



## Full wwPDB EM Validation Report ⓘ

Nov 29, 2022 – 10:32 AM JST

PDB ID : 7W9M  
EMDB ID : EMD-32370  
Title : Cryo-EM structure of human Nav1.7(E406K) in complex with auxiliary beta subunits, ProTx-II and tetrodotoxin (S6IV pi helix conformer)  
Authors : Yan, N.; Huang, G.; Liu, D.; Wei, P.; Shen, H.  
Deposited on : 2021-12-10  
Resolution : 3.00 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) 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

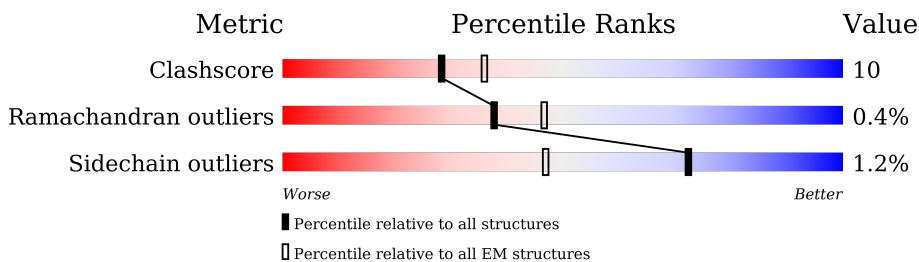
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.00 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  $\geq 3$ , 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  $\leq 5\%$ . 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	2031	
2	B	218	
3	C	215	
4	D	2	
4	E	2	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	Y01	A	2008	-	-	X	-

## 2 Entry composition i

There are 9 unique types of molecules in this entry. The entry contains 14219 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Sodium channel protein type 9 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1418	11434	7546	1800	2003	85	0	0

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-42	MET	-	expression tag	UNP Q15858
A	-41	ALA	-	expression tag	UNP Q15858
A	-40	SER	-	expression tag	UNP Q15858
A	-39	TRP	-	expression tag	UNP Q15858
A	-38	SER	-	expression tag	UNP Q15858
A	-37	HIS	-	expression tag	UNP Q15858
A	-36	PRO	-	expression tag	UNP Q15858
A	-35	GLN	-	expression tag	UNP Q15858
A	-34	PHE	-	expression tag	UNP Q15858
A	-33	GLU	-	expression tag	UNP Q15858
A	-32	LYS	-	expression tag	UNP Q15858
A	-31	GLY	-	expression tag	UNP Q15858
A	-30	GLY	-	expression tag	UNP Q15858
A	-29	GLY	-	expression tag	UNP Q15858
A	-28	ALA	-	expression tag	UNP Q15858
A	-27	ARG	-	expression tag	UNP Q15858
A	-26	GLY	-	expression tag	UNP Q15858
A	-25	GLY	-	expression tag	UNP Q15858
A	-24	SER	-	expression tag	UNP Q15858
A	-23	GLY	-	expression tag	UNP Q15858
A	-22	GLY	-	expression tag	UNP Q15858
A	-21	GLY	-	expression tag	UNP Q15858
A	-20	SER	-	expression tag	UNP Q15858
A	-19	TRP	-	expression tag	UNP Q15858
A	-18	SER	-	expression tag	UNP Q15858
A	-17	HIS	-	expression tag	UNP Q15858
A	-16	PRO	-	expression tag	UNP Q15858
A	-15	GLN	-	expression tag	UNP Q15858

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	PHE	-	expression tag	UNP Q15858
A	-13	GLU	-	expression tag	UNP Q15858
A	-12	LYS	-	expression tag	UNP Q15858
A	-11	GLY	-	expression tag	UNP Q15858
A	-10	PHE	-	expression tag	UNP Q15858
A	-9	ASP	-	expression tag	UNP Q15858
A	-8	TYR	-	expression tag	UNP Q15858
A	-7	LYS	-	expression tag	UNP Q15858
A	-6	ASP	-	expression tag	UNP Q15858
A	-5	ASP	-	expression tag	UNP Q15858
A	-4	ASP	-	expression tag	UNP Q15858
A	-3	ASP	-	expression tag	UNP Q15858
A	-2	LYS	-	expression tag	UNP Q15858
A	-1	GLY	-	expression tag	UNP Q15858
A	0	THR	-	expression tag	UNP Q15858
A	406	LYS	GLU	engineered mutation	UNP Q15858

- Molecule 2 is a protein called Sodium channel subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	173	1416	902	232	272	10	0	0

- Molecule 3 is a protein called Sodium channel subunit beta-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	119	980	615	172	183	10	4	0

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

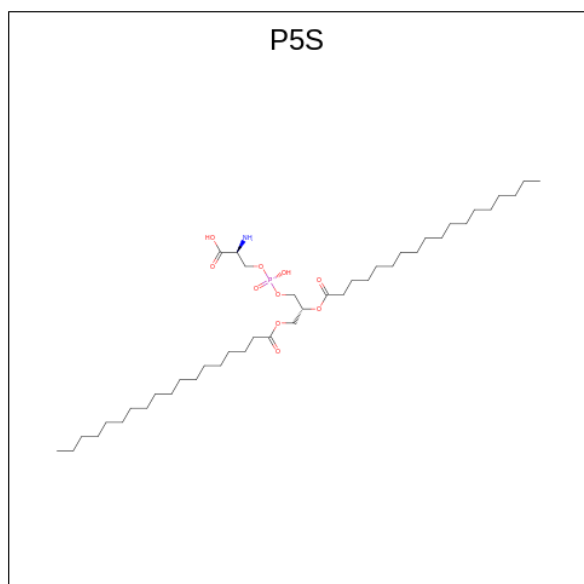


Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	E	2	28	16	2	10	0	0
4	D	2	28	16	2	10	0	0



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
6	A	1	42	24	3	15	0
6	A	1	42	24	3	15	0
6	A	1	42	24	3	15	0
6	B	1	42	24	3	15	0
6	B	1	42	24	3	15	0
6	B	1	42	24	3	15	0

- Molecule 7 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-serine (three-letter code: P5S) (formula: C<sub>42</sub>H<sub>82</sub>NO<sub>10</sub>P).

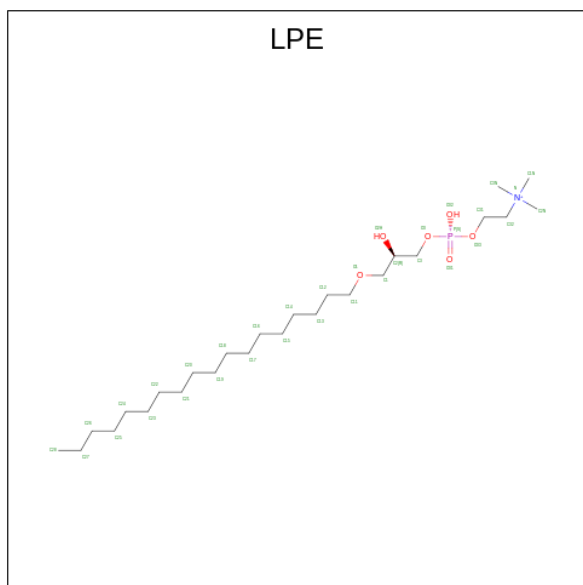


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
7	A	1	35	24	1	9	1	0

- Molecule 8 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: C<sub>31</sub>H<sub>50</sub>O<sub>4</sub>).

