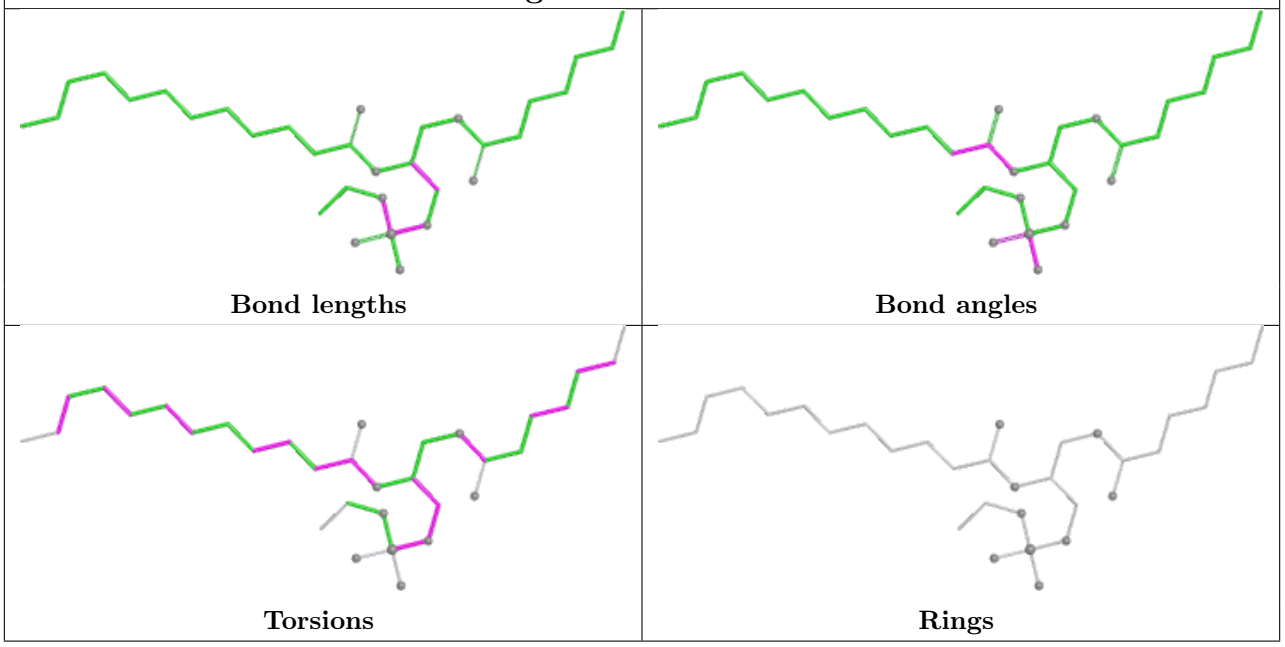
Ligand 6OU D 903



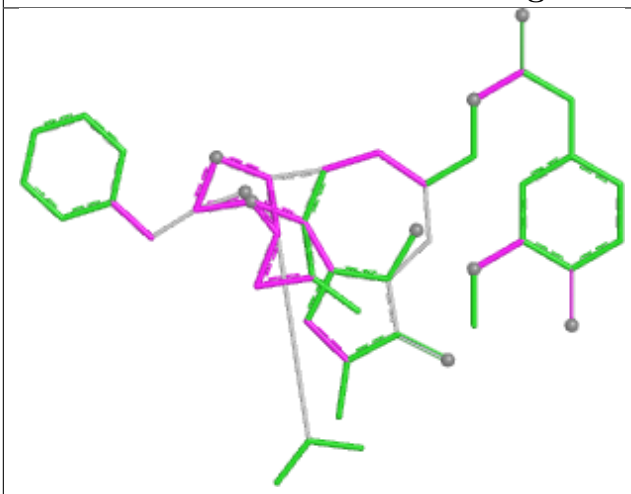
Ligand 6OU C 904



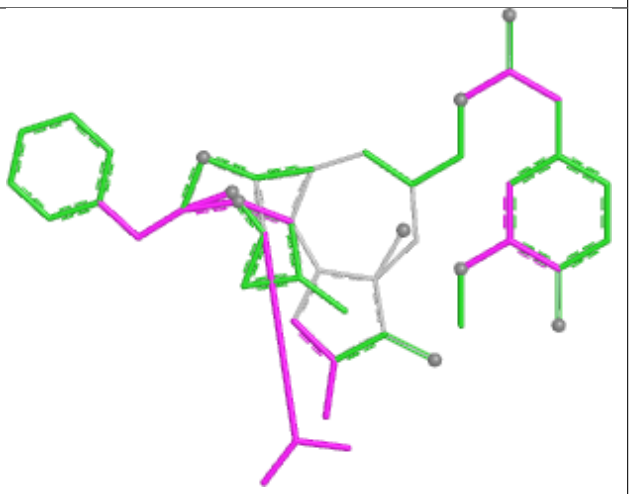
Ligand 6OU A 906



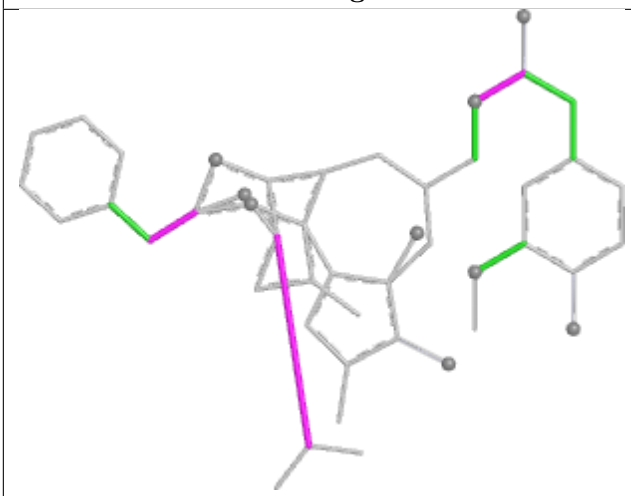
Ligand 6EU B 905



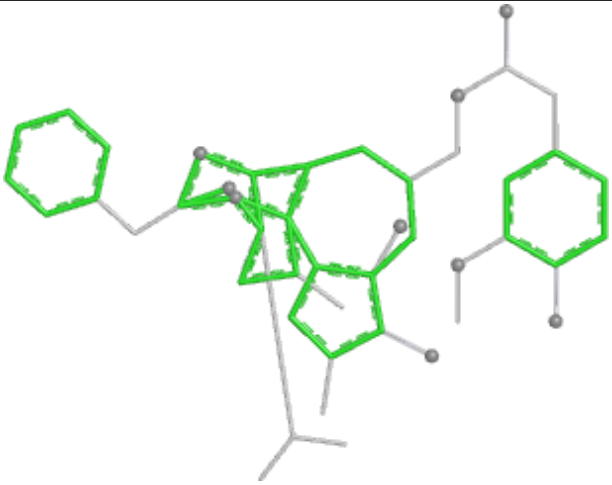
Bond lengths



Bond angles

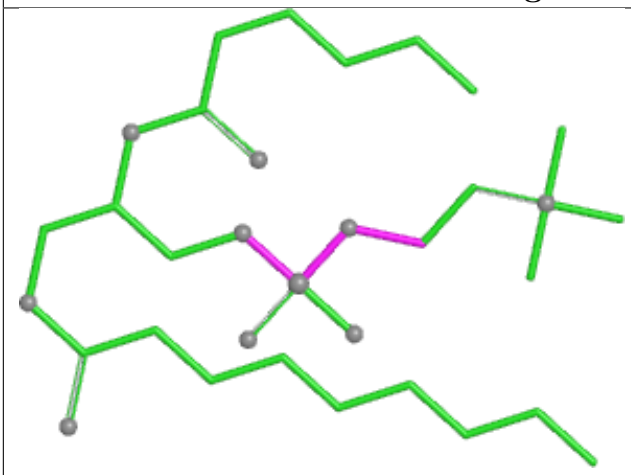


Torsions

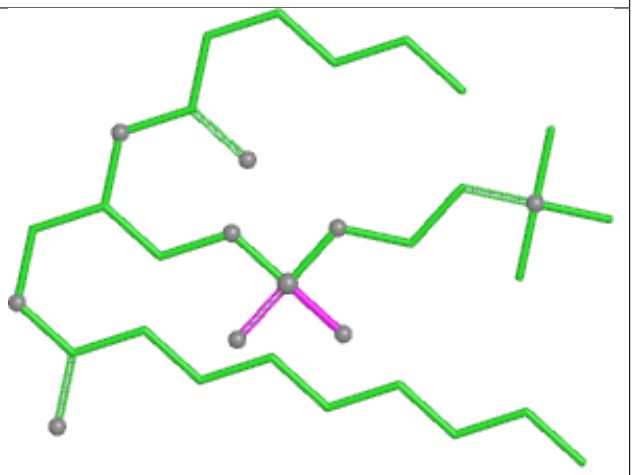


Rings

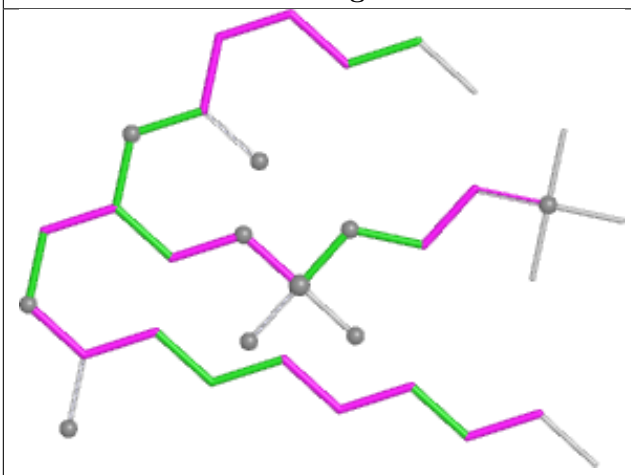
Ligand LBN B 901



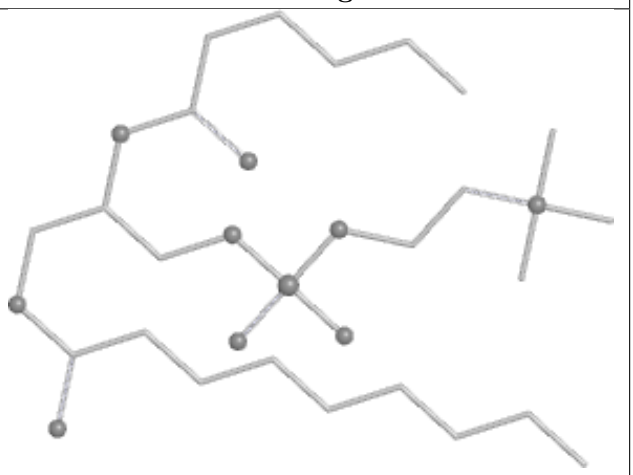
Bond lengths



Bond angles

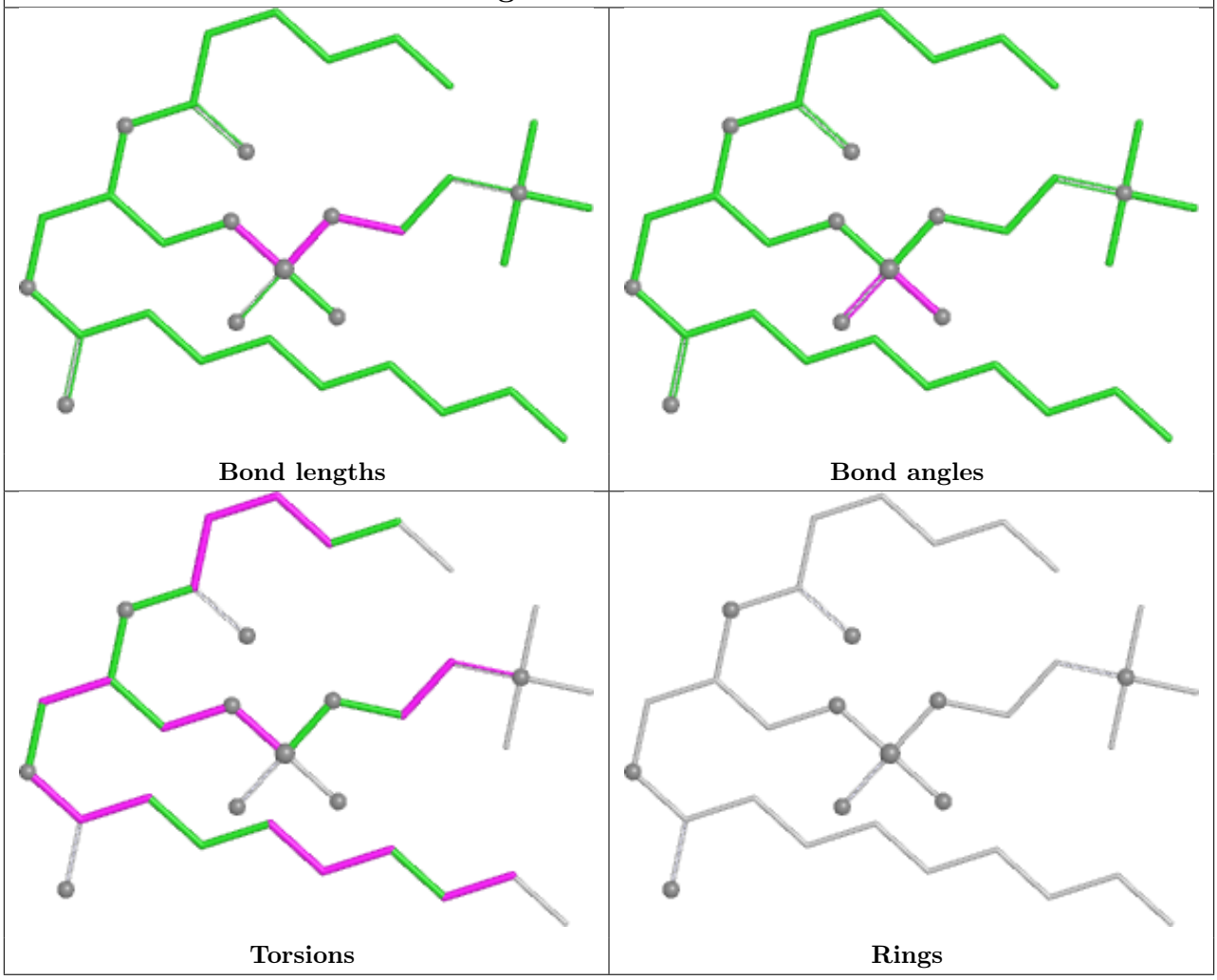


