



Full wwPDB EM Validation Report (i)

Nov 21, 2022 – 11:23 AM EST

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 (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:

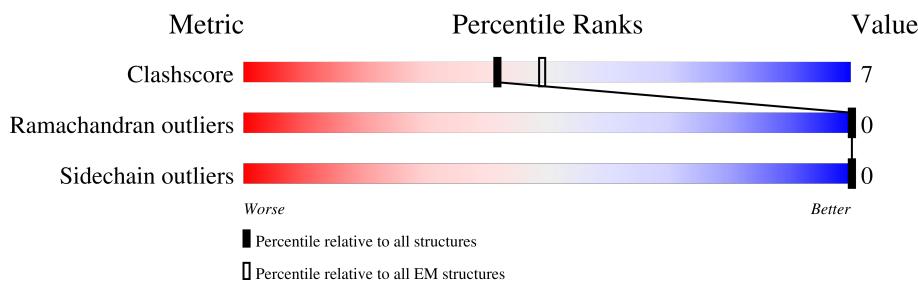
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance

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

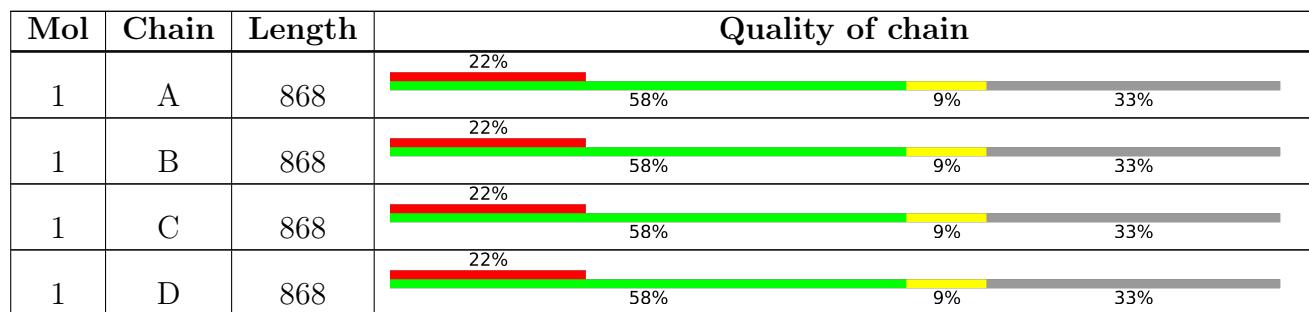
The reported resolution of this entry is 3.45 Å.

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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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



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

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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

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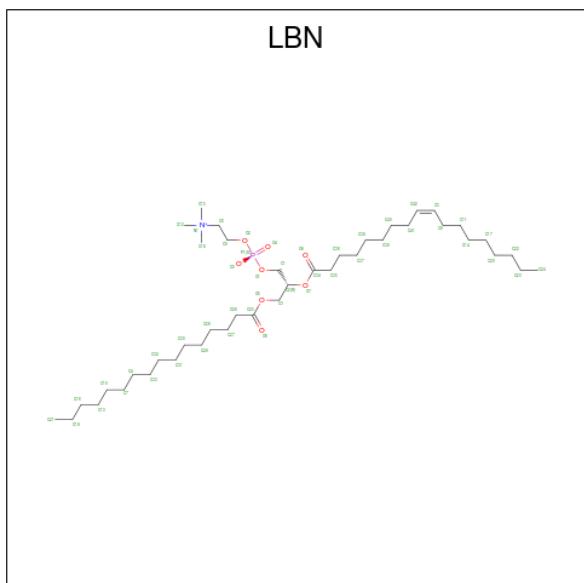
Chain	Residue	Modelled	Actual	Comment	Reference
D	842	LEU	-	expression tag	UNP O35433
D	843	GLU	-	expression tag	UNP O35433
D	844	VAL	-	expression tag	UNP O35433
D	845	LEU	-	expression tag	UNP O35433
D	846	PHE	-	expression tag	UNP O35433
D	847	GLN	-	expression tag	UNP O35433
D	848	GLY	-	expression tag	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

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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: C₄₂H₈₂NO₈P).



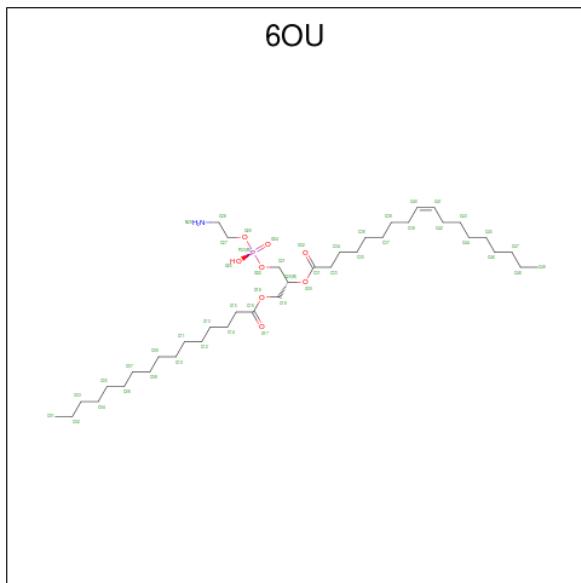
Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total		C	H	N	O	P
			77		23	44	1	8	1
2	C	1	Total		C	H	N	O	P
			77		23	44	1	8	1
2	D	1	Total		C	H	N	O	P
			77		23	44	1	8	1

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

- Molecule 3 is [(2 {R})-1-[2-azanylethoxy(oxidanyl)phosphoryl]oxy-3-hexadecanoyloxy-prop an-2-yl] ({Z})-octadec-9-enoate (three-letter code: 6OU) (formula: C₃₉H₇₆NO₈P).

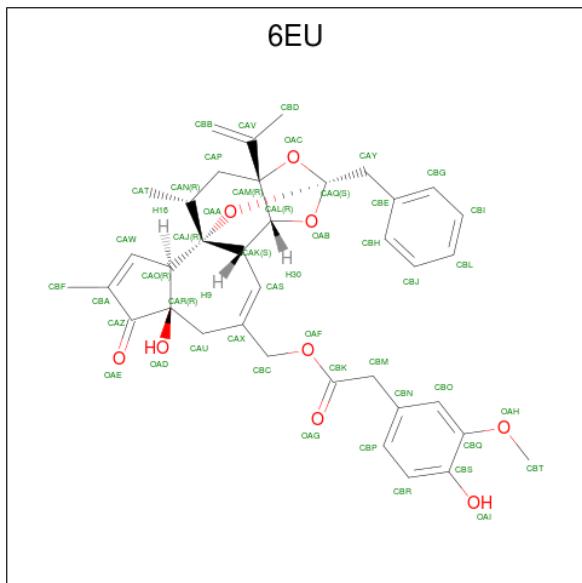


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Mol	Chain	Residues	Atoms					AltConf
3	B	1	Total	C	H	O	P	0
			183	60	105	16	2	

Mol	Chain	Residues	Atoms					AltConf
3	B	1	Total	C	H	O	P	0
			183	60	105	16	2	

- Molecule 4 is resiniferatoxin (three-letter code: 6EU) (formula: C₃₇H₄₀O₉) (labeled as "Ligand of Interest" by depositor).



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

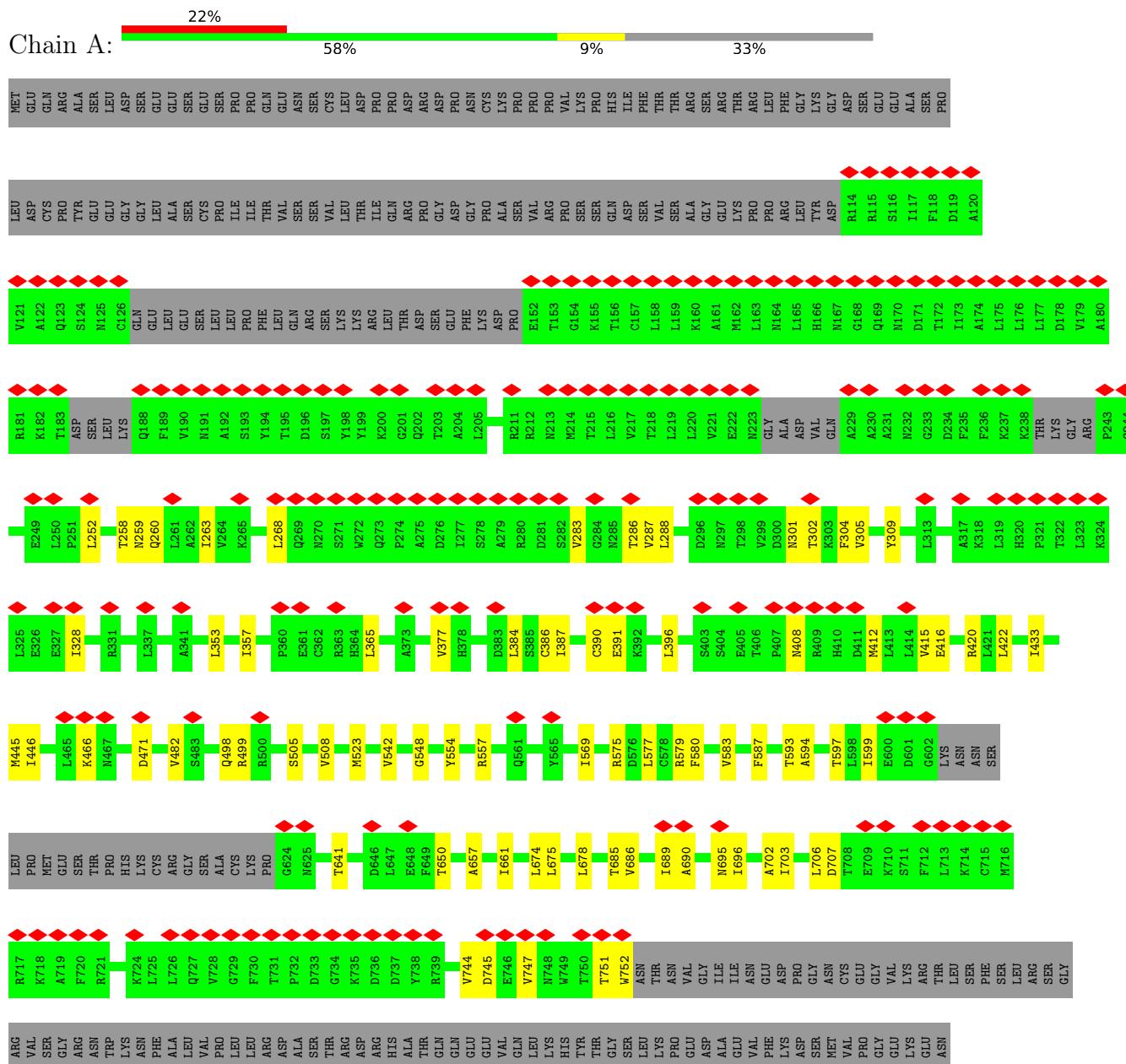
- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

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

3 Residue-property plots

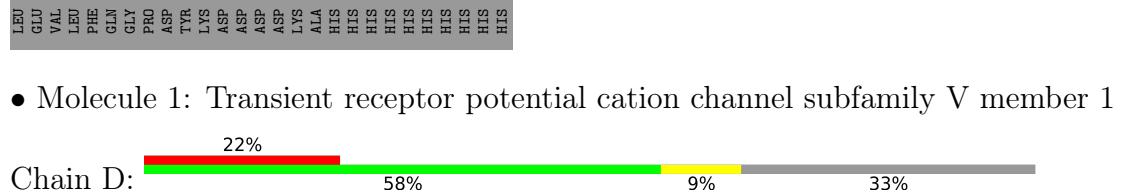
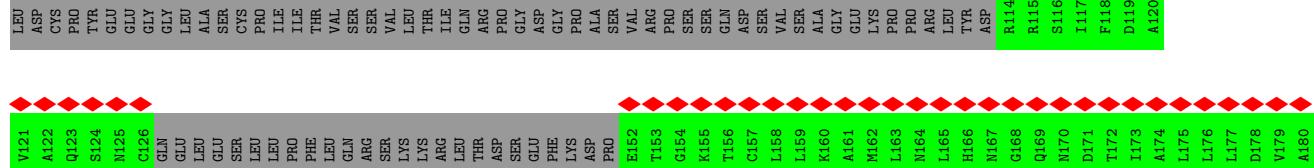
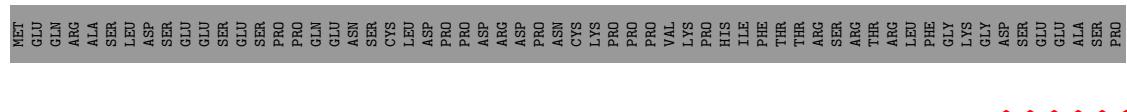
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