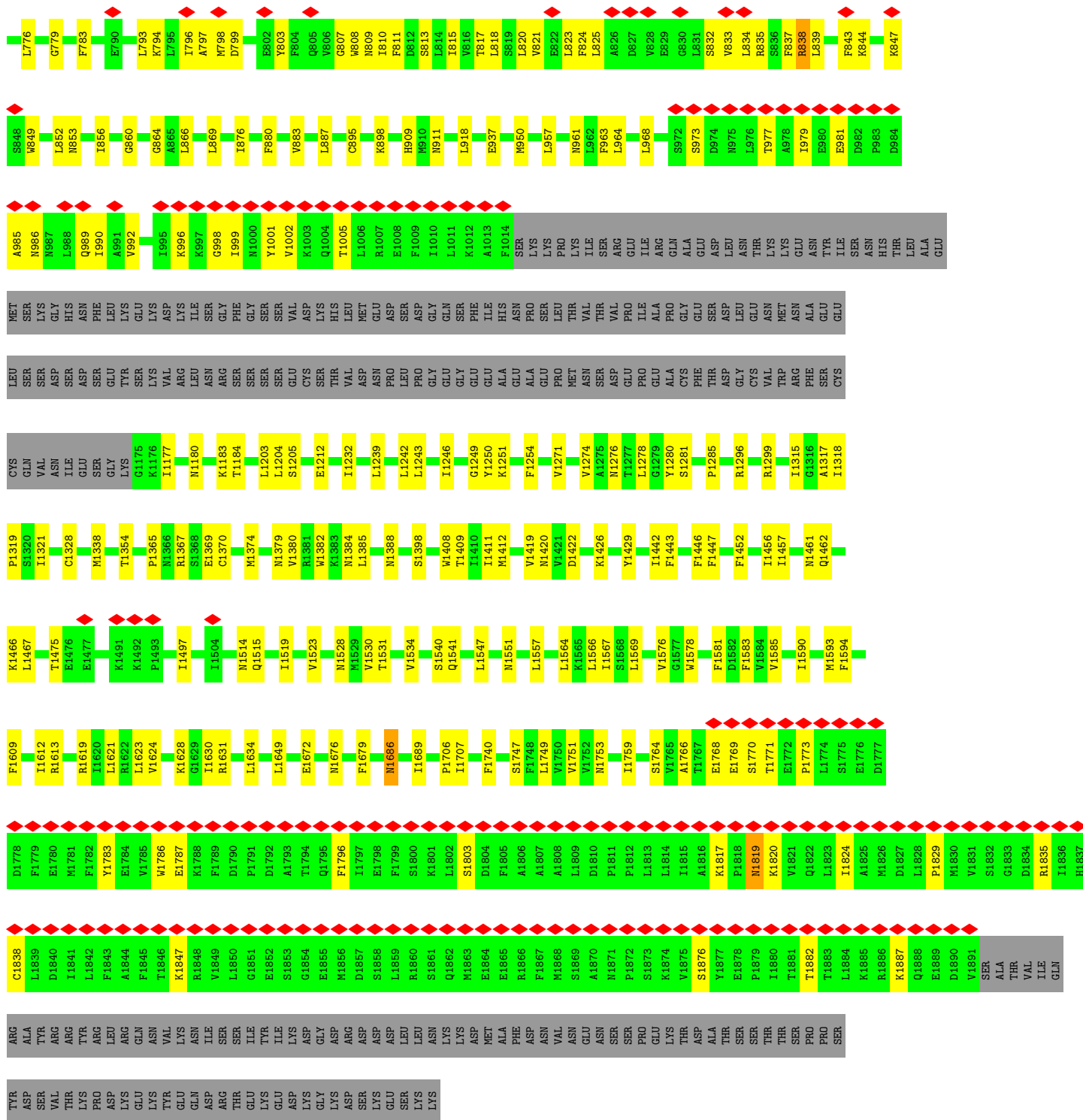






Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
9	B	1	17	9	1	6	1	0

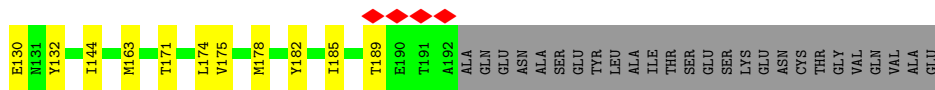




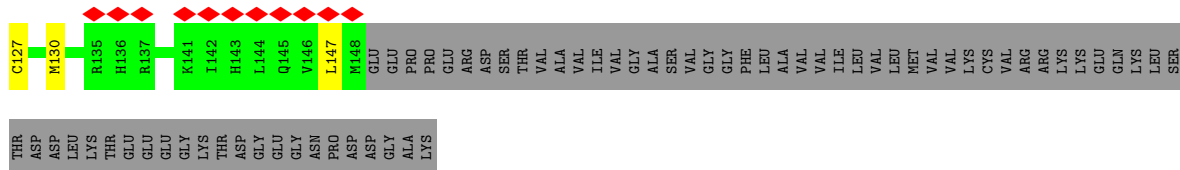
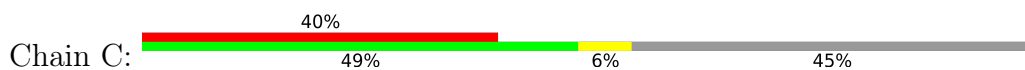
• Molecule 2: Sodium channel subunit beta-1

Chain B:





• Molecule 3: Sodium channel subunit beta-2



• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	188952	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.991	Depositor
Minimum map value	-1.381	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.104	Depositor
Recommended contour level	0.445	Depositor
Map size (Å)	261.84, 261.84, 261.84	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.091, 1.091, 1.091	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: NAG, LPE, P5S, Y01, 9SR

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	0.55	0/11707	0.57	0/15851
2	B	0.54	0/1442	0.58	0/1949
3	C	0.35	0/1011	0.58	0/1367
All	All	0.54	0/14160	0.57	0/19167

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	11434	0	11652	248	0
2	B	1416	0	1379	31	0
3	C	980	0	936	7	0
4	D	28	0	25	0	0
4	E	28	0	25	2	0
5	A	22	0	0	0	0
6	A	42	0	39	0	0
6	B	42	0	39	0	0
7	A	35	0	45	4	0
8	A	175	0	245	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	B	17	0	19	1	0
All	All	14219	0	14404	300	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 10.