Torsions

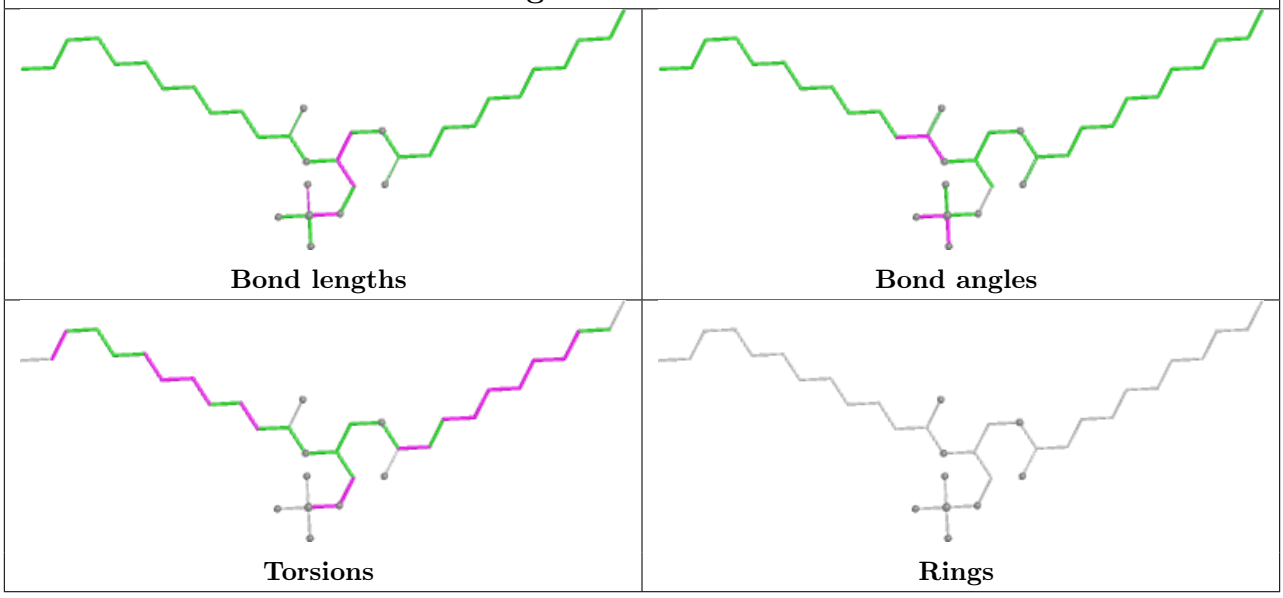


Rings

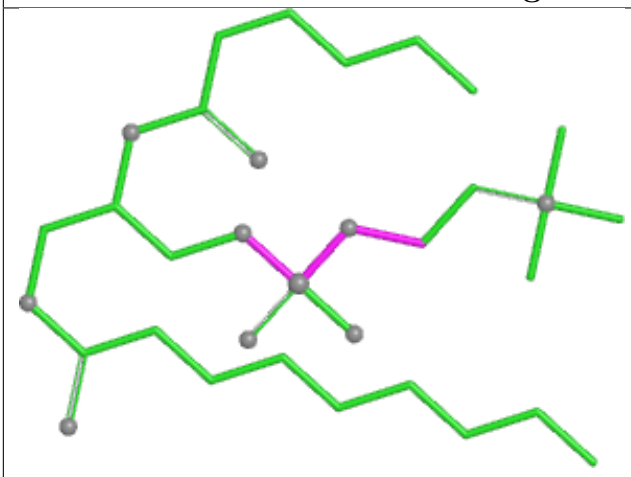
Ligand LBN C 901



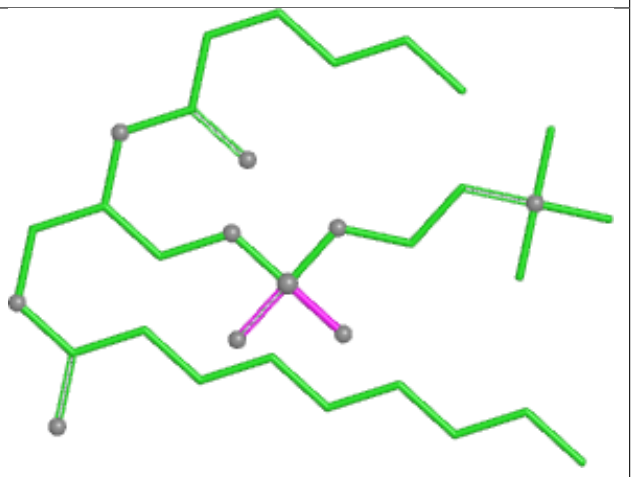
Ligand 6OU B 902



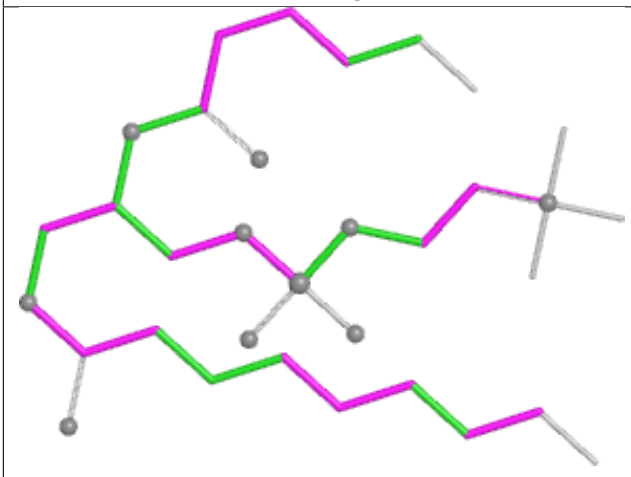
Ligand LBN D 901



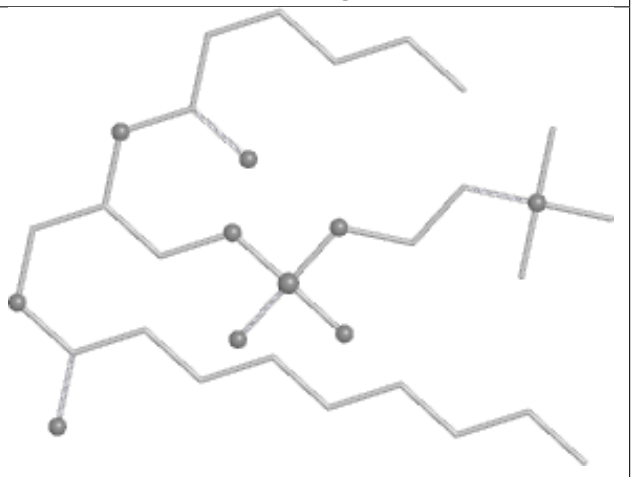
Bond lengths



Bond angles

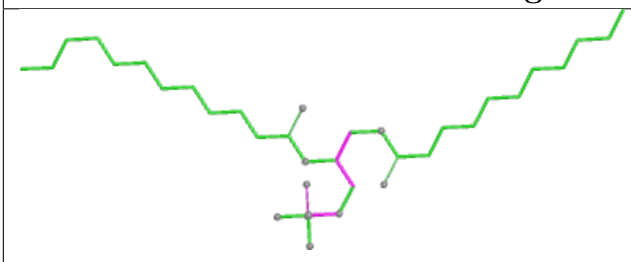


Torsions

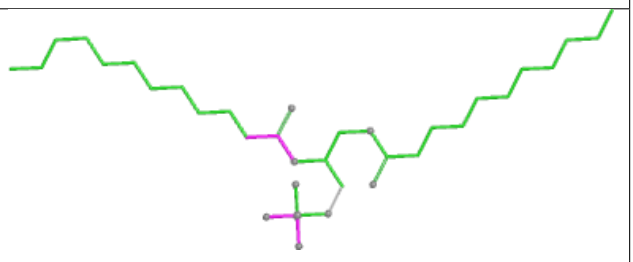


Rings

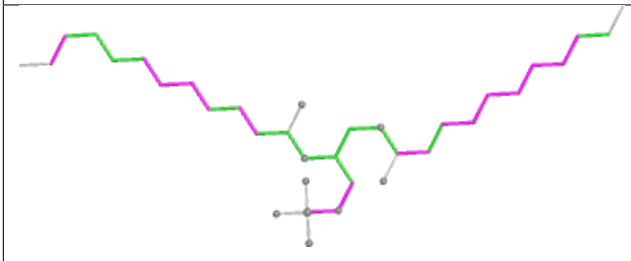
Ligand 6OU A 902



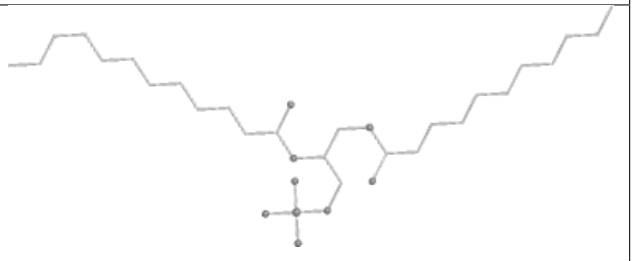
Bond lengths



Bond angles

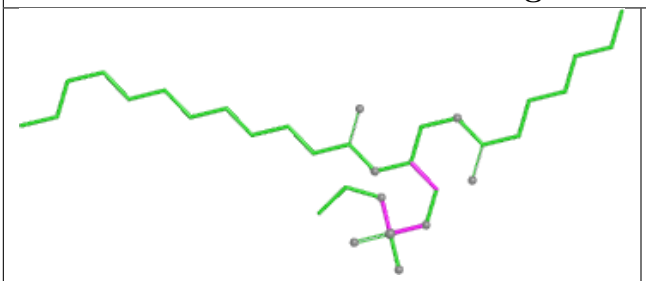