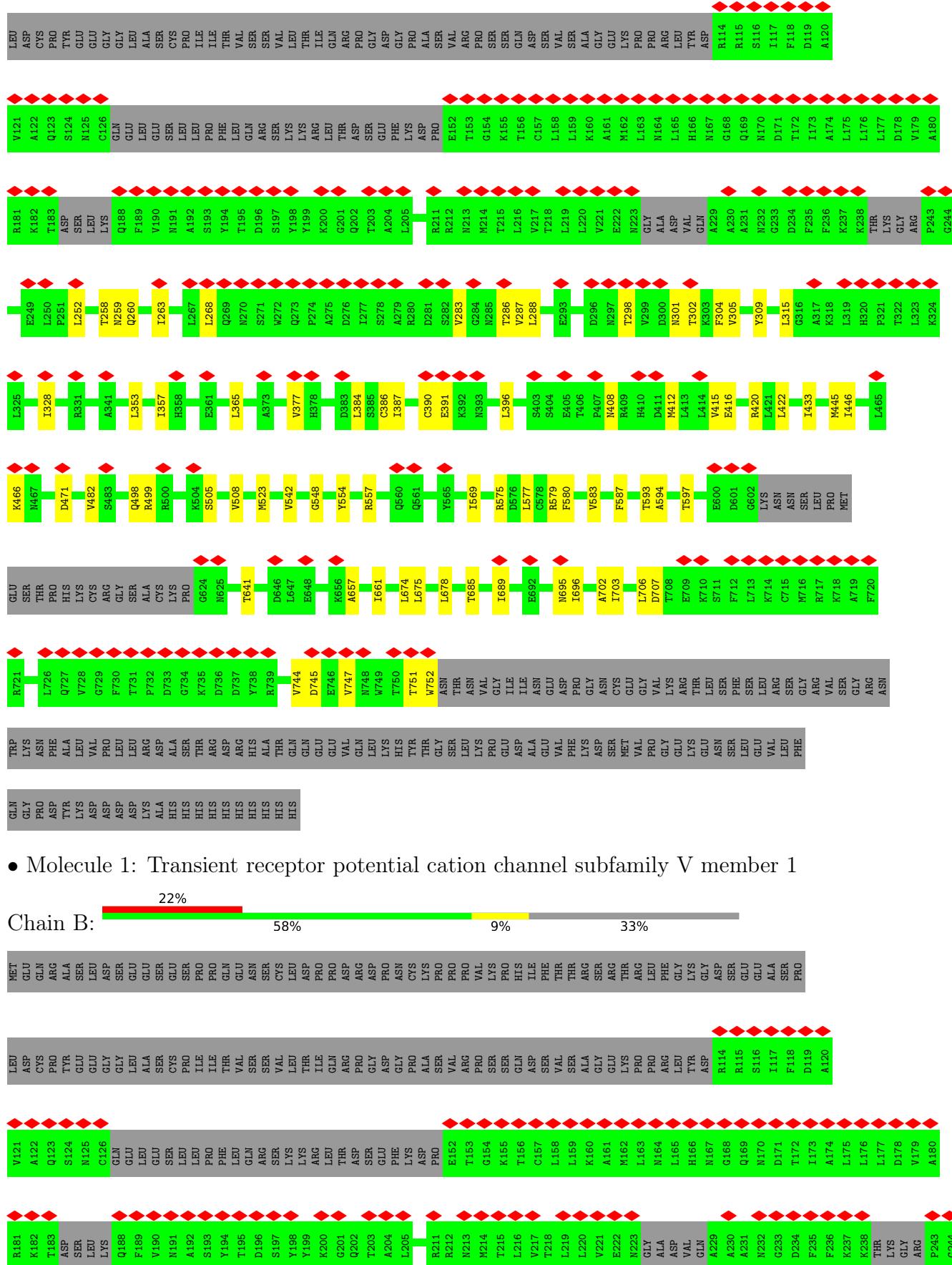
- Molecule 1: Transient receptor potential cation channel subfamily V member 1

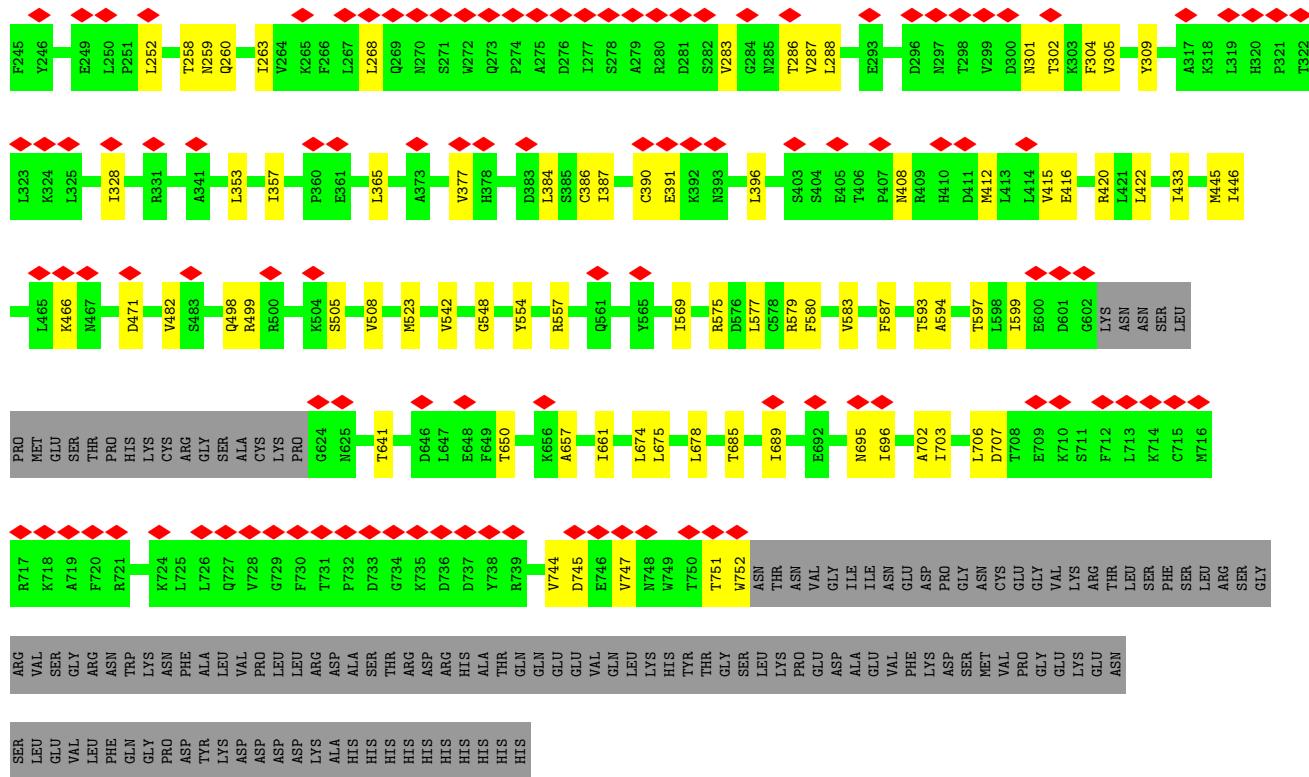


MET	LEU	SER	GLU	GLN	ARG	ALA	SER	GLY	VAL
GLU	VAL	GLN	VAL	ASP	ALA	ALA	ASP	GLY	LEU
GLN	ASP	GLY	ASP	GLN	SER	SER	GLY	GLN	PHE
ARG	TRP	VAL	PRO	ASP	LEU	LEU	PRO	GLY	GLN
ALA	LYS	ASP	PRO	ASP	ASP	ASP	ASP	ASP	ASP
SER	ASP								
GLY	ASP								
VAL	ASP								
ASP									
GLN	ASP								

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







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 ($e^-/\text{\AA}^2$)	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 i

5.1 Standard geometry i

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

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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

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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

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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

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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

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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

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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

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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 monosaccharides 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
3	6OU	D	902	-	34,34,48	1.66	4 (11%)	37,39,53	0.92	2 (5%)
3	6OU	B	904	-	9,9,48	0.71	0	8,8,53	0.40	0
3	6OU	C	903	-	32,32,48	1.52	3 (9%)	34,37,53	0.81	2 (5%)
2	LBN	B	901	-	32,32,51	1.34	3 (9%)	38,40,59	0.96	1 (2%)
3	6OU	A	904	-	9,9,48	0.71	0	8,8,53	0.40	0
4	6EU	A	905	-	43,52,52	4.41	15 (34%)	42,83,83	1.55	5 (11%)
3	6OU	A	903	-	32,32,48	1.51	3 (9%)	34,37,53	0.81	2 (5%)
3	6OU	A	902	-	34,34,48	1.66	4 (11%)	37,39,53	0.92	2 (5%)
3	6OU	B	903	-	32,32,48	1.52	3 (9%)	34,37,53	0.81	2 (5%)
2	LBN	C	901	-	32,32,51	1.34	3 (9%)	38,40,59	0.96	1 (2%)
3	6OU	C	904	-	9,9,48	0.71	0	8,8,53	0.40	0
4	6EU	D	904	-	43,52,52	4.41	15 (34%)	42,83,83	1.55	5 (11%)
4	6EU	C	905	-	43,52,52	4.40	15 (34%)	42,83,83	1.55	5 (11%)
3	6OU	C	902	-	34,34,48	1.66	4 (11%)	37,39,53	0.92	2 (5%)
3	6OU	D	903	-	9,9,48	0.71	0	8,8,53	0.41	0
3	6OU	A	906	-	32,32,48	1.52	3 (9%)	34,37,53	0.81	2 (5%)
3	6OU	B	902	-	34,34,48	1.66	4 (11%)	37,39,53	0.92	2 (5%)
2	LBN	A	901	-	32,32,51	1.35	3 (9%)	38,40,59	0.96	1 (2%)
4	6EU	B	905	-	43,52,52	4.40	15 (34%)	42,83,83	1.56	5 (11%)
2	LBN	D	901	-	32,32,51	1.35	3 (9%)	38,40,59	0.96	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	6OU	D	902	-	-	15/36/36/52	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	6OU	B	904	-	-	5/7/7/52	-
3	6OU	C	903	-	-	18/36/36/52	-
2	LBN	B	901	-	-	20/36/36/55	-
3	6OU	A	904	-	-	5/7/7/52	-
4	6EU	A	905	-	-	10/20/101/101	0/8/7/7
3	6OU	A	903	-	-	18/36/36/52	-
3	6OU	A	902	-	-	15/36/36/52	-
3	6OU	B	903	-	-	18/36/36/52	-
2	LBN	C	901	-	-	20/36/36/55	-
3	6OU	C	904	-	-	5/7/7/52	-
4	6EU	D	904	-	-	10/20/101/101	0/8/7/7
4	6EU	C	905	-	-	10/20/101/101	0/8/7/7
3	6OU	C	902	-	-	15/36/36/52	-
3	6OU	D	903	-	-	5/7/7/52	-
3	6OU	A	906	-	-	18/36/36/52	-
3	6OU	B	902	-	-	15/36/36/52	-
2	LBN	A	901	-	-	20/36/36/55	-
4	6EU	B	905	-	-	10/20/101/101	0/8/7/7
2	LBN	D	901	-	-	20/36/36/55	-

All (100) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	904	6EU	CAS-CAX	17.18	1.61	1.33
4	A	905	6EU	CAS-CAX	17.17	1.61	1.33
4	C	905	6EU	CAS-CAX	17.17	1.61	1.33
4	B	905	6EU	CAS-CAX	17.15	1.61	1.33
4	D	904	6EU	OAB-CAL	-10.90	1.27	1.43
4	A	905	6EU	OAB-CAL	-10.88	1.27	1.43
4	C	905	6EU	OAB-CAL	-10.88	1.27	1.43
4	B	905	6EU	OAB-CAL	-10.81	1.27	1.43
4	A	905	6EU	CAM-CAL	9.01	1.66	1.54
4	B	905	6EU	CAM-CAL	9.01	1.66	1.54
4	D	904	6EU	CAM-CAL	8.99	1.66	1.54
4	C	905	6EU	CAM-CAL	8.98	1.66	1.54
4	A	905	6EU	CAW-CBA	8.46	1.52	1.33
4	C	905	6EU	CAW-CBA	8.42	1.52	1.33
4	B	905	6EU	CAW-CBA	8.42	1.52	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	904	6EU	CAW-CBA	8.41	1.52	1.33
4	D	904	6EU	CAP-CAM	8.00	1.67	1.53
4	C	905	6EU	CAP-CAM	7.97	1.67	1.53
4	A	905	6EU	CAP-CAM	7.93	1.67	1.53
4	B	905	6EU	CAP-CAM	7.93	1.67	1.53
4	B	905	6EU	CAK-CAS	6.76	1.67	1.50
4	D	904	6EU	CAK-CAS	6.75	1.67	1.50
4	A	905	6EU	CAK-CAS	6.74	1.67	1.50
4	C	905	6EU	CAK-CAS	6.73	1.67	1.50
4	D	904	6EU	OAA-CAJ	6.20	1.58	1.43
4	B	905	6EU	OAA-CAJ	6.18	1.58	1.43
4	C	905	6EU	OAA-CAJ	6.17	1.58	1.43
4	A	905	6EU	OAA-CAJ	6.13	1.58	1.43
4	A	905	6EU	OAA-CAQ	5.45	1.50	1.42
4	B	905	6EU	OAA-CAQ	5.43	1.50	1.42
4	C	905	6EU	OAA-CAQ	5.42	1.50	1.42
4	D	904	6EU	OAA-CAQ	5.40	1.50	1.42
3	D	902	6OU	P23-O22	5.38	1.77	1.60
3	B	902	6OU	P23-O22	5.38	1.77	1.60
3	C	902	6OU	P23-O22	5.38	1.77	1.60
3	A	902	6OU	P23-O22	5.37	1.77	1.60
3	C	902	6OU	P23-O26	4.72	1.73	1.54
3	D	902	6OU	P23-O26	4.72	1.73	1.54
3	A	902	6OU	P23-O26	4.72	1.73	1.54
3	B	902	6OU	P23-O26	4.72	1.73	1.54
2	A	901	LBN	P1-O2	4.56	1.77	1.59
2	C	901	LBN	P1-O2	4.55	1.77	1.59
2	D	901	LBN	P1-O2	4.55	1.77	1.59
2	B	901	LBN	P1-O2	4.53	1.77	1.59
3	C	903	6OU	P23-O22	4.52	1.77	1.59
3	B	903	6OU	P23-O22	4.52	1.77	1.59
3	A	906	6OU	P23-O22	4.51	1.77	1.59
3	A	903	6OU	P23-O22	4.51	1.77	1.59
4	D	904	6EU	OAC-CAM	-4.03	1.37	1.44
4	A	905	6EU	OAC-CAM	-4.01	1.37	1.44
4	B	905	6EU	OAC-CAM	-4.01	1.37	1.44
4	C	905	6EU	OAC-CAM	-4.00	1.37	1.44
4	B	905	6EU	OAB-CAQ	-3.90	1.34	1.41
4	A	905	6EU	OAB-CAQ	-3.90	1.34	1.41
4	C	905	6EU	OAB-CAQ	-3.86	1.34	1.41
4	D	904	6EU	OAB-CAQ	-3.82	1.34	1.41
3	A	906	6OU	P23-O26	3.57	1.73	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	903	6OU	P23-O26	3.56	1.73	1.59
3	C	903	6OU	P23-O26	3.56	1.73	1.59
3	B	903	6OU	P23-O26	3.56	1.73	1.59
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	A	905	6EU	OAF-CBK	2.82	1.41	1.33
4	D	904	6EU	OAH-CBQ	2.79	1.41	1.37
4	B	905	6EU	OAH-CBQ	2.79	1.41	1.37
4	C	905	6EU	OAH-CBQ	2.79	1.41	1.37
4	A	905	6EU	OAH-CBQ	2.79	1.41	1.37
4	A	905	6EU	CAY-CBE	2.69	1.56	1.51
4	C	905	6EU	CAY-CBE	2.66	1.55	1.51
4	B	905	6EU	CAY-CBE	2.66	1.55	1.51
4	D	904	6EU	CAY-CBE	2.66	1.55	1.51
3	A	903	6OU	C21-C20	2.48	1.58	1.50
3	B	903	6OU	C21-C20	2.47	1.58	1.50
3	C	903	6OU	C21-C20	2.47	1.58	1.50
3	A	906	6OU	C21-C20	2.46	1.58	1.50
3	D	902	6OU	C21-C20	2.45	1.58	1.50
3	B	902	6OU	C21-C20	2.45	1.58	1.50
3	C	902	6OU	C21-C20	2.44	1.58	1.50
3	A	902	6OU	C21-C20	2.43	1.58	1.50
2	A	901	LBN	O2-C9	-2.43	1.34	1.44
2	C	901	LBN	O2-C9	-2.42	1.34	1.44
2	B	901	LBN	O2-C9	-2.42	1.34	1.44
2	D	901	LBN	O2-C9	-2.42	1.34	1.44
4	D	904	6EU	OAI-CBS	2.17	1.40	1.36
3	D	902	6OU	C19-C20	2.15	1.57	1.50
3	B	902	6OU	C19-C20	2.15	1.57	1.50
4	A	905	6EU	OAI-CBS	2.14	1.40	1.36
3	C	902	6OU	C19-C20	2.14	1.57	1.50
4	C	905	6EU	CAR-CAO	-2.13	1.50	1.55
4	A	905	6EU	CAR-CAO	-2.13	1.50	1.55
3	A	902	6OU	C19-C20	2.13	1.57	1.50
4	C	905	6EU	OAI-CBS	2.12	1.40	1.36
4	B	905	6EU	OAI-CBS	2.12	1.40	1.36
4	D	904	6EU	CAR-CAO	-2.10	1.50	1.55
4	B	905	6EU	CAR-CAO	-2.10	1.50	1.55
2	A	901	LBN	P1-O1	2.02	1.67	1.59
2	C	901	LBN	P1-O1	2.02	1.67	1.59
2	B	901	LBN	P1-O1	2.02	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	901	LBN	P1-O1	2.02	1.67	1.59