All (300) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:832:SER:HA	1:A:835:ARG:HD3	1.39	1.02
1:A:950:MET:CE	8:A:2008:Y01:HAC1	1.89	1.02
2:B:124:TYR:CE1	4:E:1:NAG:H62	1.98	0.98
2:B:174:LEU:CD2	2:B:178:MET:SD	2.56	0.94
1:A:1819:ASN:HD22	1:A:1819:ASN:N	1.62	0.92
1:A:212:ALA:CB	8:A:2008:Y01:CAL	2.47	0.92
1:A:212:ALA:CB	8:A:2008:Y01:HAL2	2.00	0.90
2:B:124:TYR:CD1	4:E:1:NAG:H62	2.09	0.87
2:B:78:LEU:HD21	2:B:80:LEU:HD13	1.56	0.87
1:A:950:MET:HE1	8:A:2008:Y01:HAC1	1.52	0.86
1:A:757:ASN:ND2	1:A:783:PHE:CD2	2.44	0.85
1:A:105:ALA:H	1:A:116:ARG:HH12	1.24	0.85
2:B:174:LEU:HD21	2:B:178:MET:SD	2.18	0.84
1:A:1246:ILE:HD11	7:A:2004:P5S:H53	1.60	0.83
1:A:212:ALA:HB1	8:A:2008:Y01:HAL1	1.59	0.82
1:A:212:ALA:HB2	8:A:2008:Y01:HAL2	1.61	0.81
2:B:174:LEU:HD23	2:B:178:MET:SD	2.20	0.80
1:A:909:HIS:HD2	1:A:911:ASN:H	1.29	0.80
1:A:1419:VAL:O	1:A:1420:ASN:OD1	1.99	0.80
1:A:895:CYS:HA	3:C:56:TYR:OH	1.80	0.79
1:A:212:ALA:CB	8:A:2008:Y01:HAL1	2.11	0.79
1:A:950:MET:HE3	8:A:2008:Y01:HAC1	1.65	0.79
1:A:950:MET:CE	8:A:2008:Y01:HAU2	2.13	0.77
1:A:212:ALA:HB1	8:A:2008:Y01:CAL	2.11	0.76
1:A:950:MET:HE3	8:A:2008:Y01:CAC	2.15	0.76
1:A:887:LEU:HD11	8:A:2008:Y01:HAT1	1.69	0.74
1:A:1819:ASN:HD22	1:A:1819:ASN:H	1.35	0.73
1:A:950:MET:CE	8:A:2008:Y01:CAC	2.67	0.73
1:A:104:PRO:HB2	1:A:107:TYR:HA	1.71	0.73
1:A:1249:GLY:HA2	7:A:2004:P5S:H48A	1.70	0.73
1:A:1824:ILE:HG21	1:A:1887:LYS:HE3	1.71	0.73
1:A:109:LEU:O	1:A:116:ARG:NH1	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:PHE:HD2	1:A:184:LEU:HD22	1.54	0.72
1:A:1547:LEU:O	1:A:1551:ASN:ND2	2.23	0.72
1:A:1796:PHE:HB3	1:A:1835:ARG:HG2	1.75	0.69
1:A:1593:MET:CE	1:A:1594:PHE:CE1	2.76	0.68
1:A:212:ALA:HB1	8:A:2008:Y01:OAG	1.94	0.68
1:A:53:LEU:O	1:A:99:ARG:NH2	2.26	0.67
1:A:81:TYR:O	1:A:85:LYS:NZ	2.23	0.67
1:A:1251:LYS:NZ	8:A:2006:Y01:HAR1	2.10	0.66
1:A:950:MET:HE1	8:A:2008:Y01:HAU2	1.77	0.65
1:A:1408:TRP:CE3	1:A:1412:MET:SD	2.90	0.64
1:A:1820:LYS:HD2	1:A:1820:LYS:H	1.62	0.64
1:A:1819:ASN:N	1:A:1819:ASN:ND2	2.37	0.63
1:A:101:ASN:ND2	1:A:103:THR:OG1	2.31	0.63
1:A:1278:LEU:HD23	1:A:1280:TYR:HE2	1.63	0.63
1:A:1276:ASN:HA	1:A:1281:SER:OG	1.99	0.62
2:B:58:THR:HG23	2:B:120:GLU:HB2	1.81	0.61
1:A:209:ASN:CB	8:A:2008:Y01:OAH	2.49	0.61
8:A:2005:Y01:HAE2	8:A:2005:Y01:HAC1	1.84	0.60
1:A:849:TRP:CE2	8:A:2007:Y01:HAU1	2.36	0.60
8:A:2008:Y01:HAC1	8:A:2008:Y01:HAE2	1.84	0.60
8:A:2010:Y01:HAC1	8:A:2010:Y01:HAE2	1.84	0.60
8:A:2007:Y01:HAE2	8:A:2007:Y01:HAC1	1.83	0.60
1:A:315:CYS:O	1:A:373:ALA:HA	2.02	0.60
1:A:1388:ASN:OD1	1:A:1388:ASN:N	2.32	0.59
8:A:2006:Y01:HAC1	8:A:2006:Y01:HAE2	1.83	0.59
1:A:9:PRO:HA	1:A:63:TYR:HA	1.85	0.59
1:A:1593:MET:HE3	1:A:1594:PHE:HE1	1.67	0.58
1:A:1278:LEU:HD23	1:A:1280:TYR:CE2	2.38	0.58
1:A:880:PHE:HE1	8:A:2008:Y01:HAC2	1.68	0.58
1:A:876:ILE:HD11	8:A:2008:Y01:HAB1	1.84	0.57
1:A:880:PHE:CE1	8:A:2008:Y01:HAC2	2.40	0.57
1:A:1497:ILE:HD12	1:A:1569:LEU:HA	1.86	0.57
1:A:1764:SER:O	1:A:1768:GLU:HG2	2.04	0.57
1:A:180:GLU:HG3	1:A:185:ARG:HH22	1.70	0.57
1:A:985:ALA:HB3	1:A:990:ILE:HD11	1.87	0.57
1:A:895:CYS:HA	3:C:56:TYR:CZ	2.39	0.57
1:A:91:LEU:HD21	1:A:95:LYS:HA	1.88	0.56
1:A:1672:GLU:HB2	1:A:1706:PRO:HB3	1.87	0.56
1:A:1365:PRO:HD2	1:A:1369:GLU:HG3	1.88	0.56
1:A:738:TYR:HD2	1:A:797:ALA:HB1	1.71	0.56
1:A:1246:ILE:HD11	7:A:2004:P5S:C53	2.33	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1384:ASN:OD1	1:A:1385:LEU:N	2.35	0.56
2:B:65:GLU:N	2:B:65:GLU:OE1	2.39	0.55
1:A:66:ILE:HD12	1:A:67:PRO:HD2	1.87	0.55
1:A:883:VAL:HG21	8:A:2008:Y01:HBG	1.89	0.55
1:A:1457:ILE:O	1:A:1461:ASN:ND2	2.38	0.55
1:A:758:THR:HG21	1:A:839:LEU:HD13	1.87	0.55
1:A:1239:LEU:HD21	2:B:174:LEU:HD13	1.87	0.55
1:A:1593:MET:HE2	1:A:1594:PHE:CE1	2.40	0.55
1:A:895:CYS:HA	3:C:56:TYR:HH	1.69	0.55
1:A:418:GLN:NE2	1:A:422:GLU:OE2	2.40	0.55
1:A:811:PHE:O	1:A:815:ILE:HG12	2.07	0.55
1:A:807:GLY:HA2	1:A:810:ILE:HD12	1.88	0.54
1:A:757:ASN:ND2	1:A:783:PHE:HD2	2.01	0.54
1:A:247:ASP:N	1:A:247:ASP:OD1	2.38	0.54
1:A:395:ASN:HB3	1:A:1759:ILE:HG21	1.90	0.54
2:B:129:PHE:HB2	2:B:132:TYR:HB3	1.89	0.53
1:A:285:THR:OG1	1:A:286:LEU:N	2.42	0.53
1:A:82:TYR:HB3	1:A:87:THR:HG21	1.90	0.53
1:A:1819:ASN:H	1:A:1819:ASN:ND2	2.02	0.52
1:A:139:ASN:ND2	1:A:220:ARG:HD3	2.25	0.52
1:A:417:LYS:O	1:A:421:LEU:HG	2.09	0.52
1:A:1443:PHE:HA	1:A:1447:PHE:HD2	1.74	0.52
1:A:1452:PHE:O	1:A:1456:ILE:HG13	2.08	0.52
1:A:1593:MET:HE3	1:A:1594:PHE:CE1	2.43	0.52
1:A:1747:SER:O	1:A:1751:VAL:HG12	2.09	0.52
1:A:213:LEU:HD12	1:A:214:ARG:N	2.25	0.52
1:A:963:PHE:HD1	1:A:964:LEU:HD12	1.75	0.52
2:B:78:LEU:HD12	2:B:92:TRP:HB2	1.92	0.52
3:C:47:ARG:NH2	3:C:111[B]:SER:OG	2.43	0.52
1:A:164:THR:HG21	1:A:200:TYR:HE2	1.74	0.52
1:A:251:LEU:HB2	1:A:1630:ILE:HD12	1.91	0.52
1:A:1251:LYS:NZ	8:A:2006:Y01:CAR	2.72	0.52
1:A:808:TRP:CD1	1:A:844:LYS:HG3	2.45	0.52
1:A:1354:THR:HG22	1:A:1379:ASN:HD22	1.75	0.52
1:A:1566:LEU:HD11	1:A:1583:PHE:HE1	1.75	0.52
1:A:209:ASN:CG	8:A:2008:Y01:OAH	2.48	0.51
1:A:293:LEU:HD12	1:A:298:ASP:HB3	1.92	0.51
1:A:219:LEU:HA	1:A:222:LEU:HD13	1.92	0.51
1:A:411:ALA:O	1:A:415:GLU:HG2	2.11	0.51
1:A:813:SER:O	1:A:817:THR:HG23	2.11	0.51
1:A:1422:ASP:OD2	1:A:1422:ASP:N	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:973:SER:O	1:A:977:THR:N	2.40	0.51
1:A:1251:LYS:HZ2	8:A:2006:Y01:CAT	2.24	0.51
1:A:1540:SER:OG	1:A:1541:GLN:N	2.43	0.50
1:A:1686:ASN:OD1	1:A:1686:ASN:N	2.43	0.50
8:A:2010:Y01:HAE2	8:A:2010:Y01:CAC	2.41	0.50
1:A:50:SER:OG	1:A:53:LEU:HB2	2.11	0.50
1:A:998:GLY:O	1:A:1002:VAL:HG23	2.11	0.50
1:A:757:ASN:HA	1:A:783:PHE:CE2	2.48	0.49
8:A:2007:Y01:HAE2	8:A:2007:Y01:CAC	2.41	0.49
1:A:314:LEU:HB2	1:A:372:ARG:HD2	1.94	0.49
8:A:2008:Y01:CAC	8:A:2008:Y01:HAE2	2.41	0.49
1:A:251:LEU:HD13	1:A:1630:ILE:HG23	1.95	0.49
1:A:1628:LYS:HA	1:A:1631:ARG:HH21	1.77	0.49
1:A:1001:TYR:O	1:A:1005:THR:HG23	2.13	0.49
8:A:2006:Y01:HAE2	8:A:2006:Y01:CAC	2.41	0.49
1:A:760:PHE:CE2	1:A:776:LEU:HA	2.48	0.49
1:A:221:ALA:O	1:A:224:THR:HG22	2.12	0.49
1:A:1251:LYS:NZ	8:A:2006:Y01:HAT2	2.27	0.49
1:A:90:VAL:HG21	1:A:120:ILE:HG21	1.94	0.48
1:A:1609:PHE:CZ	1:A:1613:ARG:HD2	2.48	0.48
1:A:1707:ILE:HD12	1:A:1740:PHE:HE2	1.77	0.48
1:A:957:LEU:O	1:A:961:ASN:ND2	2.38	0.48
1:A:28:ALA:HA	1:A:31:LYS:HE3	1.94	0.48
1:A:1408:TRP:HE3	1:A:1412:MET:SD	2.33	0.48
1:A:1370:CYS:SG	1:A:1382:TRP:HB2	2.53	0.48
1:A:406:LYS:HG3	1:A:968:LEU:HD21	1.96	0.48
1:A:895:CYS:HB2	1:A:898:LYS:HD2	1.95	0.48
8:A:2008:Y01:HAC1	8:A:2008:Y01:HAU2	1.96	0.48
1:A:191:LEU:O	1:A:195:VAL:HG23	2.14	0.48
1:A:1183:LYS:NZ	2:B:189:THR:OG1	2.47	0.48
1:A:1184:THR:HG21	2:B:182:TYR:HA	1.95	0.48
1:A:1876:SER:O	1:A:1876:SER:OG	2.32	0.48
1:A:1317:ALA:O	1:A:1321:ILE:HG12	2.14	0.47
8:A:2006:Y01:HAC1	8:A:2006:Y01:HAU2	1.96	0.47
1:A:1829:PRO:HA	1:A:1882:THR:HG22	1.94	0.47
8:A:2007:Y01:HAC1	8:A:2007:Y01:HAU2	1.96	0.47
1:A:225:ILE:HG23	1:A:231:LEU:HB3	1.96	0.47
1:A:758:THR:HA	1:A:761:MET:HE2	1.96	0.47