Torsions

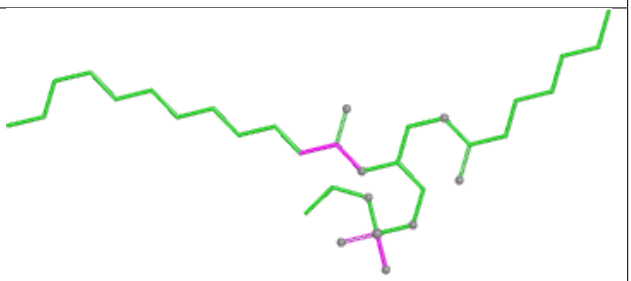


Rings

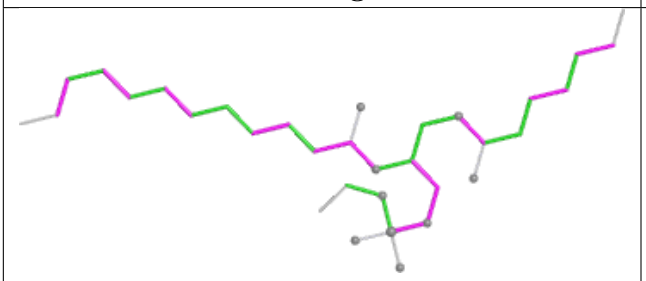
Ligand 6OU A 903



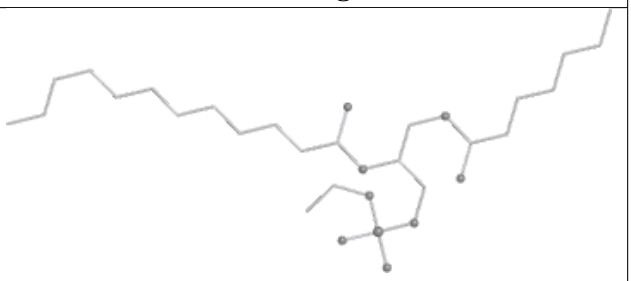
Bond lengths



Bond angles

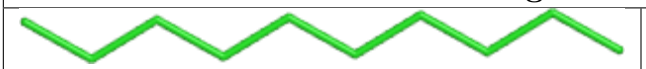


Torsions



Rings

Ligand 6OU B 904



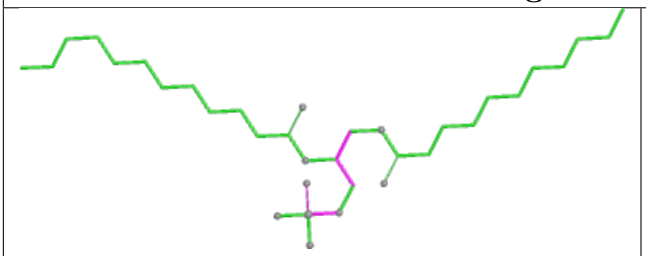
Bond lengths

Bond angles

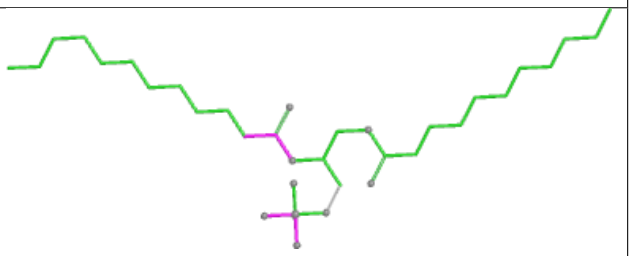
Torsions

Rings

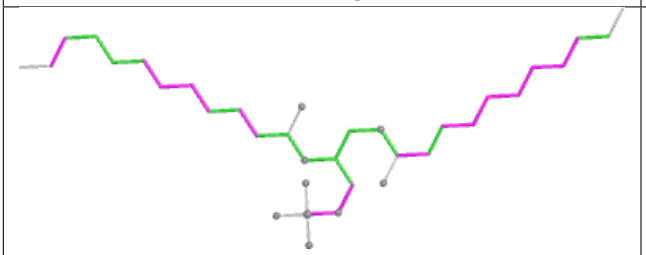
Ligand 6OU C 902



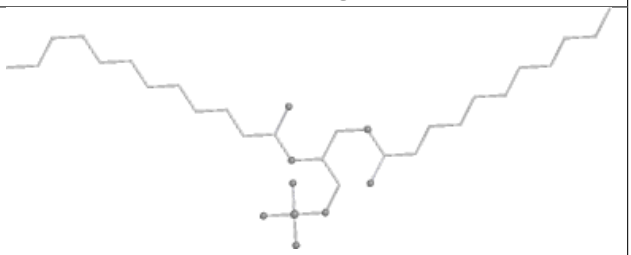
Bond lengths



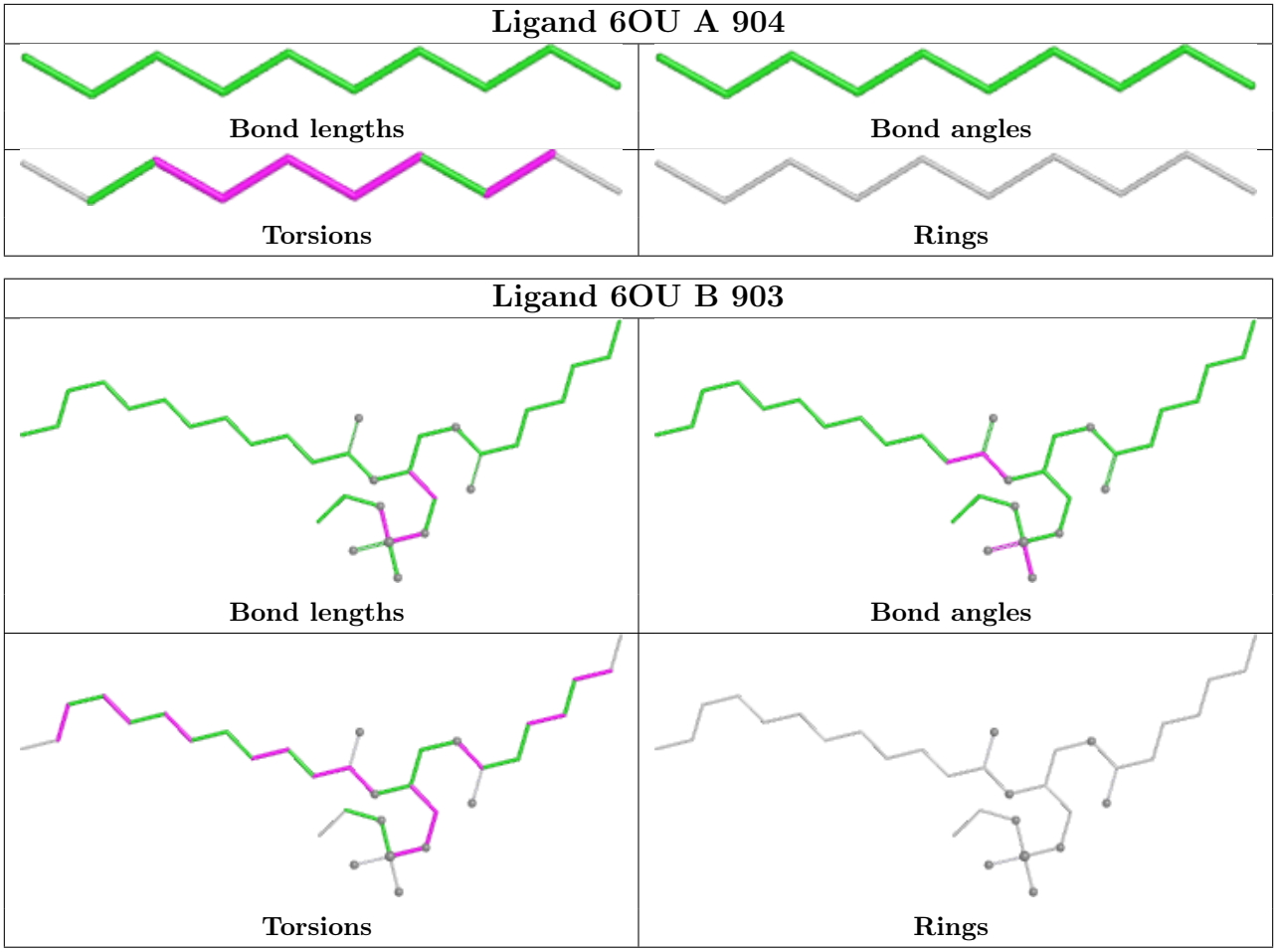