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	905	6EU	OAF-CBK-CBM	6.17	121.53	111.07
4	C	905	6EU	OAF-CBK-CBM	6.17	121.52	111.07
4	A	905	6EU	OAF-CBK-CBM	6.17	121.52	111.07
4	D	904	6EU	OAF-CBK-CBM	6.15	121.50	111.07
4	D	904	6EU	OAH-CBQ-CBS	3.74	119.99	114.57
4	B	905	6EU	OAH-CBQ-CBS	3.71	119.94	114.57
4	C	905	6EU	OAH-CBQ-CBS	3.70	119.93	114.57
4	A	905	6EU	OAH-CBQ-CBS	3.67	119.89	114.57
3	B	902	6OU	O25-P23-O24	3.48	124.31	110.68
3	C	902	6OU	O25-P23-O24	3.48	124.29	110.68
3	A	902	6OU	O25-P23-O24	3.47	124.27	110.68
3	D	902	6OU	O25-P23-O24	3.47	124.26	110.68
4	A	905	6EU	OAA-CAJ-CAK	-3.43	102.83	109.02
4	C	905	6EU	OAA-CAJ-CAK	-3.42	102.84	109.02
4	B	905	6EU	OAA-CAJ-CAK	-3.42	102.85	109.02
4	D	904	6EU	OAA-CAJ-CAK	-3.42	102.85	109.02
2	A	901	LBN	O3-P1-O4	3.31	128.60	112.24
2	C	901	LBN	O3-P1-O4	3.31	128.60	112.24
2	D	901	LBN	O3-P1-O4	3.31	128.59	112.24
2	B	901	LBN	O3-P1-O4	3.31	128.58	112.24
3	A	903	6OU	O30-C31-C33	2.41	116.68	111.50
3	C	903	6OU	O30-C31-C33	2.40	116.67	111.50
3	A	906	6OU	O25-P23-O24	2.40	124.09	112.24
3	C	903	6OU	O25-P23-O24	2.40	124.09	112.24
3	B	903	6OU	O25-P23-O24	2.40	124.09	112.24
3	B	903	6OU	O30-C31-C33	2.40	116.67	111.50
3	A	903	6OU	O25-P23-O24	2.39	124.08	112.24
3	A	906	6OU	O30-C31-C33	2.39	116.64	111.50
3	A	902	6OU	O30-C31-C33	2.30	116.45	111.50
3	D	902	6OU	O30-C31-C33	2.28	116.42	111.50
3	C	902	6OU	O30-C31-C33	2.28	116.41	111.50
3	B	902	6OU	O30-C31-C33	2.26	116.38	111.50
4	A	905	6EU	CBF-CBA-CAW	-2.19	125.91	130.48
4	C	905	6EU	CBF-CBA-CAW	-2.18	125.92	130.48
4	D	904	6EU	CBF-CBA-CAW	-2.18	125.93	130.48
4	B	905	6EU	OAH-CBQ-CBO	-2.18	120.38	124.12
4	B	905	6EU	CBF-CBA-CAW	-2.17	125.94	130.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	904	6EU	OAH-CBQ-CBO	-2.17	120.39	124.12
4	C	905	6EU	OAH-CBQ-CBO	-2.15	120.42	124.12
4	A	905	6EU	OAH-CBQ-CBO	-2.14	120.43	124.12

There are no chirality outliers.

All (272) 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
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	902	6OU	C40-C41-C42-C43
3	A	903	6OU	C21-O22-P23-O24
3	A	903	6OU	C40-C41-C42-C43
3	A	906	6OU	C21-O22-P23-O24
3	A	906	6OU	C40-C41-C42-C43
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	902	6OU	C40-C41-C42-C43
3	C	903	6OU	C21-O22-P23-O24
3	C	903	6OU	C40-C41-C42-C43
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	D	902	6OU	C40-C41-C42-C43
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	902	6OU	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
3	B	903	6OU	C21-O22-P23-O24
3	B	903	6OU	C40-C41-C42-C43
4	A	905	6EU	OAC-CAM-CAV-CBB
4	A	905	6EU	OAC-CAM-CAV-CBD
4	A	905	6EU	OAC-CAQ-CAY-CBE
4	C	905	6EU	OAC-CAM-CAV-CBB
4	C	905	6EU	OAC-CAM-CAV-CBD
4	C	905	6EU	OAC-CAQ-CAY-CBE
4	D	904	6EU	OAC-CAM-CAV-CBB
4	D	904	6EU	OAC-CAM-CAV-CBD
4	D	904	6EU	OAC-CAQ-CAY-CBE
4	B	905	6EU	OAC-CAM-CAV-CBB
4	B	905	6EU	OAC-CAM-CAV-CBD
4	B	905	6EU	OAC-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	903	6OU	C21-O22-P23-O26
3	A	906	6OU	C21-O22-P23-O26
3	C	903	6OU	C21-O22-P23-O26
3	B	903	6OU	C21-O22-P23-O26

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Mol	Chain	Res	Type	Atoms
3	A	902	6OU	C36-C37-C38-C39
3	C	902	6OU	C36-C37-C38-C39
3	D	902	6OU	C36-C37-C38-C39
3	B	902	6OU	C36-C37-C38-C39
3	A	904	6OU	C44-C45-C46-C47
3	C	904	6OU	C44-C45-C46-C47
3	D	903	6OU	C44-C45-C46-C47
3	B	904	6OU	C44-C45-C46-C47
3	A	903	6OU	C33-C34-C35-C36
3	A	906	6OU	C33-C34-C35-C36
3	C	903	6OU	C33-C34-C35-C36
3	B	903	6OU	C33-C34-C35-C36
3	A	903	6OU	C12-C13-C14-C15
3	A	906	6OU	C12-C13-C14-C15
3	C	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	D	902	6OU	C09-C10-C11-C12
3	B	902	6OU	C09-C10-C11-C12
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	902	6OU	C35-C36-C37-C38
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	A	902	6OU	C07-C08-C09-C10
3	C	902	6OU	C07-C08-C09-C10
3	D	902	6OU	C07-C08-C09-C10
3	B	902	6OU	C07-C08-C09-C10
3	A	902	6OU	C10-C11-C12-C13
3	A	903	6OU	C36-C37-C38-C39
3	A	906	6OU	C36-C37-C38-C39
3	C	902	6OU	C10-C11-C12-C13
3	C	903	6OU	C36-C37-C38-C39
3	D	902	6OU	C10-C11-C12-C13
3	B	902	6OU	C10-C11-C12-C13
3	B	903	6OU	C36-C37-C38-C39
3	A	902	6OU	C12-C13-C14-C15
3	C	902	6OU	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
3	D	902	6OU	C12-C13-C14-C15
3	B	902	6OU	C12-C13-C14-C15
2	D	901	LBN	C28-C29-C30-C31
2	B	901	LBN	C28-C29-C30-C31
2	A	901	LBN	C28-C29-C30-C31
2	C	901	LBN	C28-C29-C30-C31
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	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
4	A	905	6EU	CAP-CAM-CAV-CBD
4	C	905	6EU	CAP-CAM-CAV-CBD
4	D	904	6EU	CAP-CAM-CAV-CBD
4	B	905	6EU	CAP-CAM-CAV-CBD
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
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
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
3	A	904	6OU	C42-C43-C44-C45
3	C	904	6OU	C42-C43-C44-C45
3	D	903	6OU	C42-C43-C44-C45
3	B	904	6OU	C42-C43-C44-C45
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

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Mol	Chain	Res	Type	Atoms
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	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	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	902	6OU	C34-C35-C36-C37
3	C	902	6OU	C34-C35-C36-C37
3	B	902	6OU	C34-C35-C36-C37
3	D	902	6OU	C34-C35-C36-C37
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	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	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	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
4	A	905	6EU	OAA-CAQ-CAY-CBE
4	A	905	6EU	OAB-CAQ-CAY-CBE
4	C	905	6EU	OAA-CAQ-CAY-CBE
4	C	905	6EU	OAB-CAQ-CAY-CBE
4	D	904	6EU	OAA-CAQ-CAY-CBE
4	D	904	6EU	OAB-CAQ-CAY-CBE
4	B	905	6EU	OAA-CAQ-CAY-CBE
4	B	905	6EU	OAB-CAQ-CAY-CBE
3	D	903	6OU	C43-C44-C45-C46
3	C	904	6OU	C43-C44-C45-C46

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Mol	Chain	Res	Type	Atoms
3	B	904	6OU	C43-C44-C45-C46
3	A	904	6OU	C43-C44-C45-C46
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
3	A	902	6OU	C08-C09-C10-C11
3	C	902	6OU	C08-C09-C10-C11
3	B	902	6OU	C08-C09-C10-C11
3	D	902	6OU	C08-C09-C10-C11
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	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	C9-C6-N1-C12
2	C	901	LBN	C9-C6-N1-C12
2	D	901	LBN	C9-C6-N1-C12
2	B	901	LBN	C9-C6-N1-C12
2	A	901	LBN	O7-C34-C35-C36
2	C	901	LBN	O7-C34-C35-C36
2	D	901	LBN	O7-C34-C35-C36
2	B	901	LBN	O7-C34-C35-C36
4	A	905	6EU	CAP-CAM-CAV-CBB
4	C	905	6EU	CAP-CAM-CAV-CBB
4	D	904	6EU	CAP-CAM-CAV-CBB
4	B	905	6EU	CAP-CAM-CAV-CBB
2	A	901	LBN	C9-C6-N1-C15
2	C	901	LBN	C9-C6-N1-C15
2	D	901	LBN	C9-C6-N1-C15
2	B	901	LBN	C9-C6-N1-C15
4	A	905	6EU	OAF-CBK-CBM-CBN
4	C	905	6EU	OAF-CBK-CBM-CBN
4	D	904	6EU	OAF-CBK-CBM-CBN
4	B	905	6EU	OAF-CBK-CBM-CBN
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

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Mol	Chain	Res	Type	Atoms
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
2	A	901	LBN	C9-C6-N1-C18
2	C	901	LBN	C9-C6-N1-C18
2	D	901	LBN	C9-C6-N1-C18
2	B	901	LBN	C9-C6-N1-C18
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
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
3	A	906	6OU	C38-C39-C40-C41
3	B	903	6OU	C38-C39-C40-C41
2	A	901	LBN	C30-C31-C32-C33
2	C	901	LBN	C30-C31-C32-C33
2	D	901	LBN	C30-C31-C32-C33
2	B	901	LBN	C30-C31-C32-C33
2	C	901	LBN	O6-C25-C26-C27
2	A	901	LBN	O6-C25-C26-C27
2	D	901	LBN	O6-C25-C26-C27
2	B	901	LBN	O6-C25-C26-C27