8:A:2010:Y01:HAV2	8:A:2010:Y01:OAG	2.14	0.47
8:A:2007:Y01:OAG	8:A:2007:Y01:HAV2	2.14	0.47
1:A:1783:TYR:O	1:A:1787:GLU:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:2010:Y01:HAC1	8:A:2010:Y01:HAU2	1.96	0.47
1:A:1581:PHE:O	1:A:1585:VAL:HG13	2.15	0.47
1:A:429:ARG:O	1:A:432:LYS:HG2	2.14	0.47
1:A:880:PHE:HA	1:A:883:VAL:HG12	1.96	0.47
1:A:1205:SER:O	1:A:1296:ARG:NH2	2.46	0.47
1:A:835:ARG:O	1:A:838:ARG:HG2	2.15	0.47
1:A:52:ASP:OD1	1:A:60:PRO:HG3	2.15	0.46
1:A:429:ARG:HA	1:A:432:LYS:HD3	1.97	0.46
8:A:2005:Y01:HAC1	8:A:2005:Y01:HAU2	1.96	0.46
1:A:289:ILE:O	1:A:292:THR:HG22	2.15	0.46
1:A:793:LEU:O	1:A:796:ILE:HG13	2.15	0.46
1:A:837:PHE:O	1:A:838:ARG:C	2.54	0.46
1:A:1398:SER:HB3	1:A:1411:ILE:HD13	1.97	0.46
1:A:1374:MET:HG2	1:A:1380:VAL:HG13	1.97	0.46
1:A:1576:VAL:HG12	1:A:1578:TRP:H	1.81	0.46
1:A:1251:LYS:NZ	8:A:2006:Y01:CAT	2.79	0.46
1:A:304:TYR:HB2	1:A:328:TYR:CE2	2.51	0.46
1:A:318:SER:OG	1:A:319:THR:N	2.49	0.46
1:A:1803:SER:HB3	1:A:1820:LYS:HE3	1.97	0.46
7:A:2004:P5S:H53	7:A:2004:P5S:H56A	1.86	0.46
1:A:764:GLU:OE1	1:A:765:HIS:N	2.47	0.45
1:A:803:TYR:CE1	1:A:809:ASN:HB3	2.51	0.45
1:A:1212:GLU:OE2	1:A:1212:GLU:N	2.50	0.45
1:A:1497:ILE:CD1	1:A:1569:LEU:HA	2.46	0.45
1:A:1232:ILE:HD11	2:B:163:MET:HA	1.97	0.45
1:A:1232:ILE:HG13	2:B:163:MET:HG3	1.98	0.45
1:A:1623:LEU:HD23	1:A:1623:LEU:HA	1.72	0.45
1:A:1676:ASN:OD1	1:A:1679:PHE:HB2	2.16	0.45
1:A:139:ASN:HD21	1:A:220:ARG:HD3	1.82	0.45
1:A:203:GLU:HG3	1:A:204:PHE:HD1	1.81	0.45
1:A:1242:LEU:O	1:A:1246:ILE:HG12	2.17	0.45
1:A:1564:LEU:O	1:A:1567:ILE:HG22	2.17	0.45
2:B:24:VAL:HG12	2:B:25:ASP:H	1.81	0.45
2:B:182:TYR:CE2	9:B:304:LPE:O33	2.70	0.45
1:A:1817:LYS:HA	1:A:1819:ASN:ND2	2.31	0.45
1:A:216:PHE:O	1:A:219:LEU:HG	2.16	0.45
1:A:13:VAL:HG23	1:A:76:GLU:HB2	1.98	0.45
1:A:51:SER:O	1:A:57:LYS:NZ	2.34	0.45
1:A:909:HIS:CD2	1:A:911:ASN:H	2.21	0.45
1:A:1442:ILE:O	1:A:1446:PHE:HB3	2.17	0.45
1:A:1649:LEU:HD23	1:A:1649:LEU:HA	1.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:130:GLU:OE1	2:B:130:GLU:N	2.45	0.45
8:A:2005:Y01:HAE2	8:A:2005:Y01:CAC	2.41	0.45
1:A:115:LEU:HD12	1:A:115:LEU:H	1.82	0.44
1:A:318:SER:OG	1:A:320:ASP:OD1	2.25	0.44
2:B:37:LYS:HB2	2:B:107:PHE:HD1	1.82	0.44
2:B:24:VAL:HG12	2:B:25:ASP:N	2.33	0.44
1:A:1296:ARG:HG2	1:A:1299:ARG:NH2	2.33	0.44
8:A:2010:Y01:HAN2	8:A:2010:Y01:HAC3	2.00	0.44
1:A:1766:ALA:C	1:A:1768:GLU:H	2.20	0.44
1:A:853:ASN:HA	1:A:856:ILE:HG22	1.99	0.44
1:A:367:TYR:OH	1:A:1689:ILE:HG23	2.18	0.44
2:B:92:TRP:CZ2	2:B:94:GLY:HA3	2.52	0.44
1:A:111:PRO:HA	1:A:116:ARG:HD3	1.98	0.44
3:C:67:TRP:CZ2	3:C:127:CYS:HB3	2.52	0.44
1:A:1251:LYS:HZ2	8:A:2006:Y01:HAR1	1.83	0.43
1:A:1315:ILE:O	1:A:1318:ILE:HG22	2.18	0.43
2:B:38:ILE:O	2:B:105:SER:HB3	2.18	0.43
1:A:12:PHE:HZ	1:A:63:TYR:HB3	1.83	0.43
1:A:423:PHE:HA	1:A:426:MET:HG2	1.99	0.43
1:A:1426:LYS:HB2	1:A:1429:TYR:HB2	1.99	0.43
1:A:1514:ASN:OD1	1:A:1515:GLN:N	2.52	0.43
1:A:1621:LEU:O	1:A:1624:VAL:HG22	2.18	0.43
1:A:364:GLU:O	1:A:368:GLN:HG3	2.18	0.43
1:A:820:LEU:O	1:A:823:LEU:HB3	2.17	0.43
1:A:989:GLN:HA	1:A:992:VAL:HG12	2.00	0.43
2:B:73:TYR:HD1	2:B:78:LEU:HB2	1.83	0.43
1:A:1456:ILE:HD12	1:A:1753:ASN:ND2	2.33	0.43
1:A:27:ILE:HD13	1:A:84:ASP:HB2	2.00	0.43
1:A:106:LEU:HA	1:A:178:VAL:HG11	2.01	0.43
1:A:866:LEU:HD12	1:A:869:LEU:HD23	2.00	0.43
1:A:388:LEU:O	1:A:392:TYR:HB3	2.18	0.43
1:A:794:LYS:HA	1:A:794:LYS:HD3	1.84	0.43
1:A:1243:LEU:HA	1:A:1243:LEU:HD23	1.71	0.43
1:A:209:ASN:HB2	8:A:2008:Y01:OAH	2.17	0.43
1:A:1250:TYR:HD1	1:A:1254:PHE:HE2	1.67	0.43
1:A:833:VAL:HG12	1:A:1338:MET:HG3	2.00	0.42
1:A:1590:ILE:HG23	1:A:1594:PHE:CE2	2.54	0.42
1:A:82:TYR:HA	1:A:85:LYS:HE2	2.00	0.42
1:A:1676:ASN:OD1	1:A:1676:ASN:N	2.52	0.42
1:A:1769:GLU:O	1:A:1771:THR:N	2.52	0.42
2:B:171:THR:O	2:B:175:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:833:VAL:HG23	1:A:834:LEU:HG	2.00	0.42
1:A:24:GLU:HG3	1:A:86:LYS:NZ	2.34	0.42
1:A:735:LYS:HD3	1:A:735:LYS:HA	1.77	0.42
1:A:1528:ASN:HD21	1:A:1619:ARG:HH11	1.68	0.42
8:A:2005:Y01:HAE1	8:A:2005:Y01:HAS2	1.81	0.42
8:A:2007:Y01:HAN2	8:A:2007:Y01:HAC3	2.00	0.42
1:A:261:LEU:HD23	1:A:261:LEU:HA	1.83	0.42
1:A:837:PHE:O	1:A:839:LEU:N	2.51	0.42
1:A:1278:LEU:HD12	1:A:1278:LEU:HA	1.83	0.42
1:A:30:ARG:O	1:A:34:GLU:HG3	2.20	0.42
1:A:860:GLY:O	1:A:864:GLY:N	2.53	0.42
1:A:832:SER:O	1:A:835:ARG:HB2	2.20	0.42
1:A:431:LYS:HD3	1:A:431:LYS:HA	1.74	0.42
1:A:65:ASP:OD1	1:A:66:ILE:N	2.53	0.42
1:A:1318:ILE:N	1:A:1319:PRO:HD2	2.35	0.42
1:A:1820:LYS:HD2	1:A:1820:LYS:N	2.33	0.42
2:B:185:ILE:HA	2:B:185:ILE:HD13	1.80	0.42
1:A:729:TYR:HD1	1:A:732:LYS:HE2	1.85	0.41
2:B:144:ILE:HD13	2:B:144:ILE:HA	1.89	0.41
1:A:876:ILE:CD1	8:A:2008:Y01:HAB1	2.50	0.41
3:C:65:LEU:HB3	3:C:83:PHE:HB3	2.02	0.41
1:A:58:GLN:OE1	1:A:95:LYS:HB2	2.20	0.41
1:A:296:GLU:OE2	1:A:300:ARG:NE	2.52	0.41
1:A:843:PHE:CD1	1:A:852:LEU:HD21	2.55	0.41
1:A:339:TYR:HB3	1:A:937:GLU:OE2	2.21	0.41
2:B:98:THR:C	2:B:100:ASP:H	2.23	0.41
1:A:760:PHE:CE2	1:A:779:GLY:HA3	2.55	0.41
1:A:1242:LEU:HA	1:A:1242:LEU:HD13	1.76	0.41
1:A:1271:VAL:HA	1:A:1274:VAL:HG12	2.02	0.41
1:A:1634:LEU:HD23	1:A:1634:LEU:HA	1.87	0.41
2:B:62:LYS:HB3	2:B:62:LYS:HE2	1.80	0.41
1:A:824:PHE:O	1:A:825:LEU:C	2.58	0.41
1:A:1177:ILE:HA	1:A:1180:ASN:ND2	2.35	0.41
1:A:1462:GLN:O	1:A:1466:LYS:HG2	2.20	0.41
1:A:918:LEU:HA	1:A:918:LEU:HD23	1.82	0.41
1:A:1593:MET:CE	1:A:1594:PHE:HE1	2.23	0.41
1:A:1749:LEU:HD13	1:A:1749:LEU:HA	1.90	0.41
1:A:104:PRO:HA	1:A:109:LEU:O	2.20	0.41
1:A:996:LYS:HA	1:A:999:ILE:HG12	2.03	0.41
1:A:1367:ARG:HB2	1:A:1382:TRP:CZ2	2.55	0.41
1:A:1519:ILE:O	1:A:1523:VAL:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1566:LEU:HA	1:A:1566:LEU:HD23	1.82	0.41
1:A:1612:ILE:HA	1:A:1612:ILE:HD12	1.78	0.41
2:B:112:THR:OG1	2:B:113:TYR:N	2.54	0.41
1:A:818:LEU:HA	1:A:821:VAL:HG12	2.03	0.41
2:B:65:GLU:O	2:B:65:GLU:HG2	2.21	0.41
1:A:396:LEU:HD23	1:A:396:LEU:HA	1.81	0.40
1:A:798:MET:O	1:A:799:ASP:HB2	2.20	0.40
1:A:979:ILE:HD11	1:A:981:GLU:HB2	2.03	0.40
1:A:1203:LEU:HD23	1:A:1203:LEU:HA	1.89	0.40
1:A:1531:THR:O	1:A:1534:VAL:HG12	2.21	0.40
8:A:2007:Y01:HAE1	8:A:2007:Y01:HAS2	1.81	0.40
1:A:225:ILE:HA	1:A:231:LEU:HD12	2.02	0.40
1:A:1609:PHE:O	1:A:1612:ILE:HG22	2.21	0.40
3:C:38:LEU:HD23	3:C:48:LEU:HD22	2.04	0.40
1:A:1567:ILE:HD12	1:A:1567:ILE:HA	1.94	0.40
1:A:1786:TRP:CZ2	1:A:1838:CYS:HB2	2.56	0.40
1:A:53:LEU:HD23	1:A:53:LEU:HA	1.88	0.40
1:A:377:THR:C	1:A:379:MET:N	2.74	0.40
1:A:973:SER:O	1:A:977:THR:HG23	2.22	0.40
1:A:986:ASN:HB3	1:A:989:GLN:HG3	2.03	0.40
1:A:1408:TRP:O	1:A:1409:THR:C	2.56	0.40
2:B:101:LEU:HD23	2:B:101:LEU:HA	1.85	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	1408/2031 (69%)	1319 (94%)	83 (6%)	6 (0%)	34 72
2	B	171/218 (78%)	157 (92%)	14 (8%)	0	100 100
3	C	120/215 (56%)	117 (98%)	3 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1699/2464 (69%)	1593 (94%)	100 (6%)	6 (0%)	38 72