Bond angles



Torsions



Rings



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

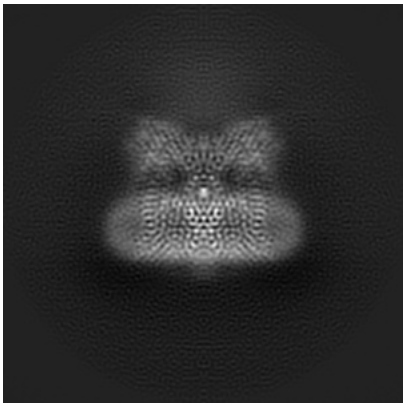
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24637. These allow visual inspection of the internal detail of the map and identification of artifacts.

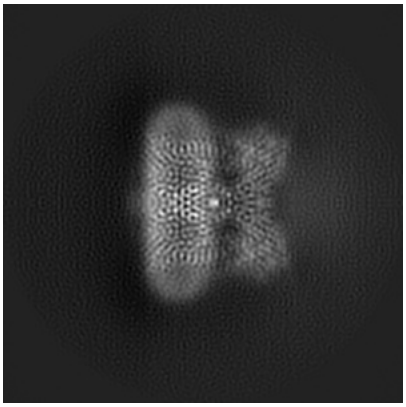
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

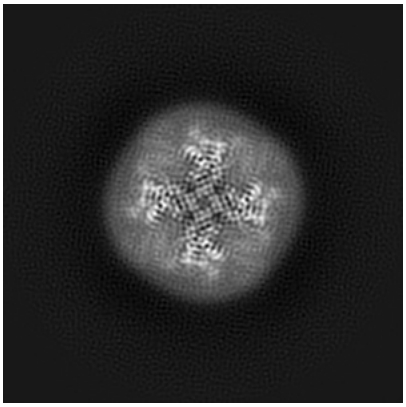
6.1.1 Primary map



X



Y

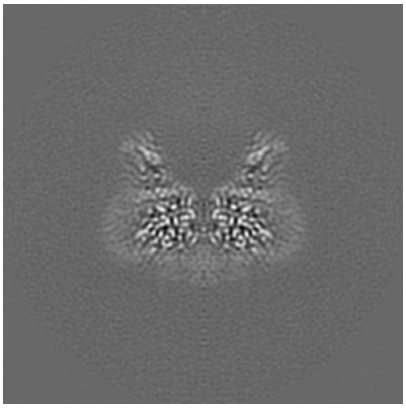


Z

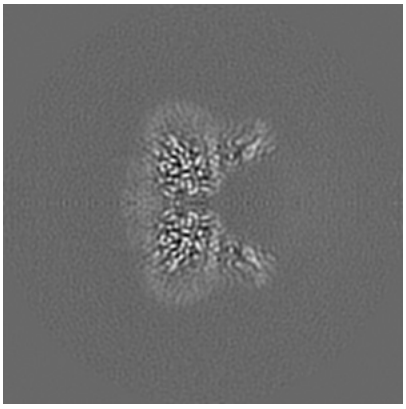
The images above show the map projected in three orthogonal directions.