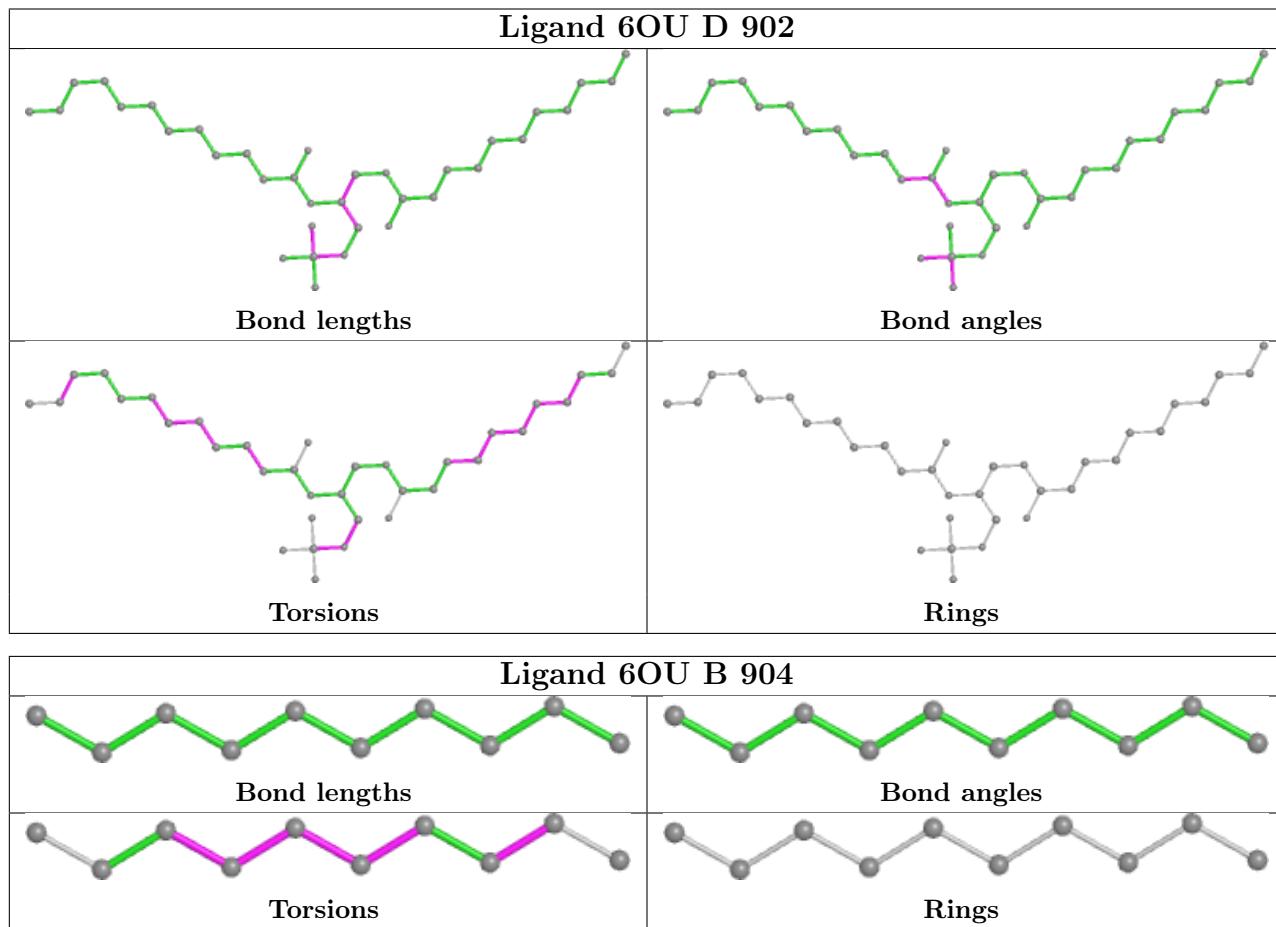
There are no ring outliers.

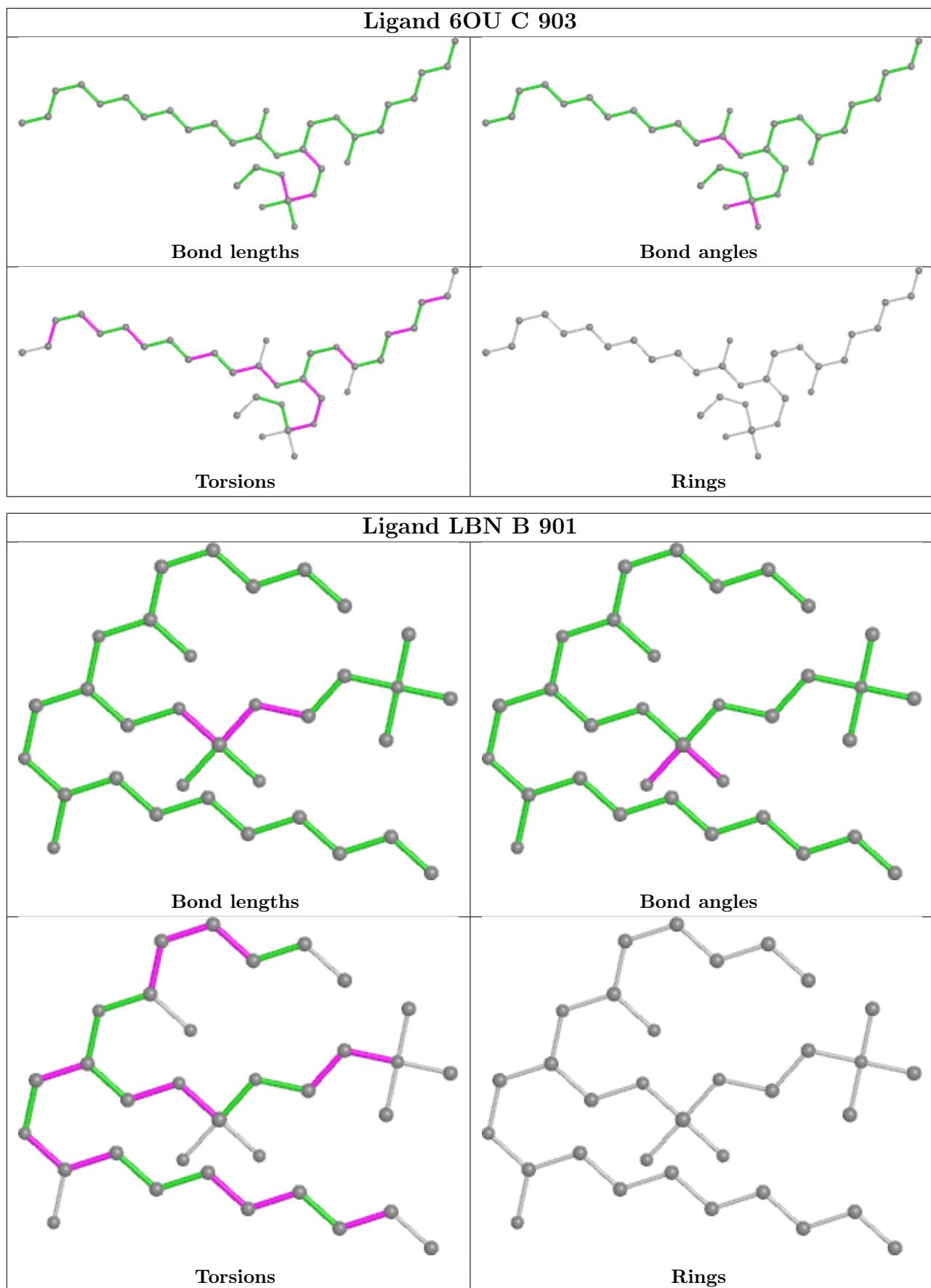
4 monomers are involved in 4 short contacts:

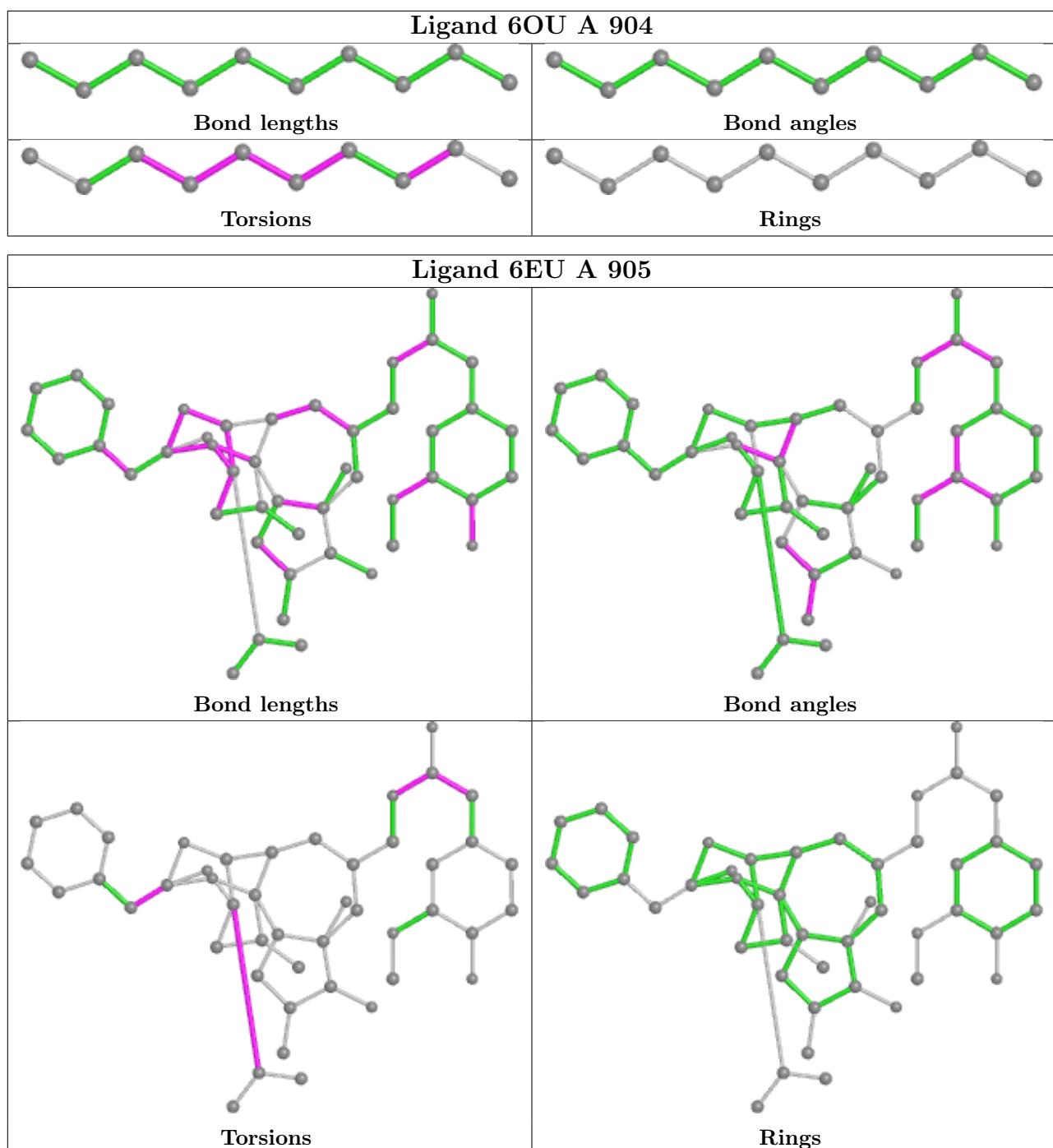
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	905	6EU	1	0
4	D	904	6EU	1	0
4	C	905	6EU	1	0
4	B	905	6EU	1	0

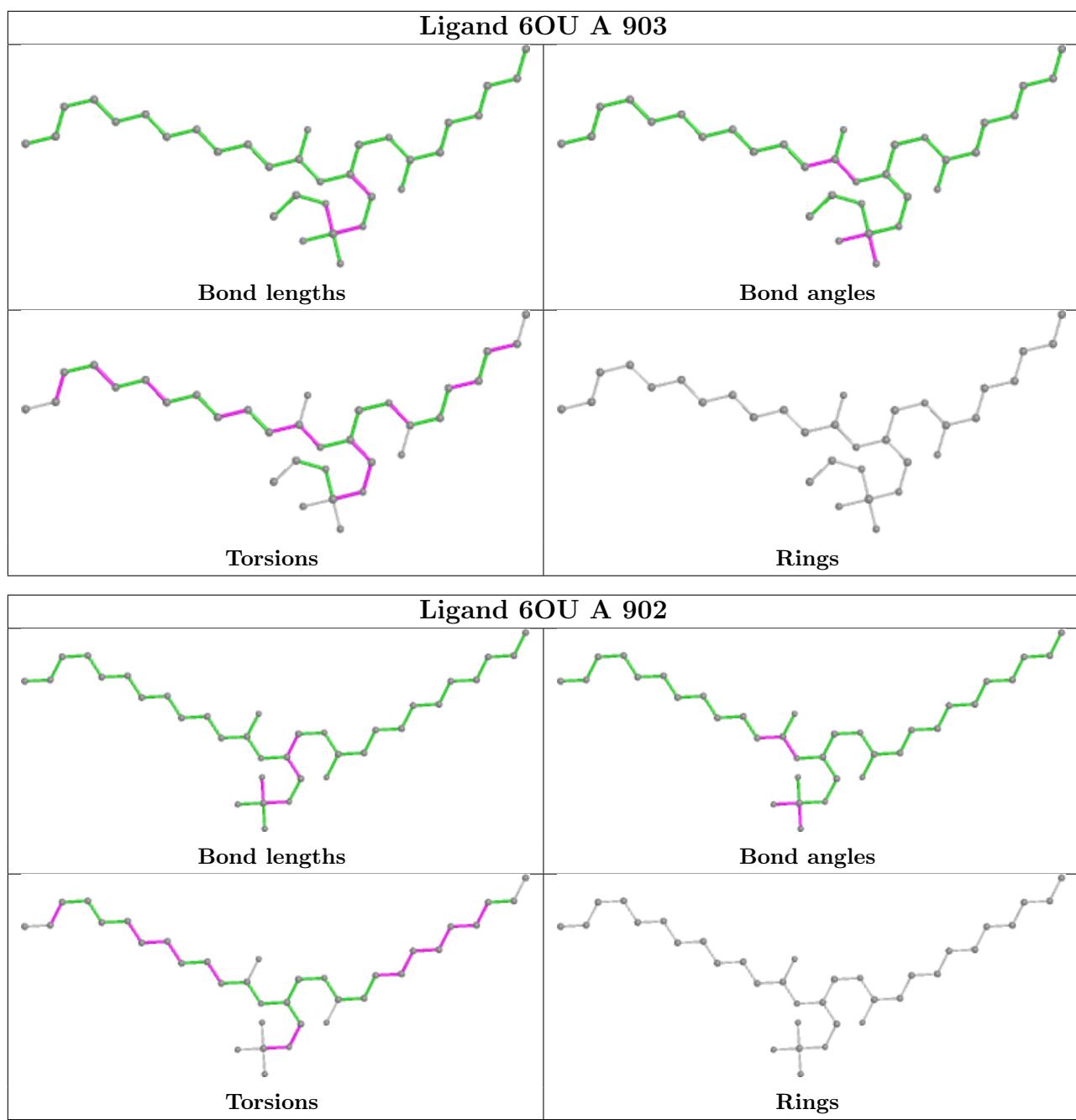
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