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	838	ARG
1	A	1770	SER
1	A	1773	PRO
1	A	847	LYS
1	A	740	ILE
1	A	1285	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1268/1809 (70%)	1255 (99%)	13 (1%)	76 91
2	B	157/190 (83%)	156 (99%)	1 (1%)	86 95
3	C	114/193 (59%)	110 (96%)	4 (4%)	36 71
All	All	1539/2192 (70%)	1521 (99%)	18 (1%)	72 90

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	20	LEU
1	A	388	LEU
1	A	740	ILE
1	A	1204	LEU
1	A	1328	CYS
1	A	1467	LEU
1	A	1475	THR
1	A	1530	VAL
1	A	1557	LEU

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Mol	Chain	Res	Type
1	A	1686	ASN
1	A	1819	ASN
1	A	1847	LYS
2	B	93	ASN
3	C	55	CYS
3	C	71	GLU
3	C	130	MET
3	C	147	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	154	ASN
1	A	395	ASN
1	A	424	GLN
1	A	809	ASN
1	A	909	HIS
1	A	941	GLN
1	A	1478	GLN
1	A	1721	HIS
1	A	1819	ASN
2	B	102	GLN
2	B	115	HIS
2	B	134	HIS
3	C	53	ASN
3	C	82	GLN
3	C	118	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

4 monosaccharides are modelled in this entry.



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	NAG	D	1	4,1	14,14,15	0.23	0	17,19,21	0.46	0
4	NAG	D	2	4	14,14,15	0.25	0	17,19,21	0.37	0
4	NAG	E	1	2,4	14,14,15	0.57	0	17,19,21	1.19	2 (11%)
4	NAG	E	2	4	14,14,15	0.32	0	17,19,21	0.70	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	NAG	E	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
4	E	1	NAG	C1-O5-C5	2.72	115.88	112.19
4	E	1	NAG	C3-C4-C5	-2.66	105.49	110.24

There are no chirality outliers.

All (6) torsion outliers are listed below:

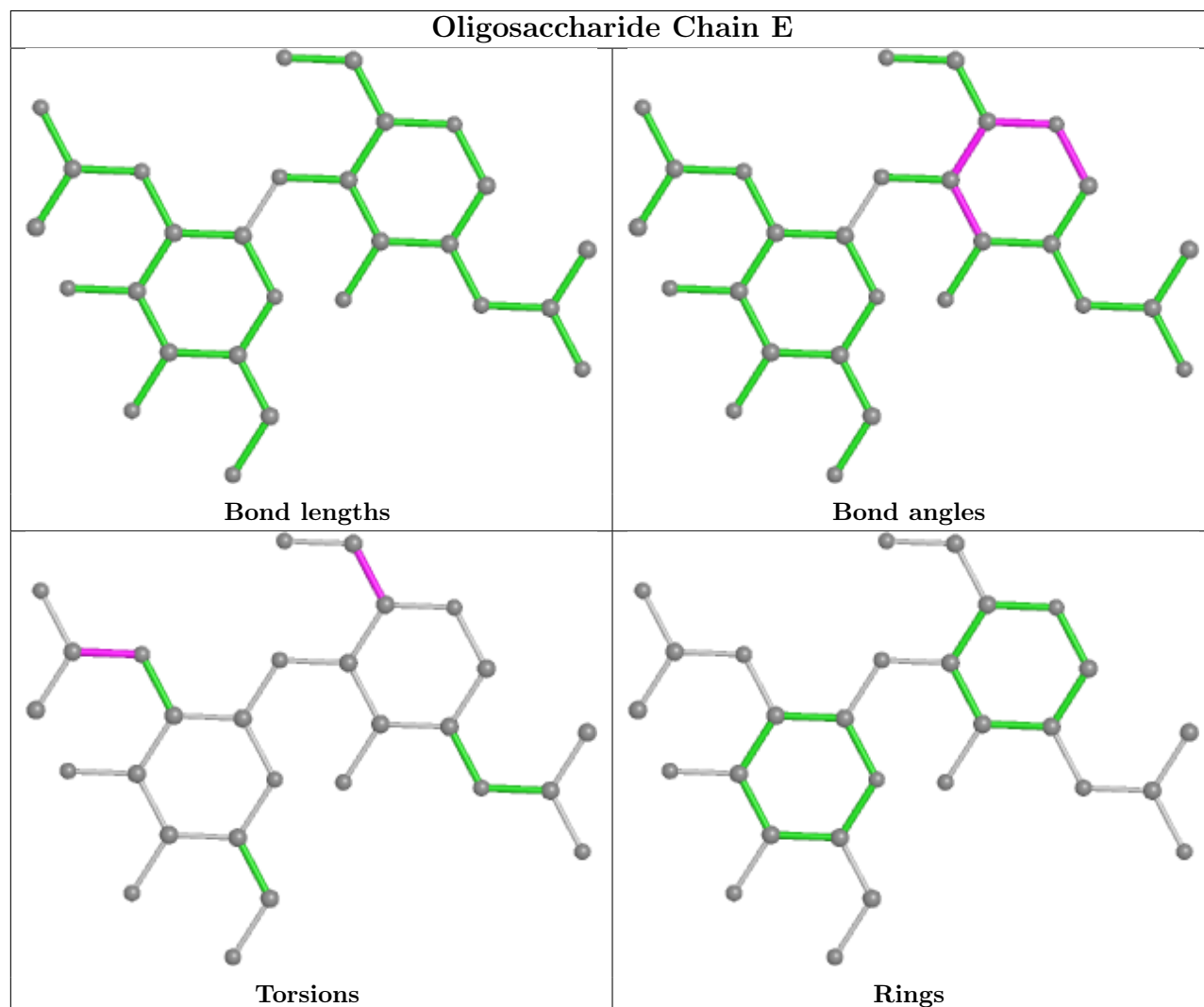
Mol	Chain	Res	Type	Atoms
4	E	2	NAG	C8-C7-N2-C2
4	E	2	NAG	O7-C7-N2-C2
4	D	1	NAG	C4-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6