6.2 Central slices

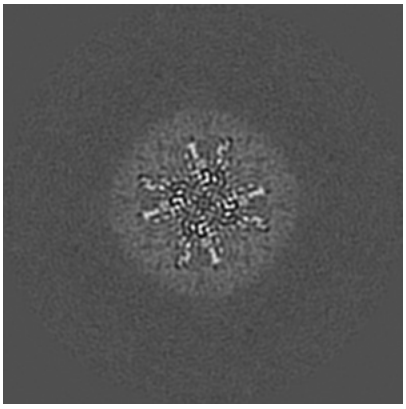
6.2.1 Primary map



X Index: 128



Y Index: 128

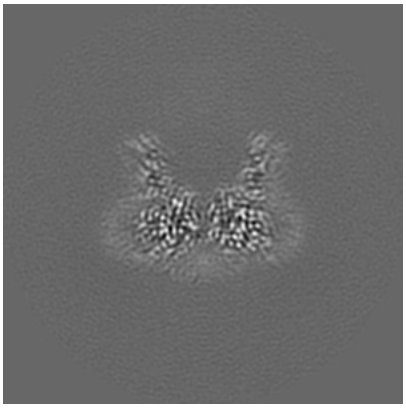


Z Index: 128

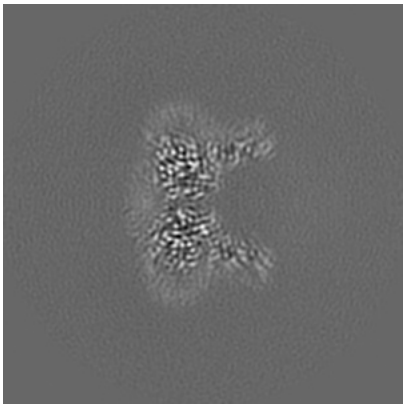
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

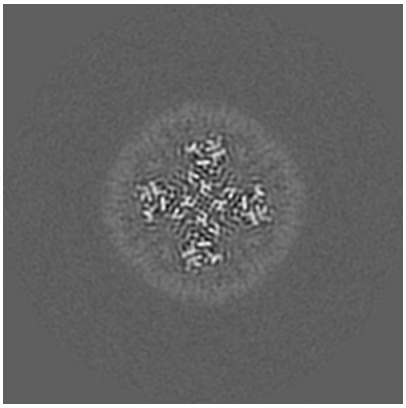
6.3.1 Primary map



X Index: 126



Y Index: 130

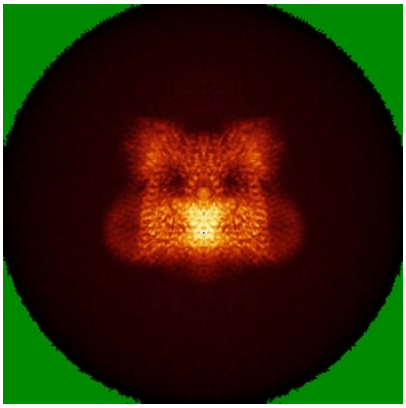


Z Index: 119

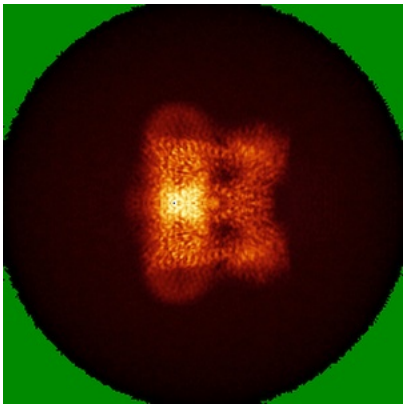
The images above show the largest variance slices of the map in three orthogonal directions.