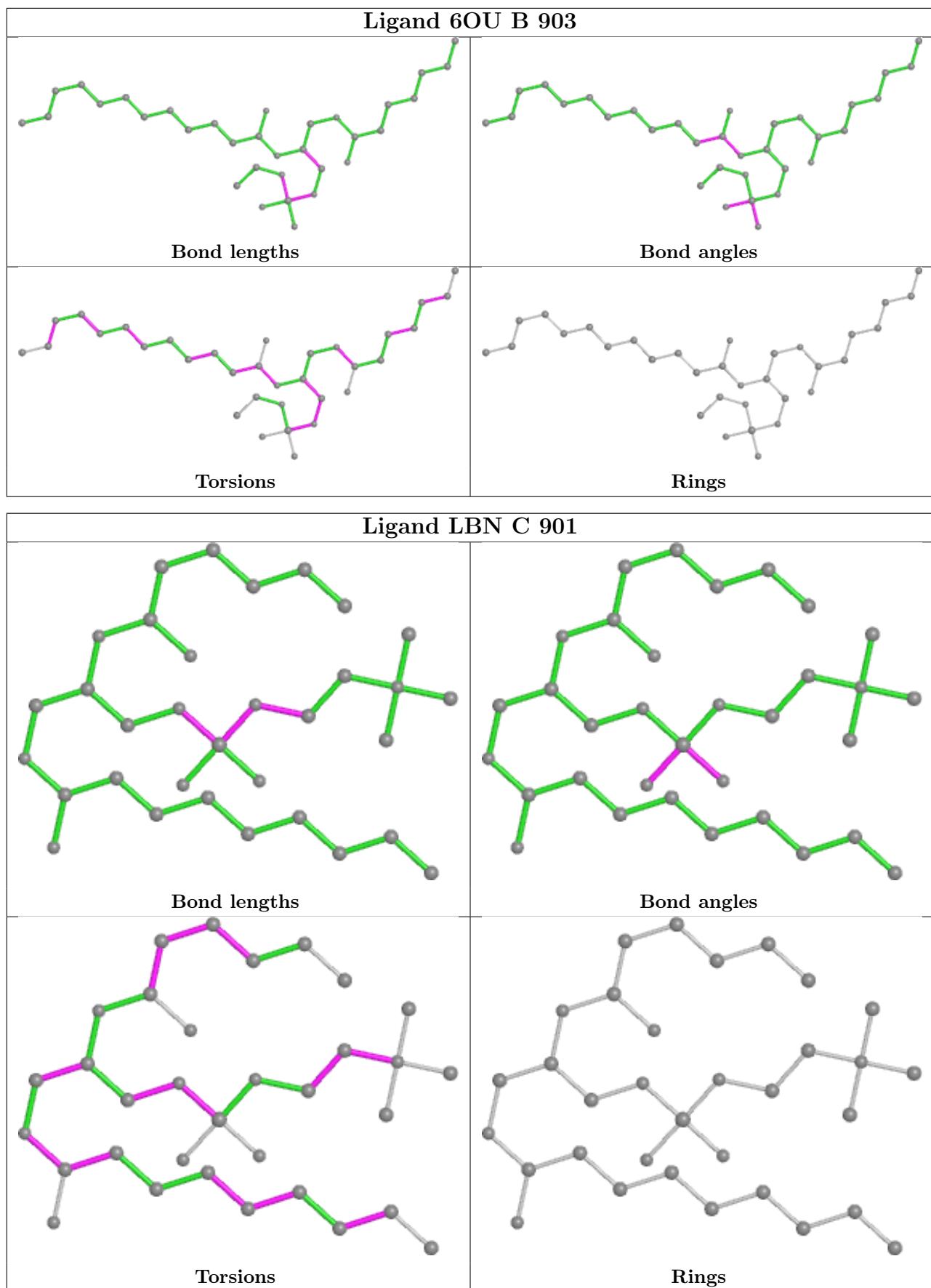
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.

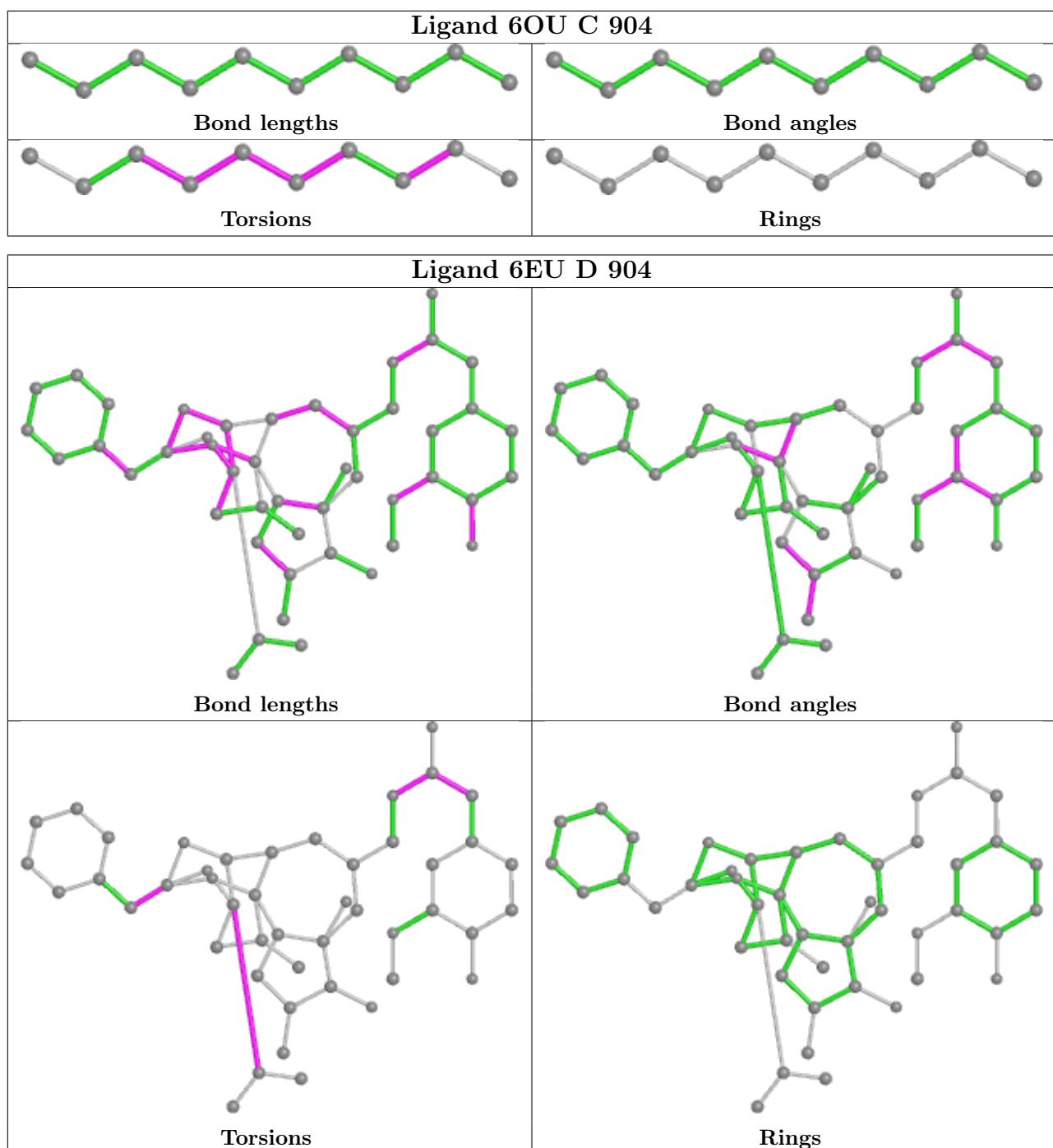


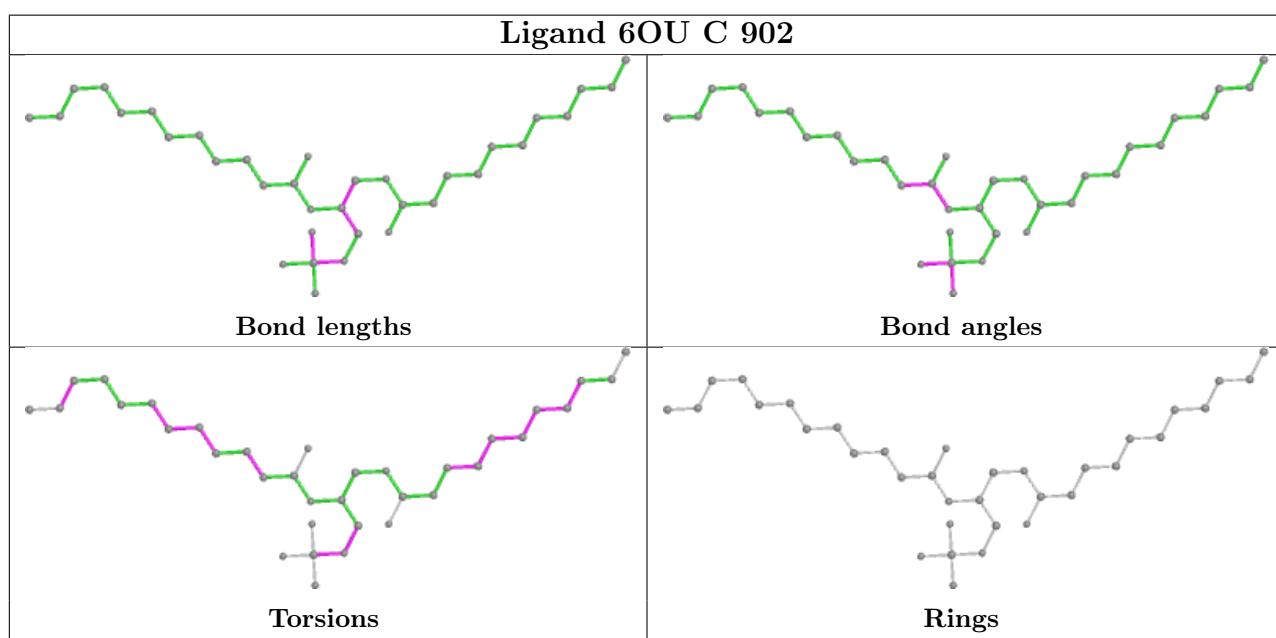
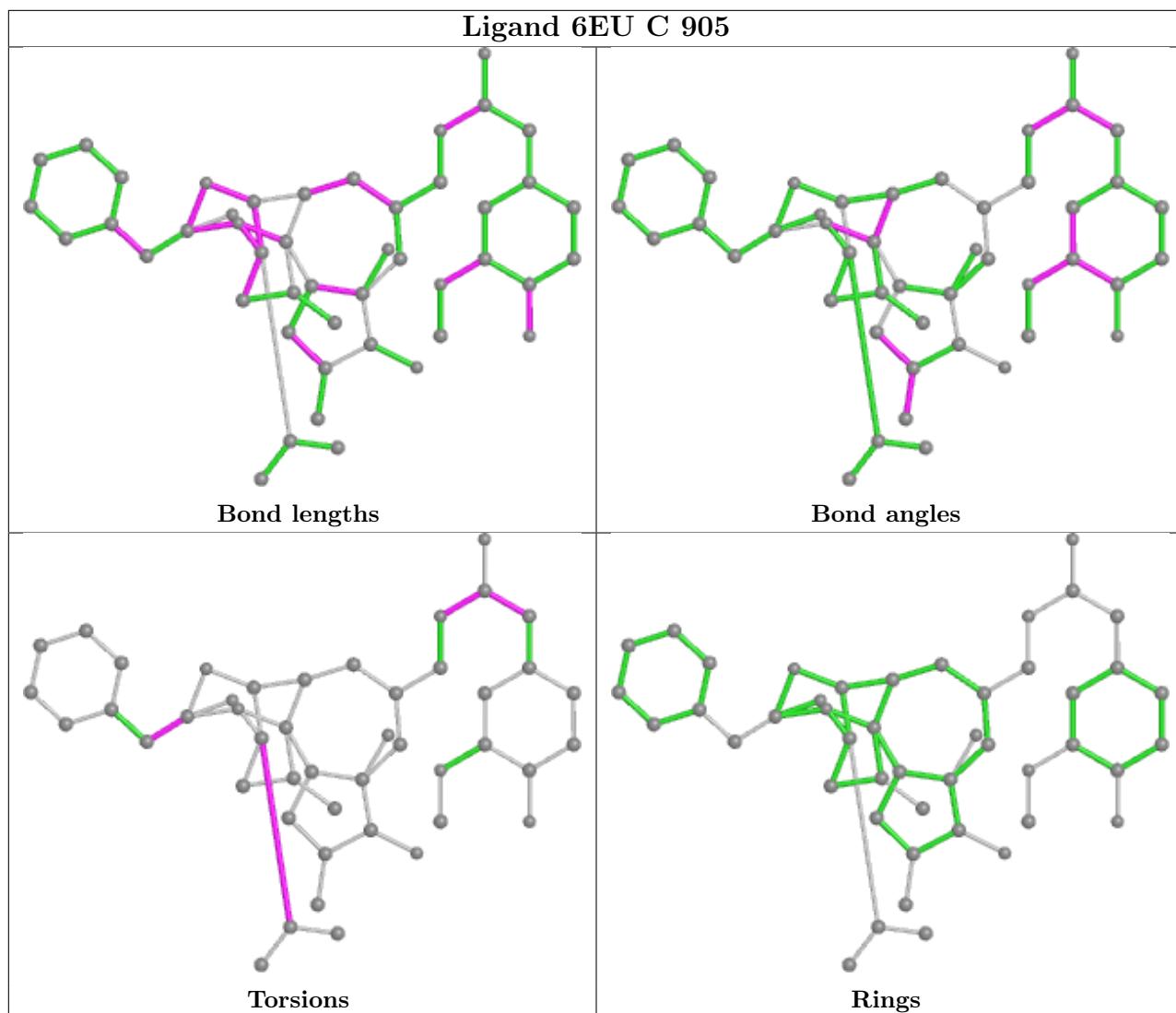