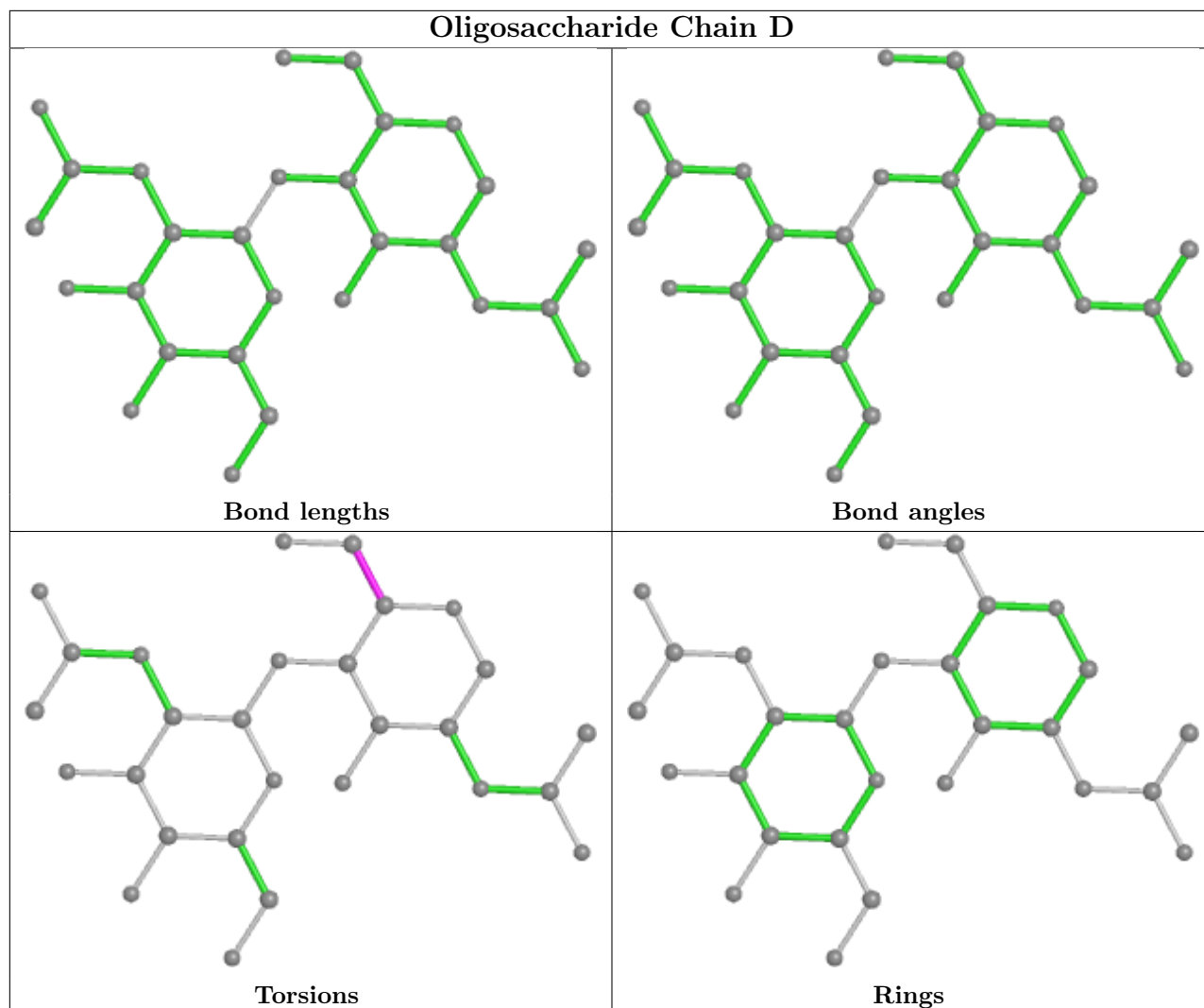
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1	NAG	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





## 5.6 Ligand geometry [i](#)

14 ligands are modelled in this entry.

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$
8	Y01	A	2008	-	38,38,38	0.66	1 (2%)	57,57,57	1.78	10 (17%)
8	Y01	A	2006	-	38,38,38	0.66	1 (2%)	57,57,57	1.79	11 (19%)
9	LPE	B	304	-	16,16,33	0.66	0	20,22,39	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	A	2002	1	14,14,15	0.36	0	17,19,21	0.44	0
6	NAG	B	302	2	14,14,15	0.20	0	17,19,21	0.41	0
8	Y01	A	2005	-	38,38,38	0.66	1 (2%)	57,57,57	1.78	11 (19%)
8	Y01	A	2010	-	38,38,38	1.16	4 (10%)	57,57,57	1.74	11 (19%)
7	P5S	A	2004	-	33,34,53	0.76	1 (3%)	36,40,60	1.80	5 (13%)
6	NAG	B	303	2	14,14,15	0.26	0	17,19,21	0.42	0
6	NAG	A	2003	1	14,14,15	0.19	0	17,19,21	0.46	0
8	Y01	A	2007	-	38,38,38	1.16	4 (10%)	57,57,57	1.74	11 (19%)
5	9SR	A	2001	-	16,25,25	2.73	6 (37%)	18,44,44	1.74	2 (11%)
6	NAG	B	301	2	14,14,15	0.63	0	17,19,21	0.97	0
6	NAG	A	2009	1	14,14,15	0.30	0	17,19,21	1.00	1 (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
8	Y01	A	2008	-	-	0/19/77/77	0/4/4/4
8	Y01	A	2006	-	-	0/19/77/77	0/4/4/4
9	LPE	B	304	-	-	9/17/17/34	-
6	NAG	A	2002	1	-	2/6/23/26	0/1/1/1
6	NAG	B	302	2	-	0/6/23/26	0/1/1/1
8	Y01	A	2005	-	-	0/19/77/77	0/4/4/4
8	Y01	A	2010	-	-	4/19/77/77	0/4/4/4
7	P5S	A	2004	-	-	28/39/39/59	-
6	NAG	B	303	2	-	0/6/23/26	0/1/1/1
6	NAG	A	2003	1	-	2/6/23/26	0/1/1/1
8	Y01	A	2007	-	-	4/19/77/77	0/4/4/4
5	9SR	A	2001	-	-	0/3/70/70	0/5/4/4
6	NAG	B	301	2	-	0/6/23/26	0/1/1/1
6	NAG	A	2009	1	-	2/6/23/26	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2001	9SR	C21-C03	5.18	1.63	1.52
5	A	2001	9SR	C13-N18	4.59	1.45	1.34
5	A	2001	9SR	C03-C05	-4.26	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2001	9SR	C03-C02	-4.13	1.45	1.53
5	A	2001	9SR	O20-C19	-3.67	1.35	1.42
8	A	2007	Y01	OAW-CAY	3.63	1.44	1.34
8	A	2010	Y01	OAW-CAY	3.62	1.44	1.34
7	A	2004	P5S	O37-C38	3.39	1.43	1.34
5	A	2001	9SR	O04-C03	-2.78	1.39	1.43
8	A	2007	Y01	CAM-CAY	2.38	1.57	1.50
8	A	2010	Y01	CAM-CAY	2.34	1.57	1.50
8	A	2010	Y01	CAL-CAX	2.25	1.55	1.50
8	A	2007	Y01	CAL-CAX	2.24	1.55	1.50
8	A	2006	Y01	CBH-CBF	-2.23	1.52	1.56
8	A	2010	Y01	CBH-CBF	-2.21	1.52	1.56
8	A	2007	Y01	CBH-CBF	-2.19	1.52	1.56
8	A	2005	Y01	CBH-CBF	-2.17	1.52	1.56
8	A	2008	Y01	CBH-CBF	-2.15	1.52	1.56