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

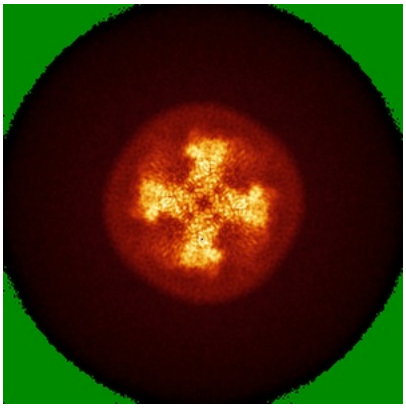
6.4.1 Primary map



X



Y

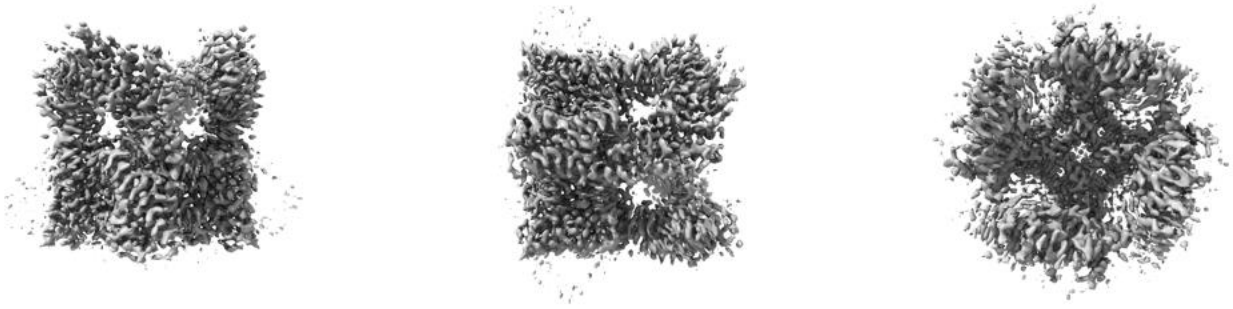


Z

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 0.0254. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

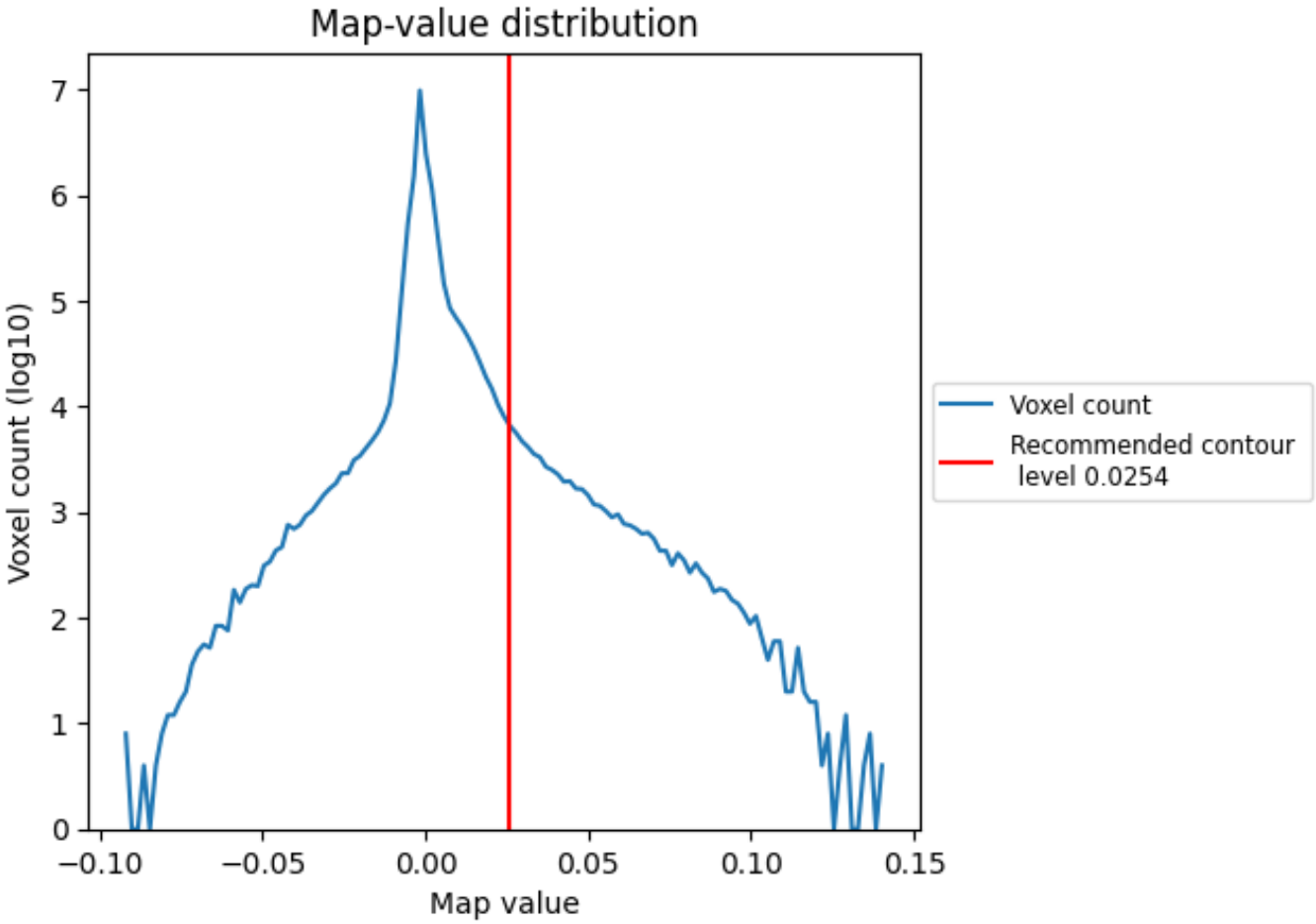
6.6 Mask visualisation (i)