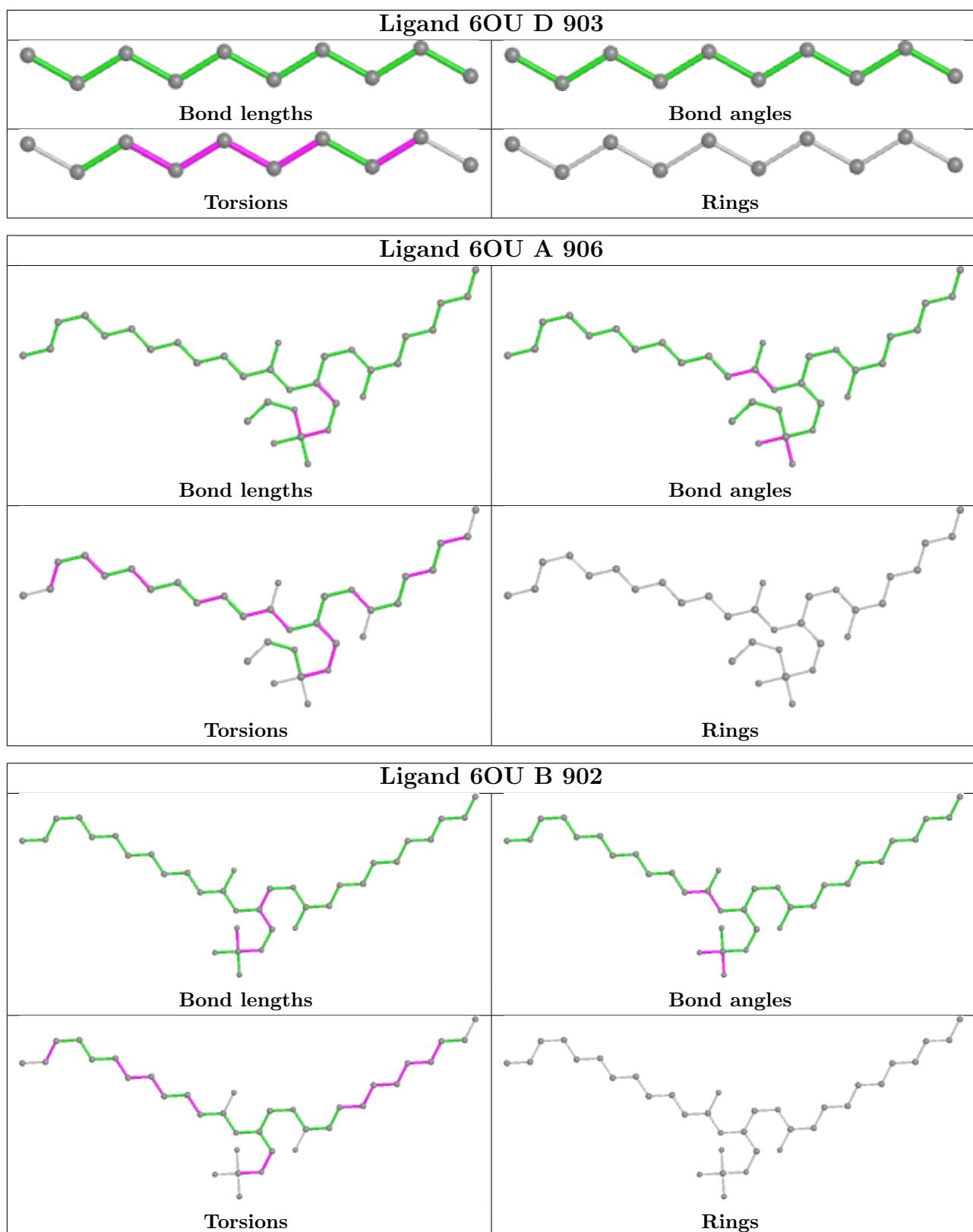


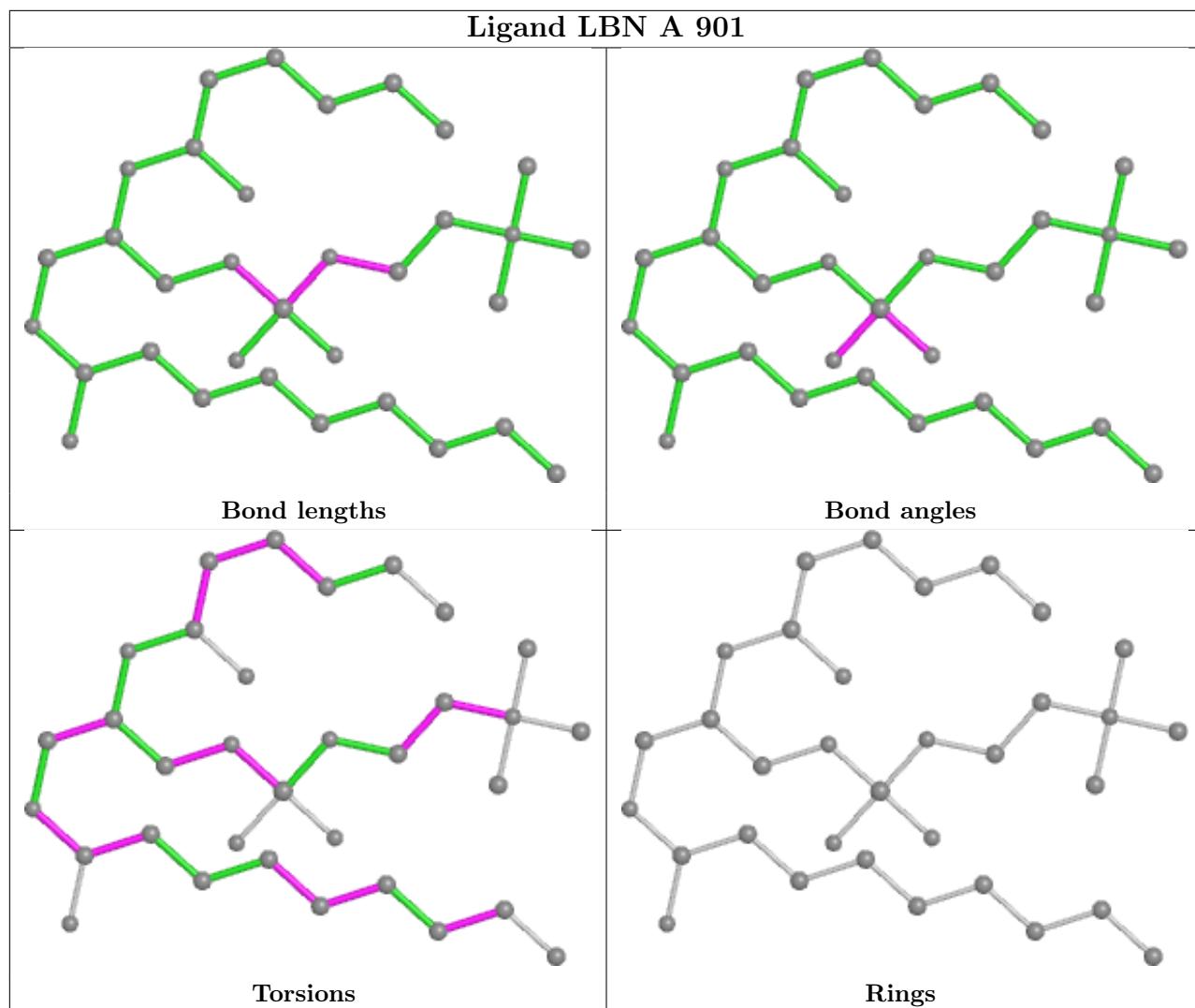


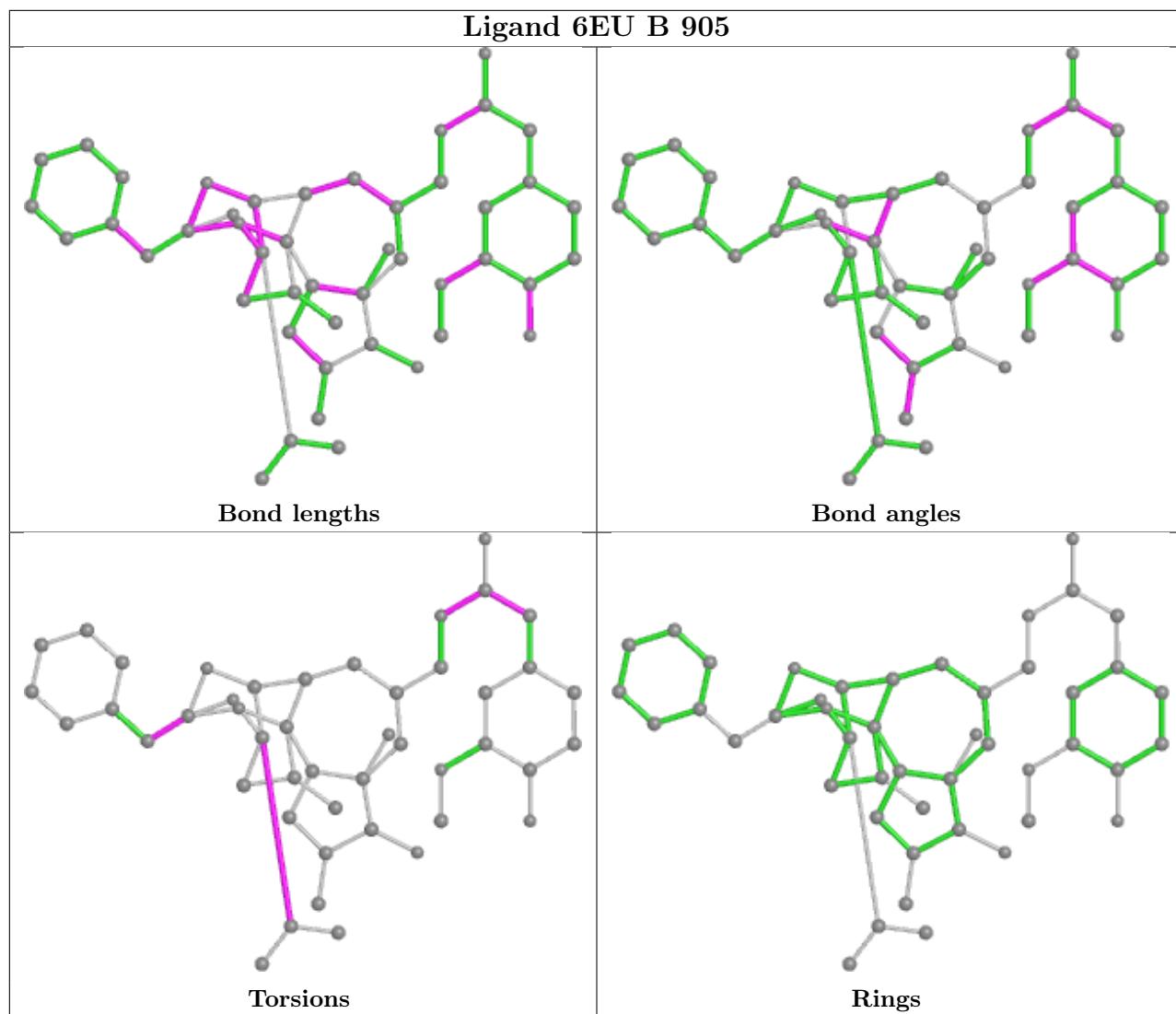


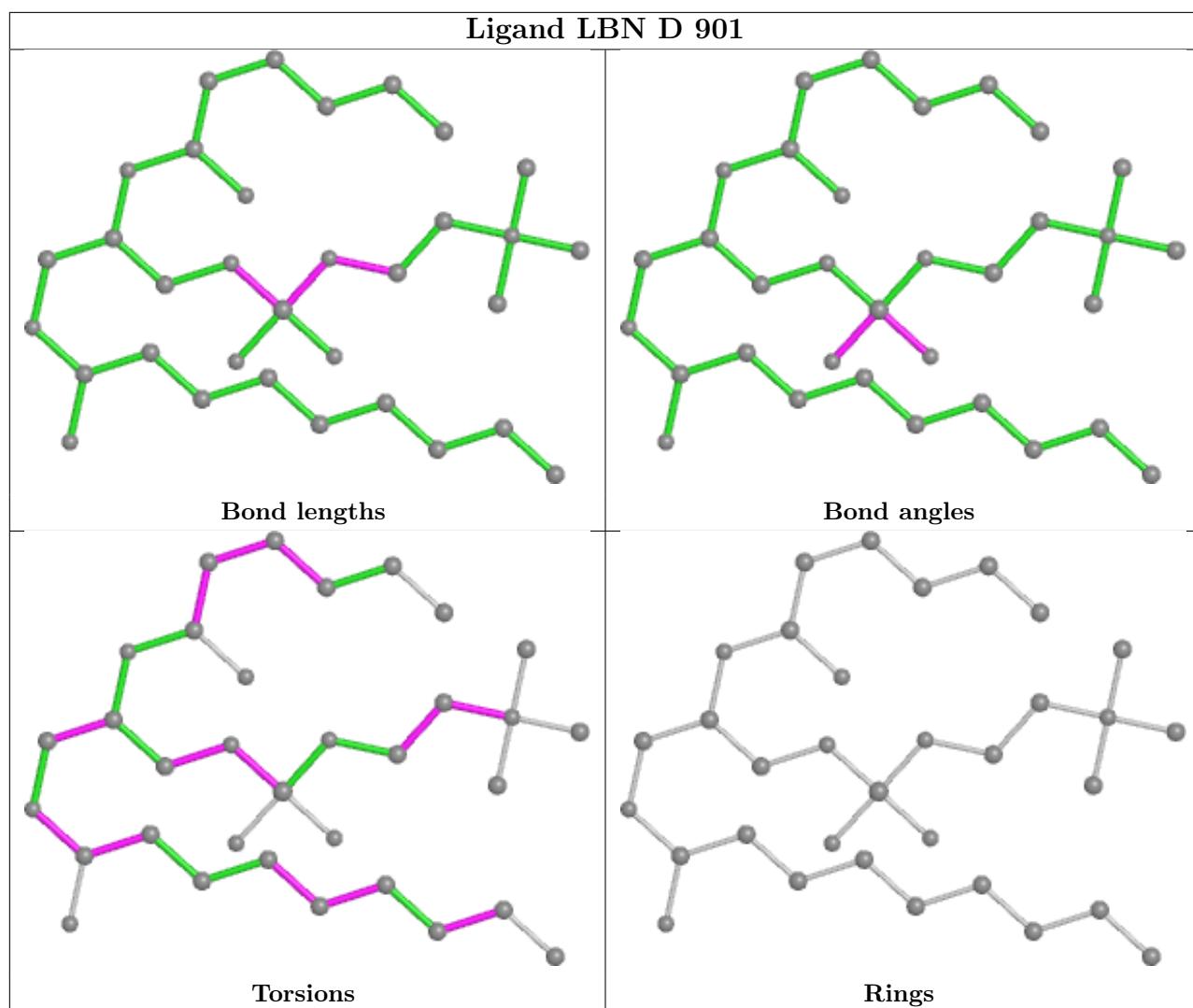












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

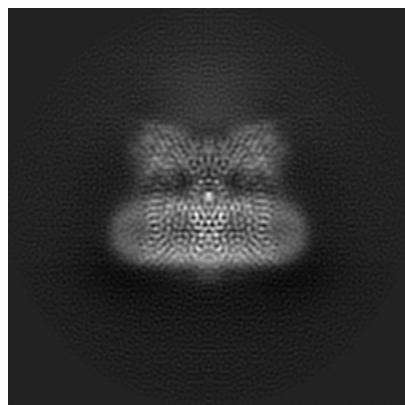
6 Map visualisation (i)