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	2004	P5S	OG-CB-CA	7.03	114.19	108.06
8	A	2010	Y01	CBI-CBE-CBB	-5.96	110.15	119.49
8	A	2008	Y01	CBI-CBE-CBB	-5.93	110.20	119.49
8	A	2007	Y01	CBI-CBE-CBB	-5.90	110.24	119.49
8	A	2006	Y01	CBI-CBE-CBB	-5.90	110.25	119.49
8	A	2005	Y01	CBI-CBE-CBB	-5.90	110.25	119.49
5	A	2001	9SR	C17-C11-N12	5.58	114.28	108.12
8	A	2006	Y01	CBI-CBG-CBD	-4.82	107.25	114.38
8	A	2008	Y01	CBI-CBG-CBD	-4.80	107.28	114.38
8	A	2007	Y01	CBI-CBG-CBD	-4.75	107.35	114.38
8	A	2005	Y01	CBI-CBG-CBD	-4.74	107.36	114.38
8	A	2010	Y01	CBI-CBG-CBD	-4.66	107.48	114.38
7	A	2004	P5S	OXT-C-O	-4.06	114.86	124.09
8	A	2006	Y01	OAW-CAY-CAM	3.98	120.07	111.50
8	A	2008	Y01	OAW-CAY-CAM	3.97	120.06	111.50
8	A	2005	Y01	OAW-CAY-CAM	3.96	120.03	111.50
8	A	2010	Y01	OAW-CAY-CAM	3.75	119.58	111.50
8	A	2007	Y01	OAW-CAY-CAM	3.71	119.49	111.50
7	A	2004	P5S	O37-C38-C39	3.69	119.44	111.50
8	A	2007	Y01	CAS-CAU-CBI	-3.33	107.07	112.78
8	A	2005	Y01	CAS-CAU-CBI	-3.33	107.07	112.78
8	A	2006	Y01	CAS-CAU-CBI	-3.32	107.08	112.78
8	A	2010	Y01	CAS-CAU-CBI	-3.30	107.11	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2008	Y01	CAS-CAU-CBI	-3.28	107.16	112.78
7	A	2004	P5S	OXT-C-CA	2.94	123.39	113.38
8	A	2006	Y01	CAD-CBH-CBF	-2.93	108.19	111.68
8	A	2005	Y01	CAD-CBH-CBF	-2.92	108.19	111.68
8	A	2007	Y01	CAD-CBH-CBF	-2.91	108.21	111.68
8	A	2010	Y01	CAD-CBH-CBF	-2.90	108.22	111.68
6	A	2009	NAG	C4-C3-C2	-2.88	106.80	111.02
8	A	2008	Y01	CAD-CBH-CBF	-2.85	108.28	111.68
8	A	2010	Y01	CBG-CBI-CBE	2.74	103.32	100.07
8	A	2005	Y01	CBG-CBI-CBE	2.73	103.31	100.07
8	A	2008	Y01	CBG-CBI-CBE	2.73	103.30	100.07
8	A	2007	Y01	CBG-CBI-CBE	2.70	103.27	100.07
8	A	2006	Y01	CBG-CBI-CBE	2.69	103.25	100.07
5	A	2001	9SR	C03-C02-C19	-2.62	110.28	114.38
8	A	2008	Y01	CAS-CBF-CBH	-2.59	109.67	113.08
8	A	2006	Y01	CAS-CBF-CBH	-2.51	109.77	113.08
8	A	2005	Y01	CBD-CAK-CAI	-2.49	109.16	112.73
8	A	2005	Y01	CAS-CBF-CBH	-2.49	109.81	113.08
8	A	2007	Y01	CAS-CBF-CBH	-2.48	109.82	113.08
8	A	2010	Y01	CBD-CAK-CAI	-2.47	109.18	112.73
8	A	2010	Y01	CAS-CBF-CBH	-2.46	109.84	113.08
8	A	2007	Y01	CBD-CAK-CAI	-2.45	109.21	112.73
8	A	2006	Y01	CBD-CAK-CAI	-2.43	109.24	112.73
8	A	2008	Y01	CBD-CAK-CAI	-2.41	109.27	112.73
8	A	2010	Y01	CBF-CBH-CAZ	2.35	113.34	109.65
8	A	2005	Y01	CBF-CBH-CAZ	2.34	113.32	109.65
8	A	2008	Y01	CBF-CBH-CAZ	2.32	113.28	109.65
8	A	2007	Y01	CBF-CBH-CAZ	2.31	113.28	109.65
7	A	2004	P5S	C2-O37-C38	-2.31	112.10	117.79
8	A	2006	Y01	CBF-CBH-CAZ	2.30	113.27	109.65
8	A	2008	Y01	CAC-CBB-CBE	-2.26	109.47	112.92
8	A	2006	Y01	CAC-CBB-CBE	-2.24	109.49	112.92
8	A	2007	Y01	CAC-CBB-CBE	-2.24	109.49	112.92
8	A	2005	Y01	CAC-CBB-CBE	-2.23	109.50	112.92
8	A	2010	Y01	CAC-CBB-CBE	-2.16	109.62	112.92
8	A	2005	Y01	CAQ-CBG-CBD	-2.05	115.71	119.08
8	A	2006	Y01	CAQ-CBG-CBD	-2.05	115.71	119.08
8	A	2010	Y01	CAQ-CBG-CBD	-2.02	115.75	119.08
8	A	2007	Y01	CAQ-CBG-CBD	-2.01	115.76	119.08

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	2004	P5S	C-CA-CB-OG
7	A	2004	P5S	N-CA-CB-OG
7	A	2004	P5S	CB-OG-P12-O13
7	A	2004	P5S	C3-O16-P12-OG
7	A	2004	P5S	C3-O16-P12-O13
7	A	2004	P5S	C3-O16-P12-O15
9	B	304	LPE	C3-O3-P-O31
9	B	304	LPE	C3-O3-P-O32
9	B	304	LPE	C3-O3-P-O33
6	A	2002	NAG	O5-C5-C6-O6
6	A	2003	NAG	O5-C5-C6-O6
6	A	2002	NAG	C4-C5-C6-O6
6	A	2009	NAG	C8-C7-N2-C2
8	A	2007	Y01	CAR-CBC-OAW-CAY
8	A	2010	Y01	CAR-CBC-OAW-CAY
6	A	2009	NAG	O7-C7-N2-C2
6	A	2003	NAG	C4-C5-C6-O6
7	A	2004	P5S	C38-C39-C40-C41
7	A	2004	P5S	CB-OG-P12-O16
9	B	304	LPE	C31-O33-P-O3
8	A	2007	Y01	CAV-CBC-OAW-CAY
8	A	2010	Y01	CAV-CBC-OAW-CAY
7	A	2004	P5S	C46-C48-C49-C50
7	A	2004	P5S	C51-C52-C53-C54
7	A	2004	P5S	C41-C42-C43-C44
7	A	2004	P5S	C52-C53-C54-C55
7	A	2004	P5S	C48-C49-C50-C51
7	A	2004	P5S	C39-C38-O37-C2
7	A	2004	P5S	O47-C38-O37-C2
7	A	2004	P5S	C1-C2-C3-O16
9	B	304	LPE	C2-C3-O3-P
7	A	2004	P5S	C2-C3-O16-P12
8	A	2010	Y01	CAO-CAJ-CAN-CBA
8	A	2007	Y01	CAO-CAJ-CAN-CBA
7	A	2004	P5S	O37-C2-C3-O16
7	A	2004	P5S	C40-C41-C42-C43
9	B	304	LPE	C2-C1-O1-C11
7	A	2004	P5S	CB-OG-P12-O15
9	B	304	LPE	C31-O33-P-O31
9	B	304	LPE	C32-C31-O33-P
9	B	304	LPE	O33-C31-C32-N
7	A	2004	P5S	C50-C51-C52-C53
7	A	2004	P5S	C43-C44-C45-C46

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Mol	Chain	Res	Type	Atoms
7	A	2004	P5S	C39-C40-C41-C42
7	A	2004	P5S	O19-C1-C2-O37
7	A	2004	P5S	C53-C54-C55-C56
7	A	2004	P5S	C49-C50-C51-C52
7	A	2004	P5S	O37-C38-C39-C40
8	A	2007	Y01	CAN-CAJ-CAO-CBB
8	A	2010	Y01	CAN-CAJ-CAO-CBB
7	A	2004	P5S	O47-C38-C39-C40

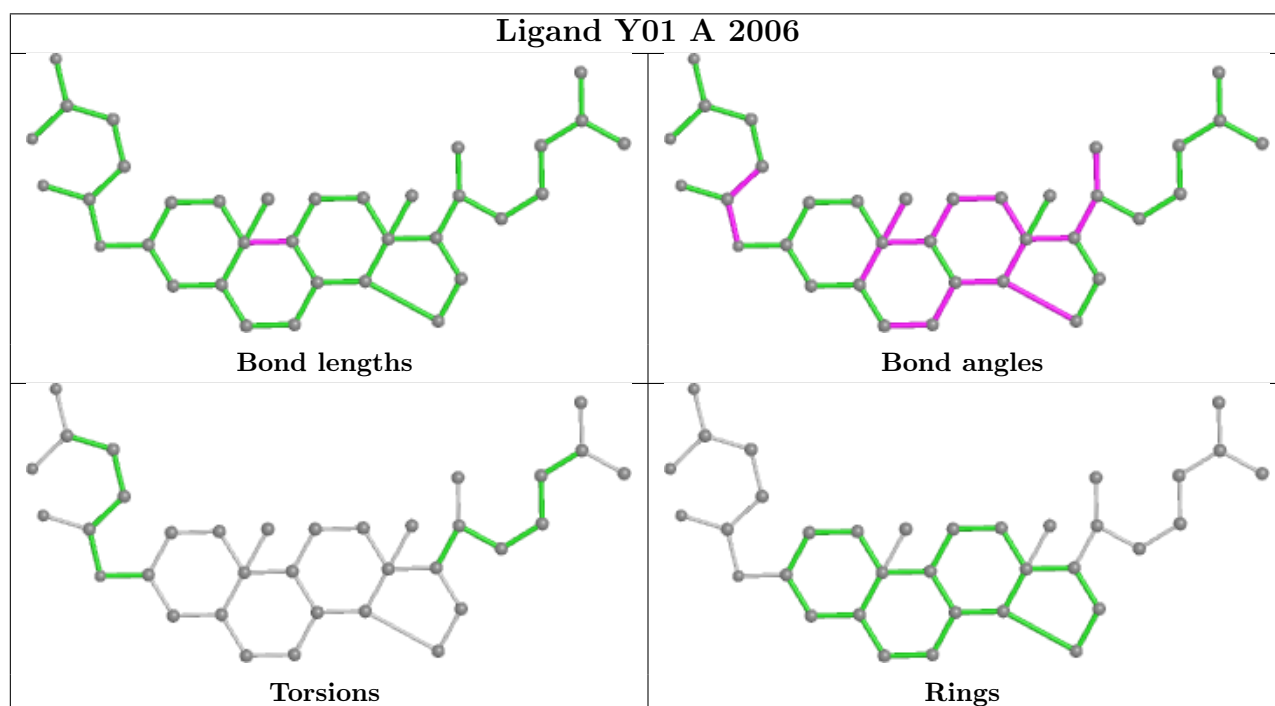
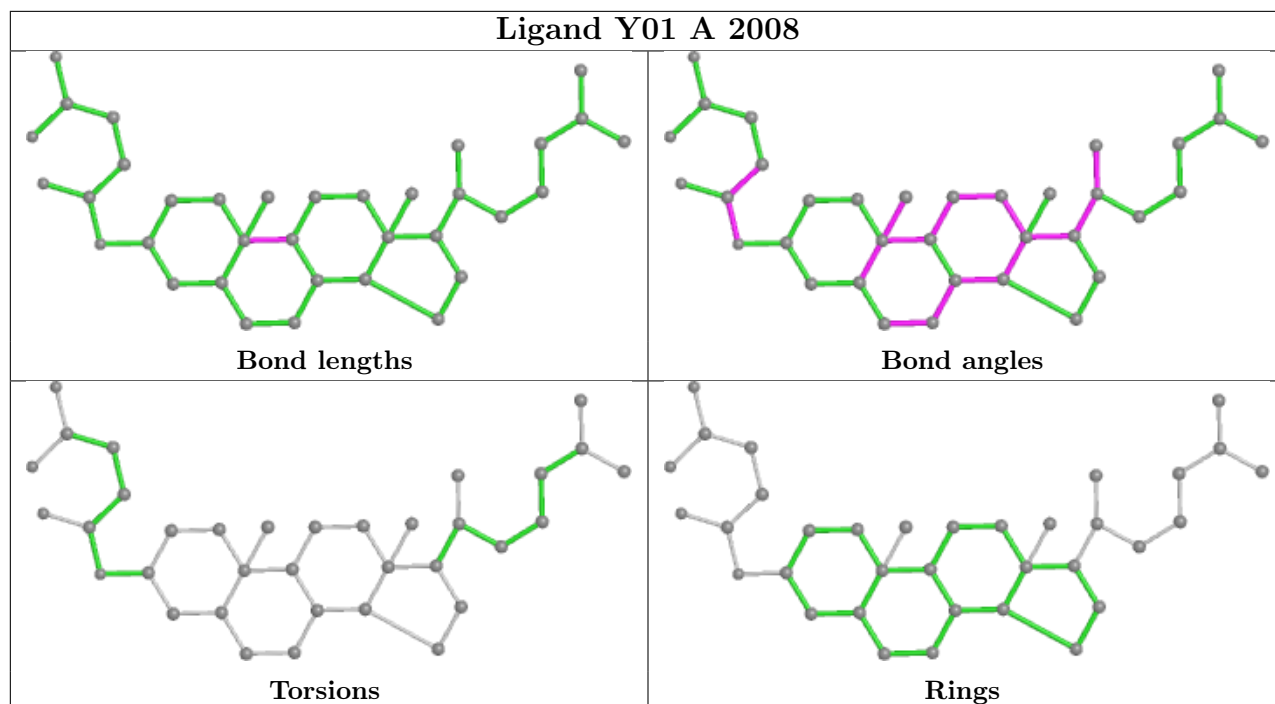
There are no ring outliers.