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

7 Map analysis

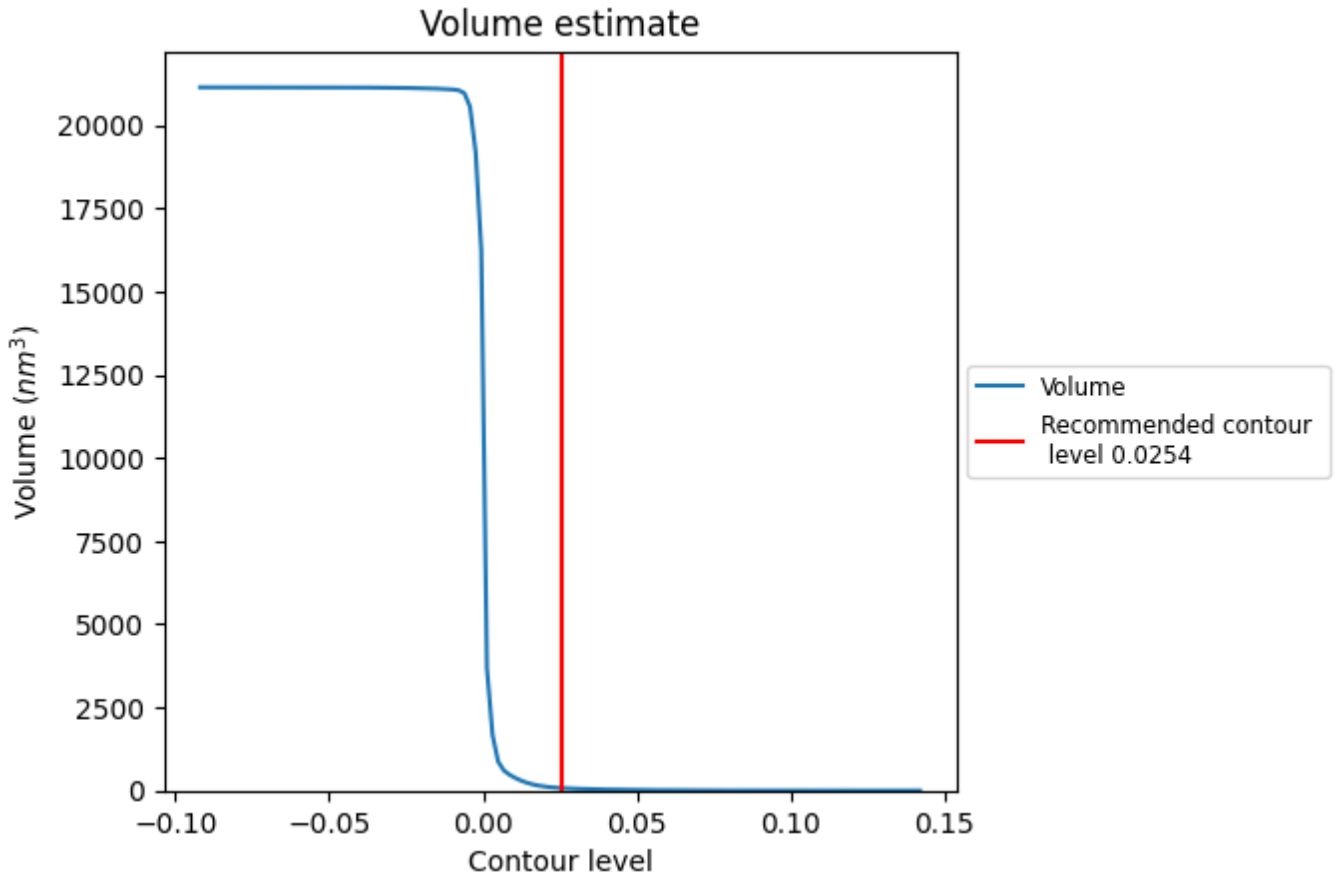
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

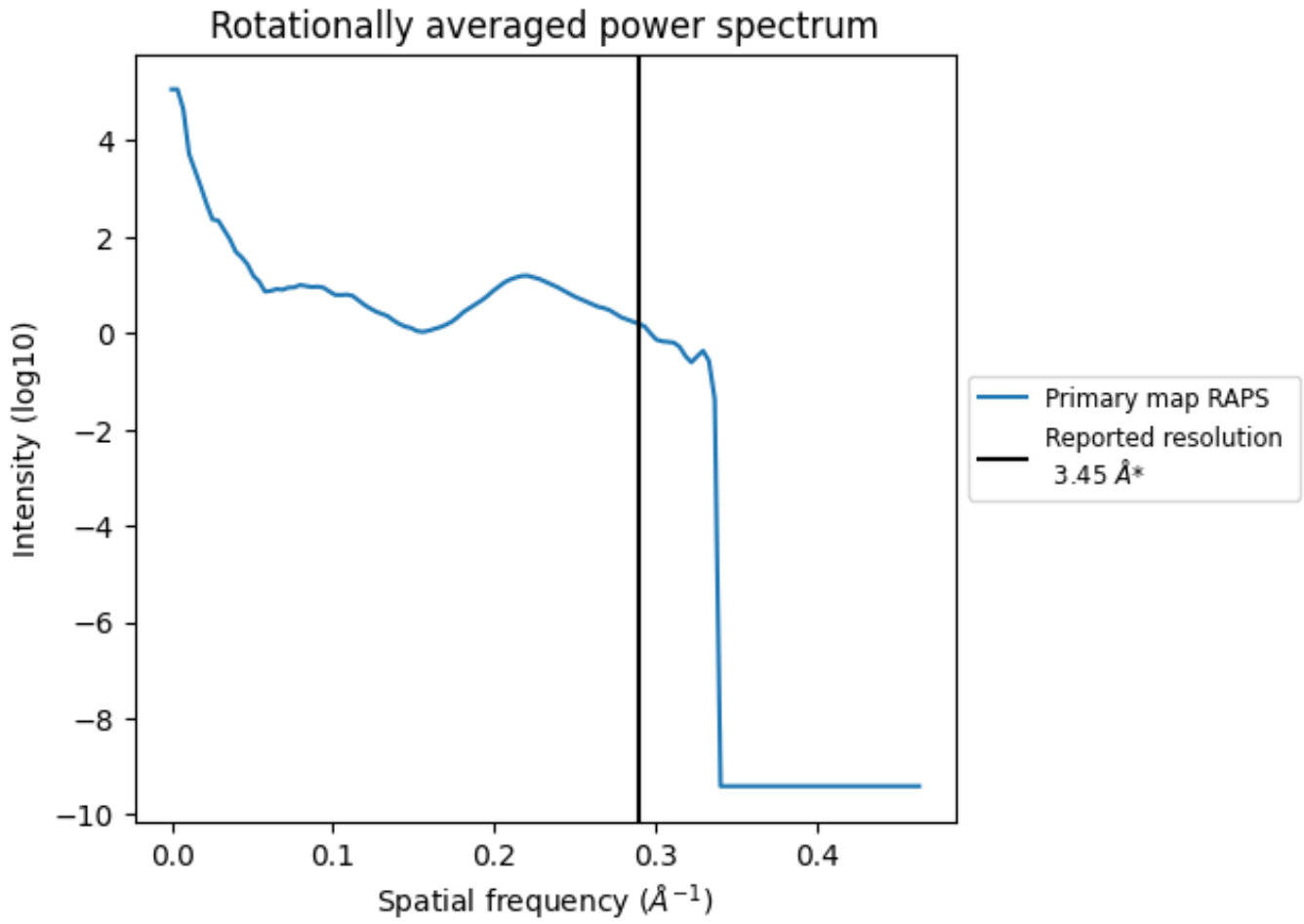
7.2 Volume estimate



The volume at the recommended contour level is 76 nm^3; this corresponds to an approximate mass of 69 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 0.290 Å^{-1}

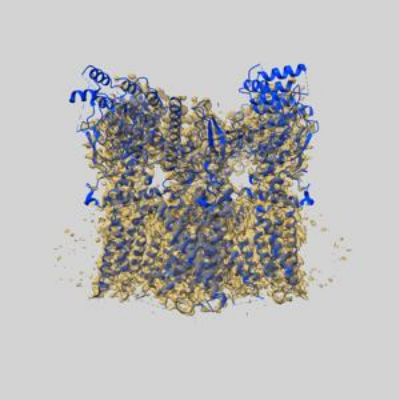
8 Fourier-Shell correlation

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

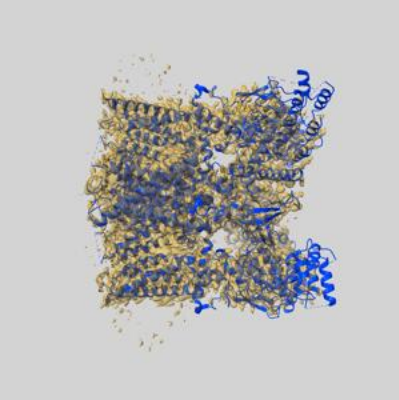
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-24637 and PDB model 7RQV. Per-residue inclusion information can be found in section 3 on page 9.