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

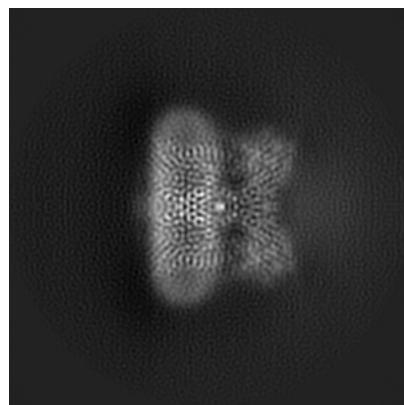
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

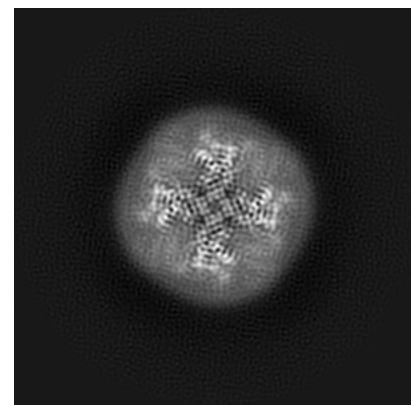
6.1.1 Primary map



X



Y

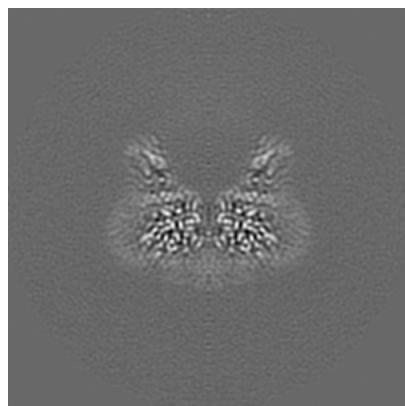


Z

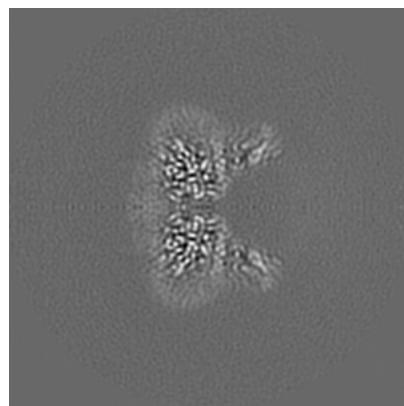
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

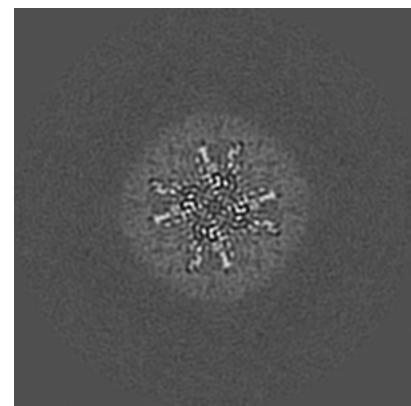
6.2.1 Primary map



X Index: 128



Y Index: 128

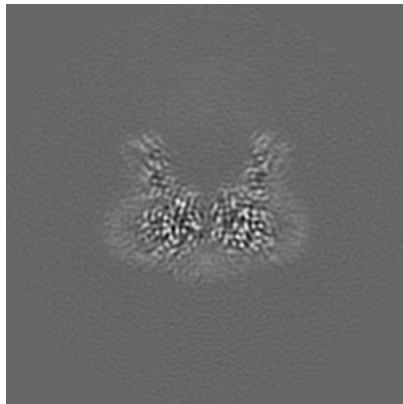


Z Index: 128

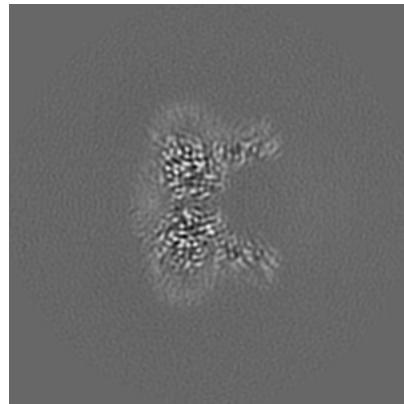
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [\(i\)](#)

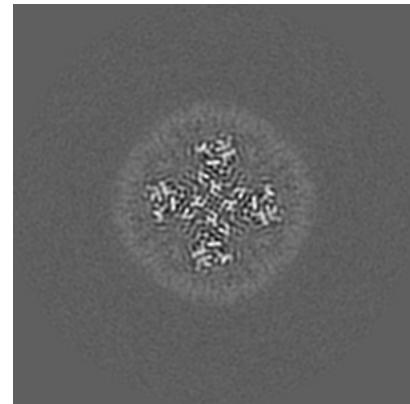
6.3.1 Primary map



X Index: 126



Y Index: 130

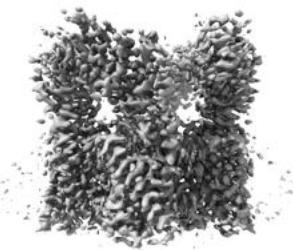


Z Index: 119

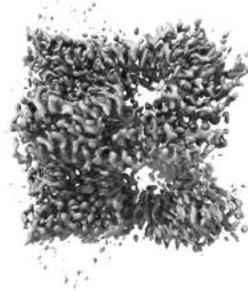
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [\(i\)](#)

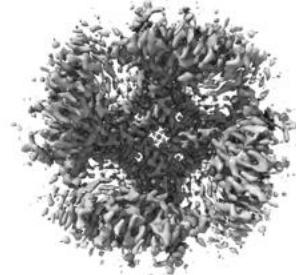
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0254. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

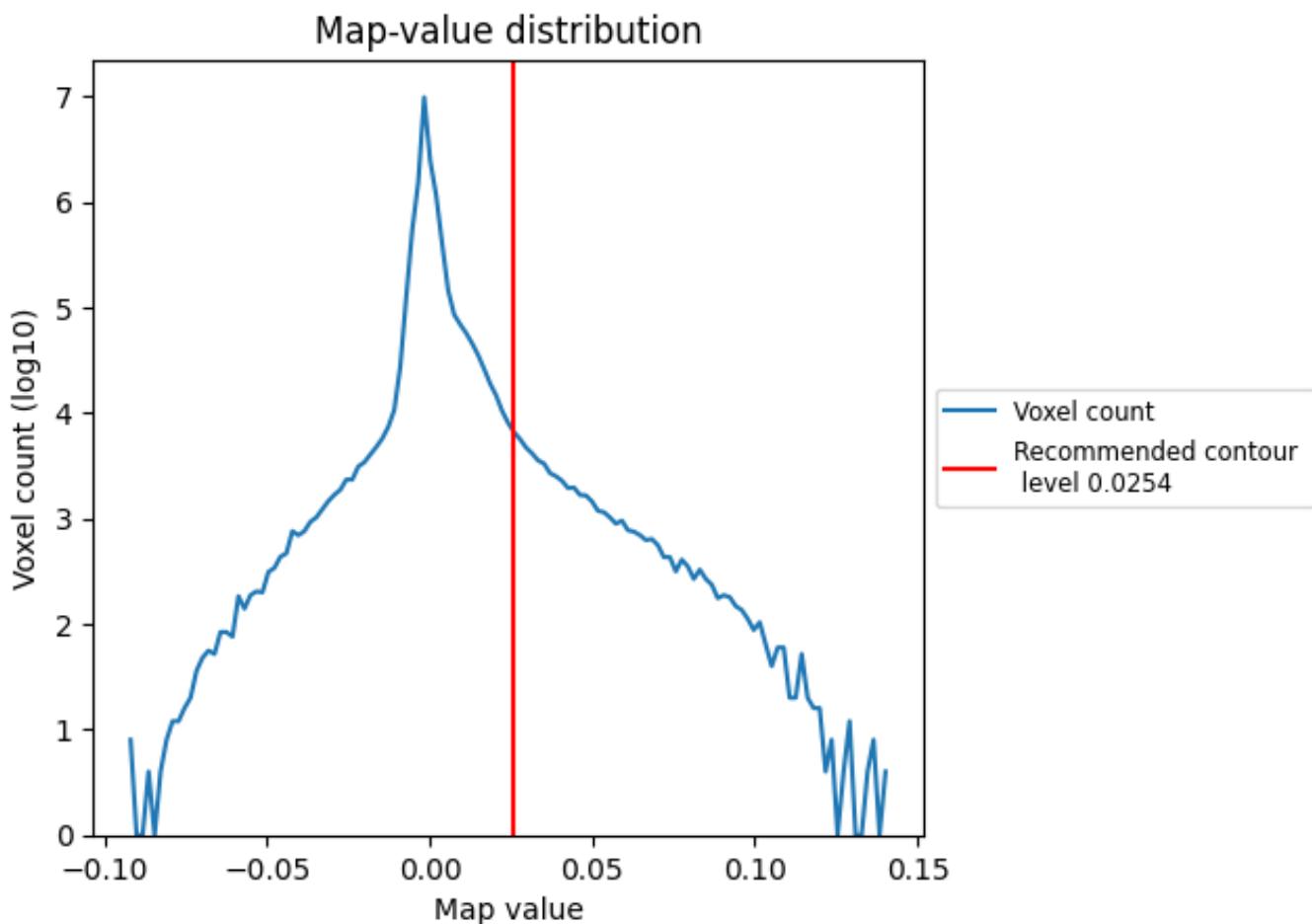
6.5 Mask visualisation

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

7 Map analysis (i)

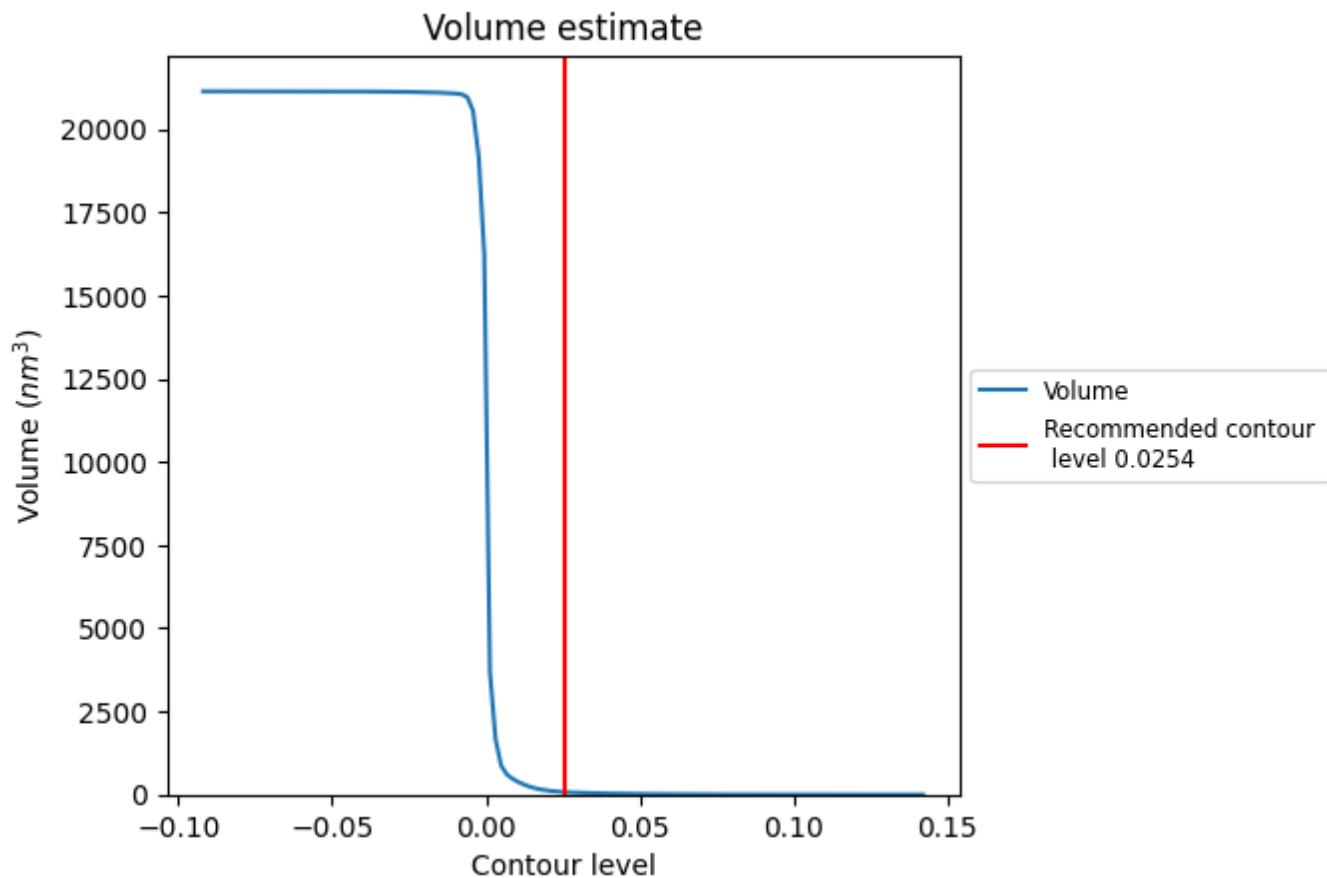
This section contains the results of statistical analysis of the map.