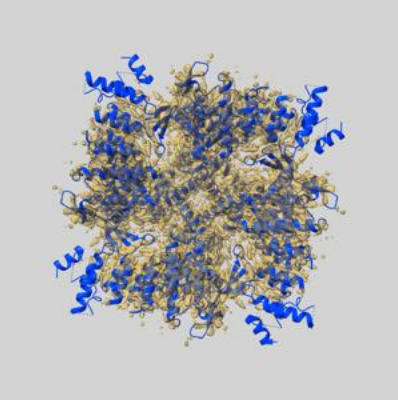
9.1 Map-model overlay



X



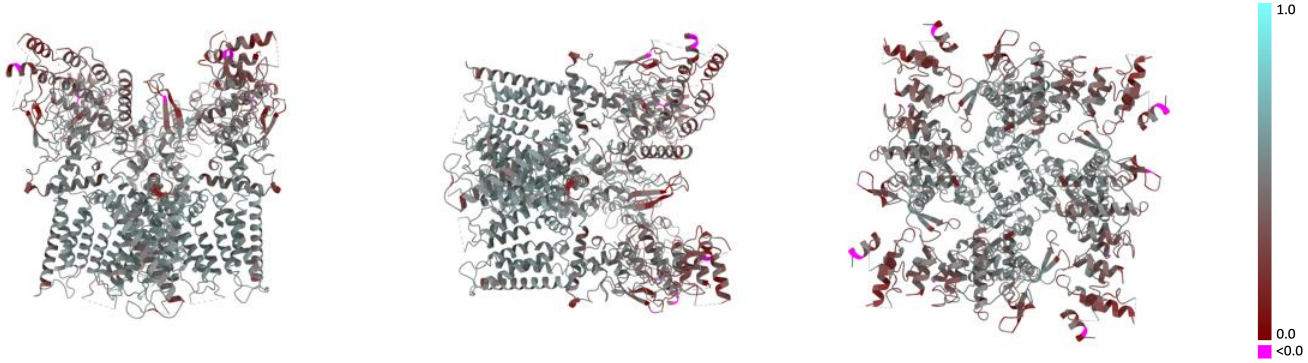
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0254 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.

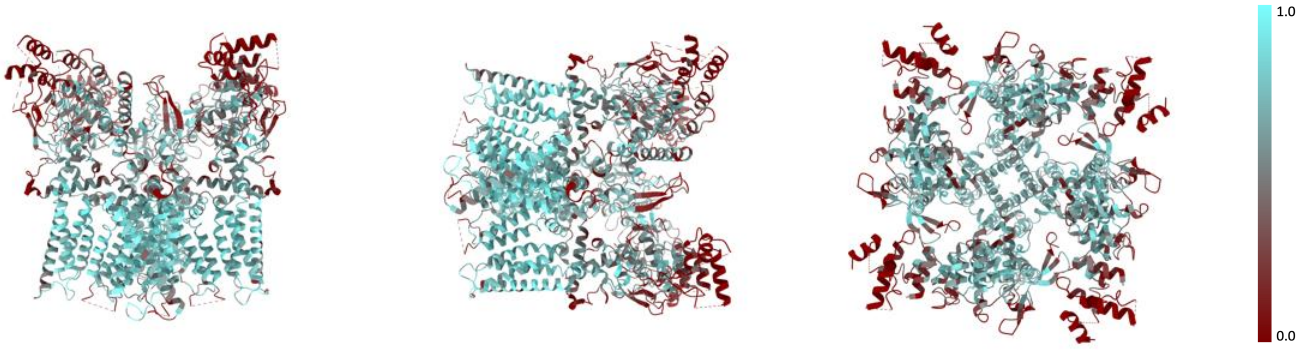
9.2 Q-score mapped to coordinate model (i)



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.

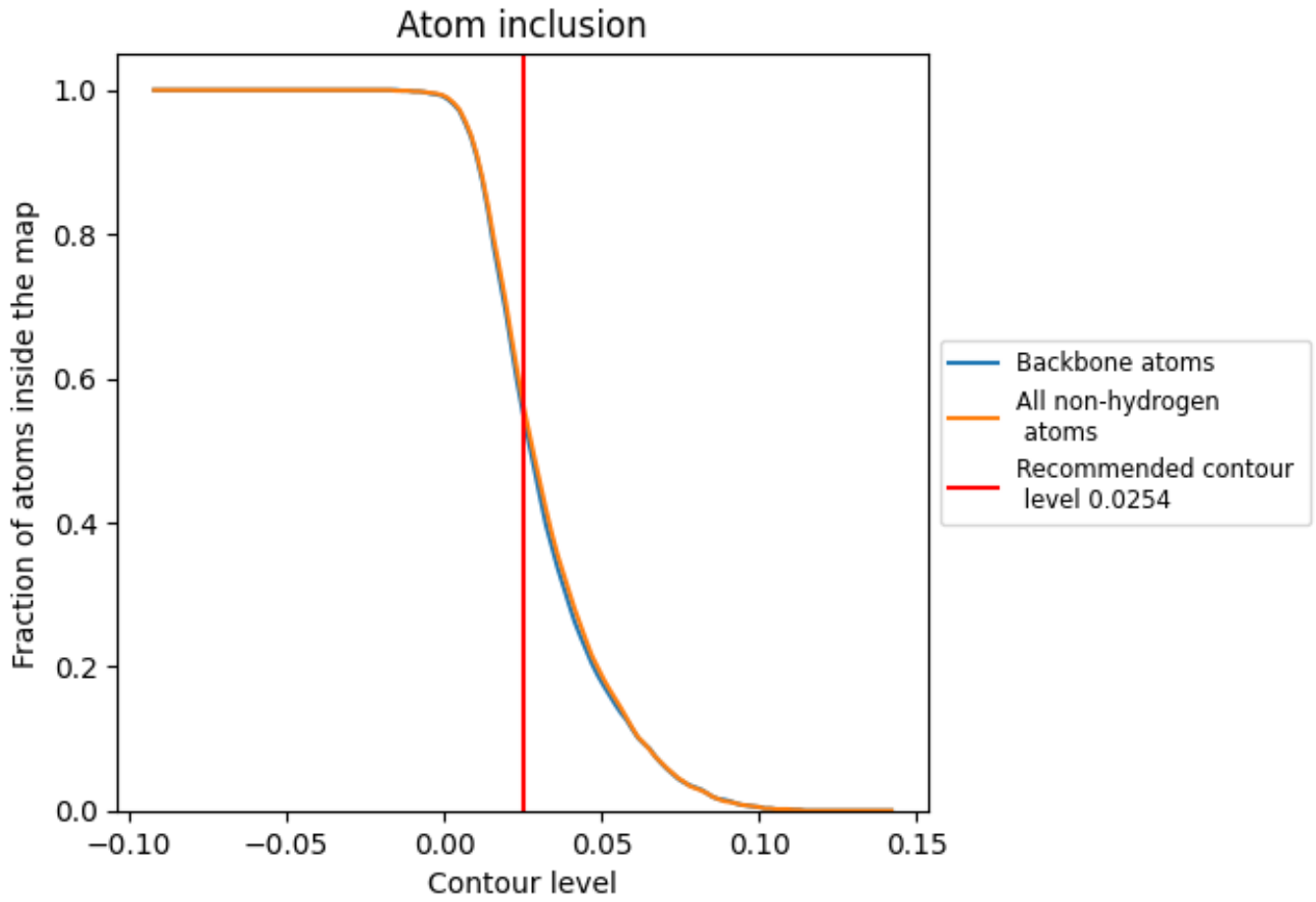
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0254).

9.4 Atom inclusion (i)



At the recommended contour level, 55% of all backbone atoms, 56% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0254) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5590	0.4660
A	0.5730	0.4670
B	0.5730	0.4660
C	0.5730	0.4640
D	0.5760	0.4650