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.

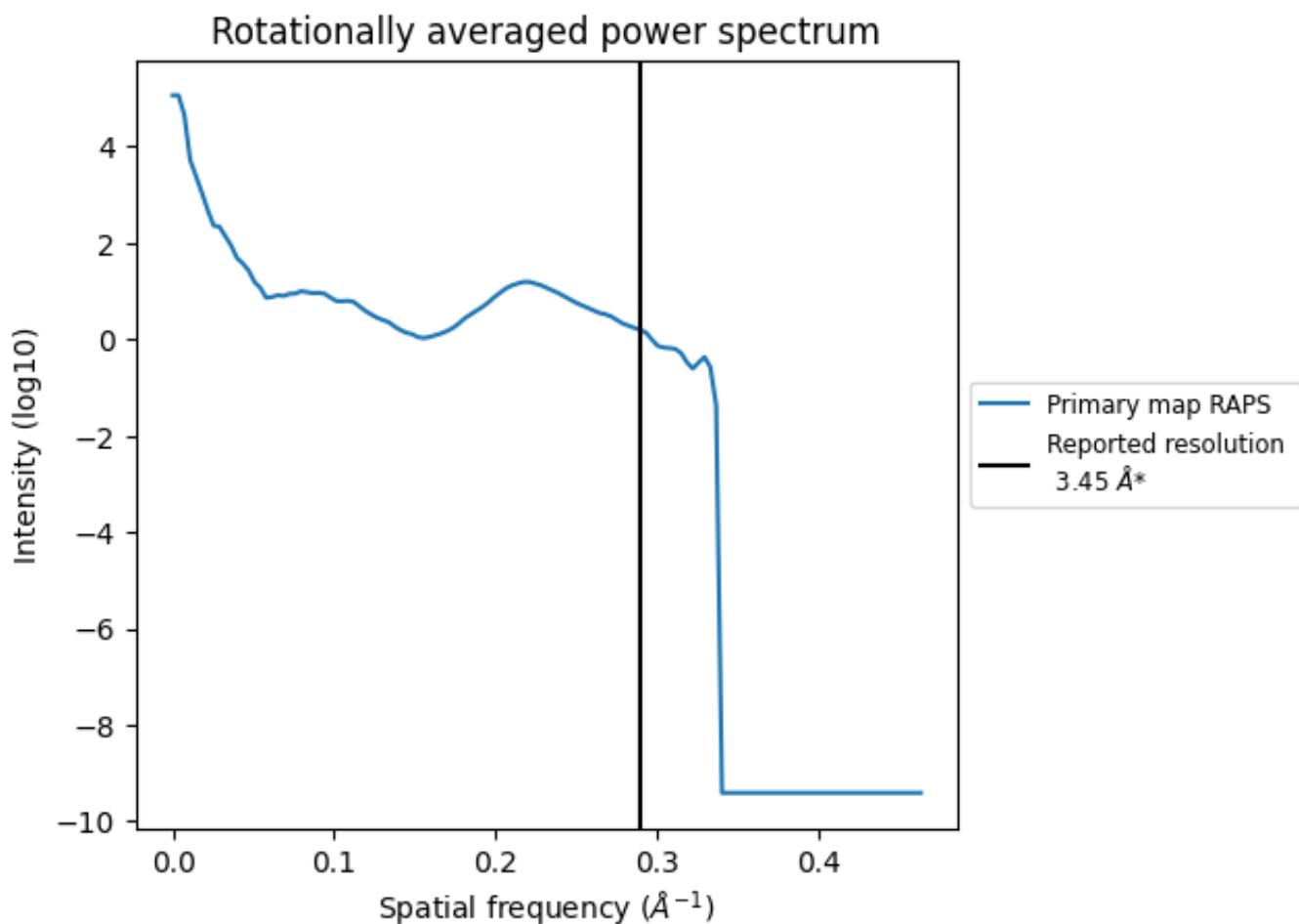
7.2 Volume estimate (i)



The volume at the recommended contour level is 76 nm³; 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 \AA^{-1}

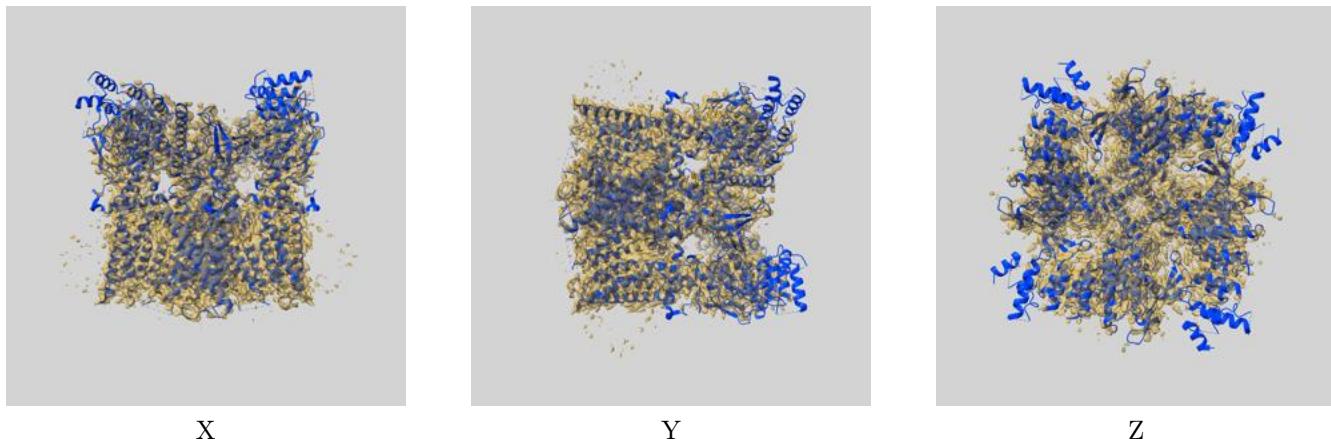
8 Fourier-Shell correlation

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

9 Map-model fit i

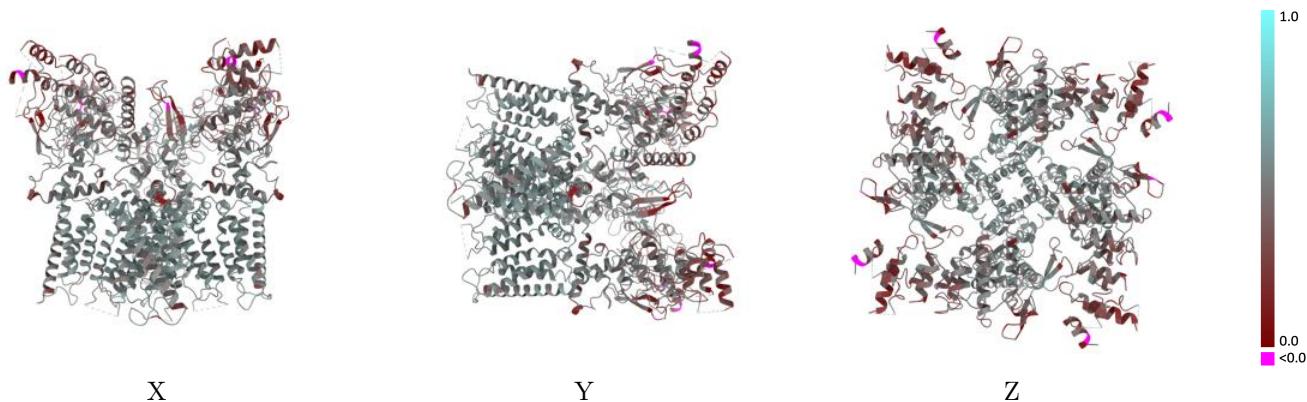
This section contains information regarding the fit between EMDB map EMD-24637 and PDB model 7RQV. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay i



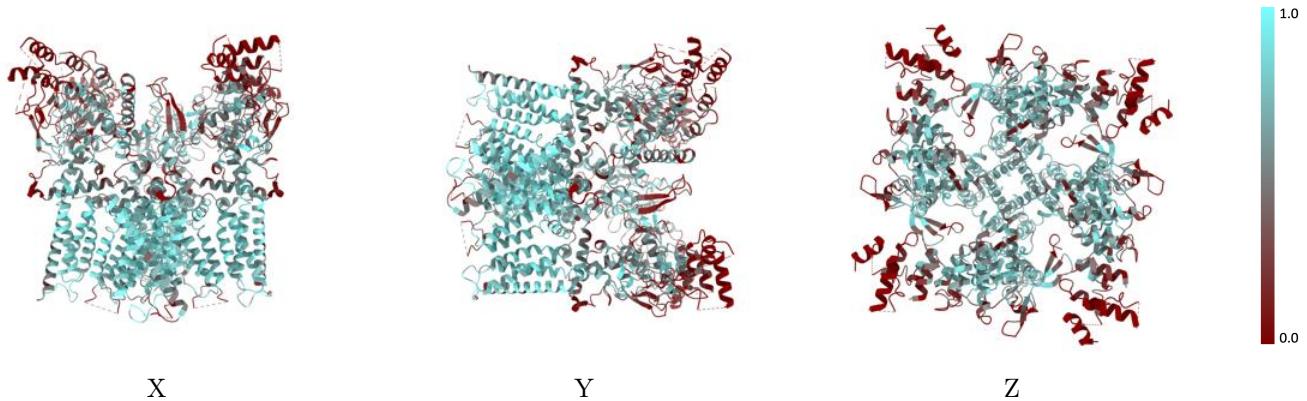
The images above show the 3D surface view of the map at the recommended contour level 0.0254 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



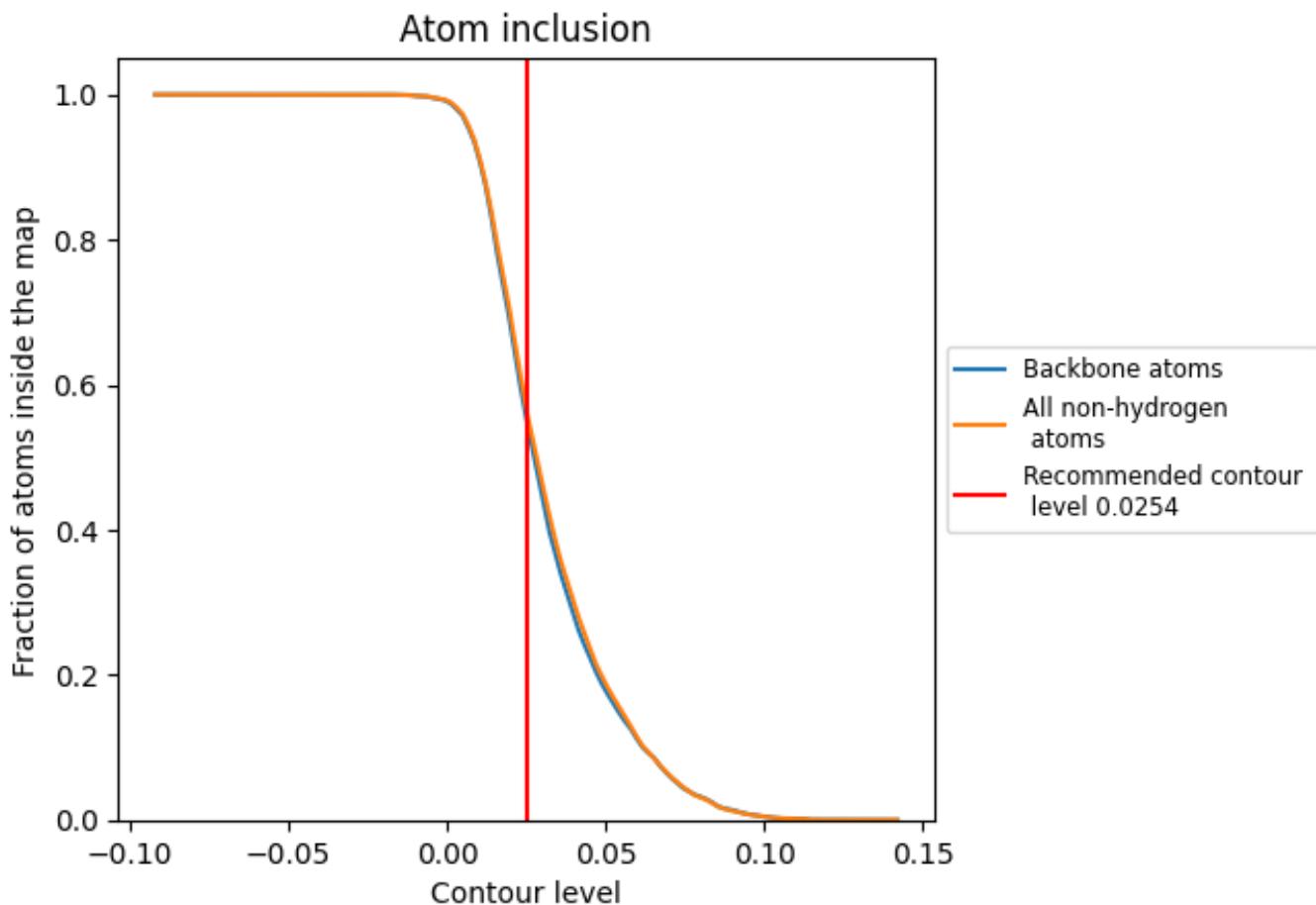
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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)



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 [\(i\)](#)

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	0.5587	0.4660
A	0.5733	0.4670
B	0.5731	0.4660
C	0.5731	0.4640
D	0.5758	0.4650