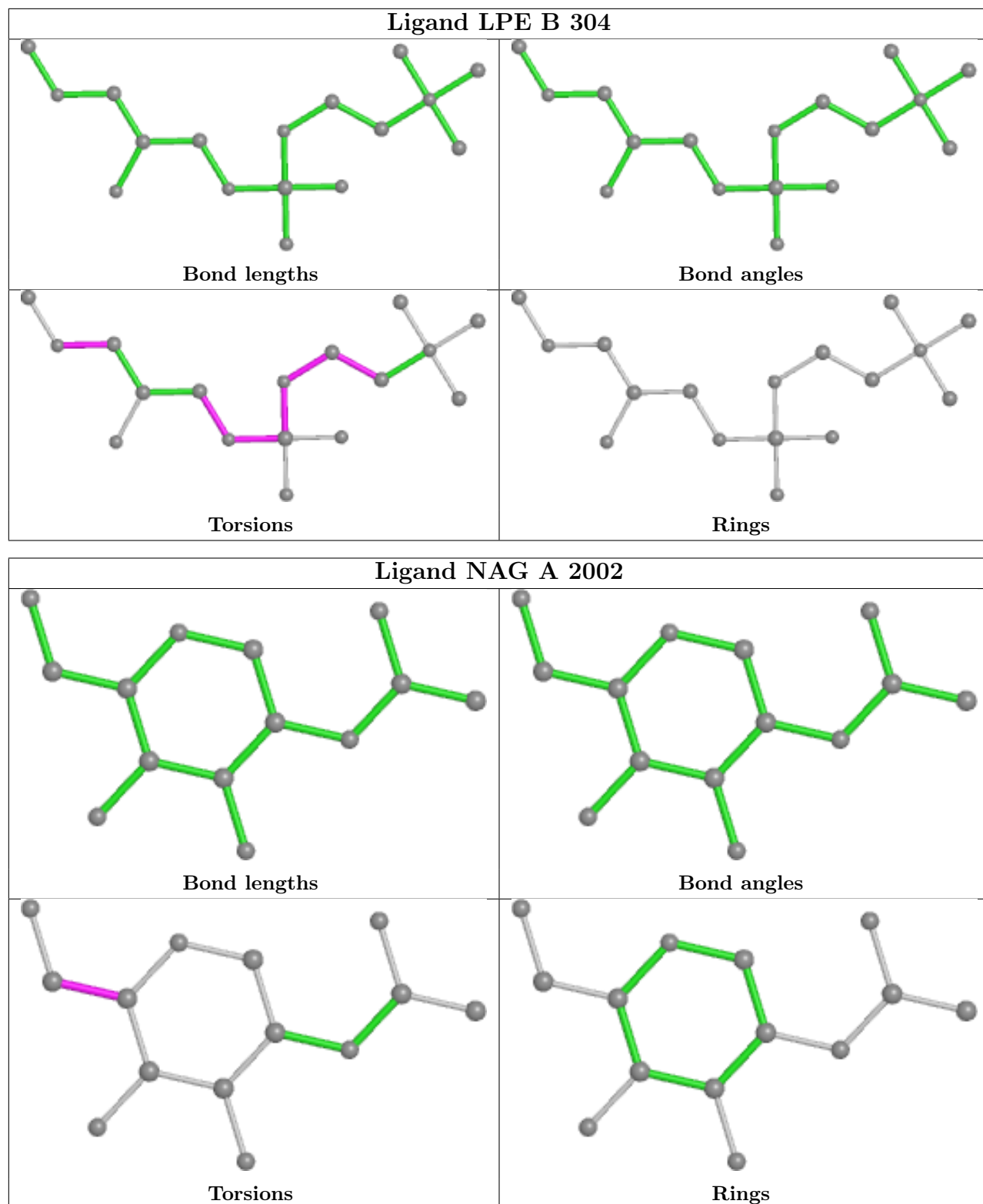
7 monomers are involved in 56 short contacts:

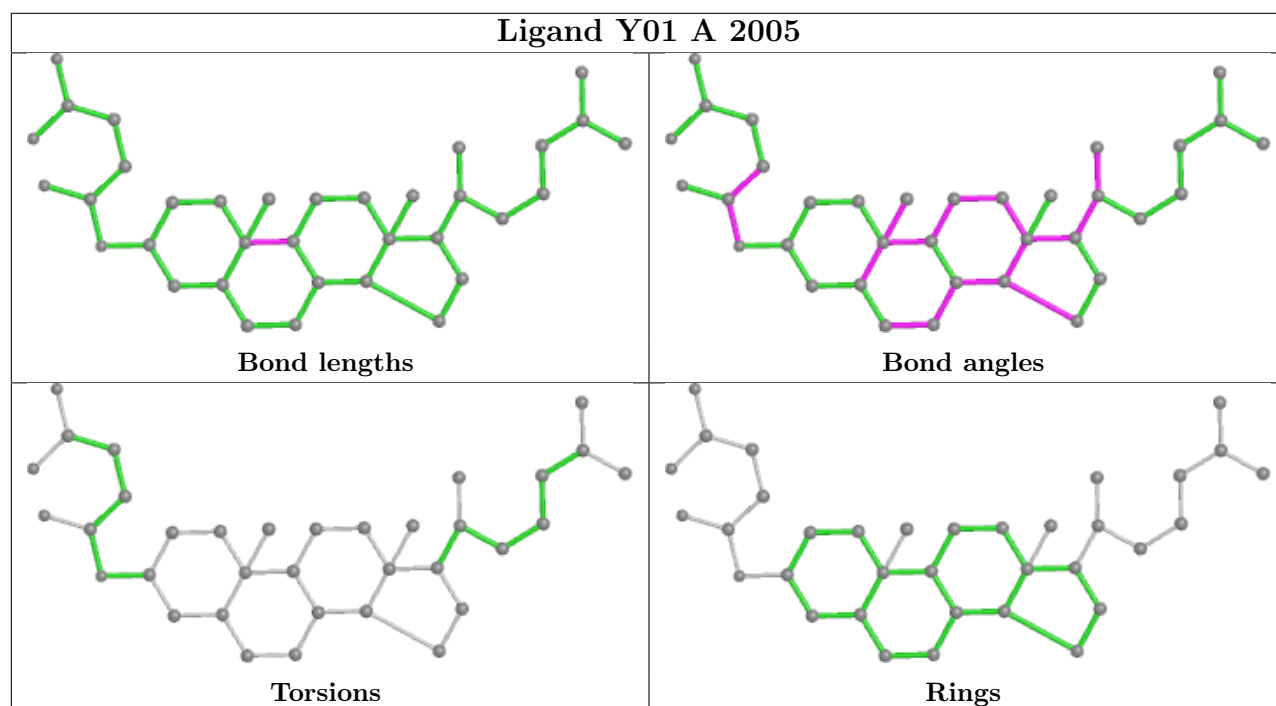
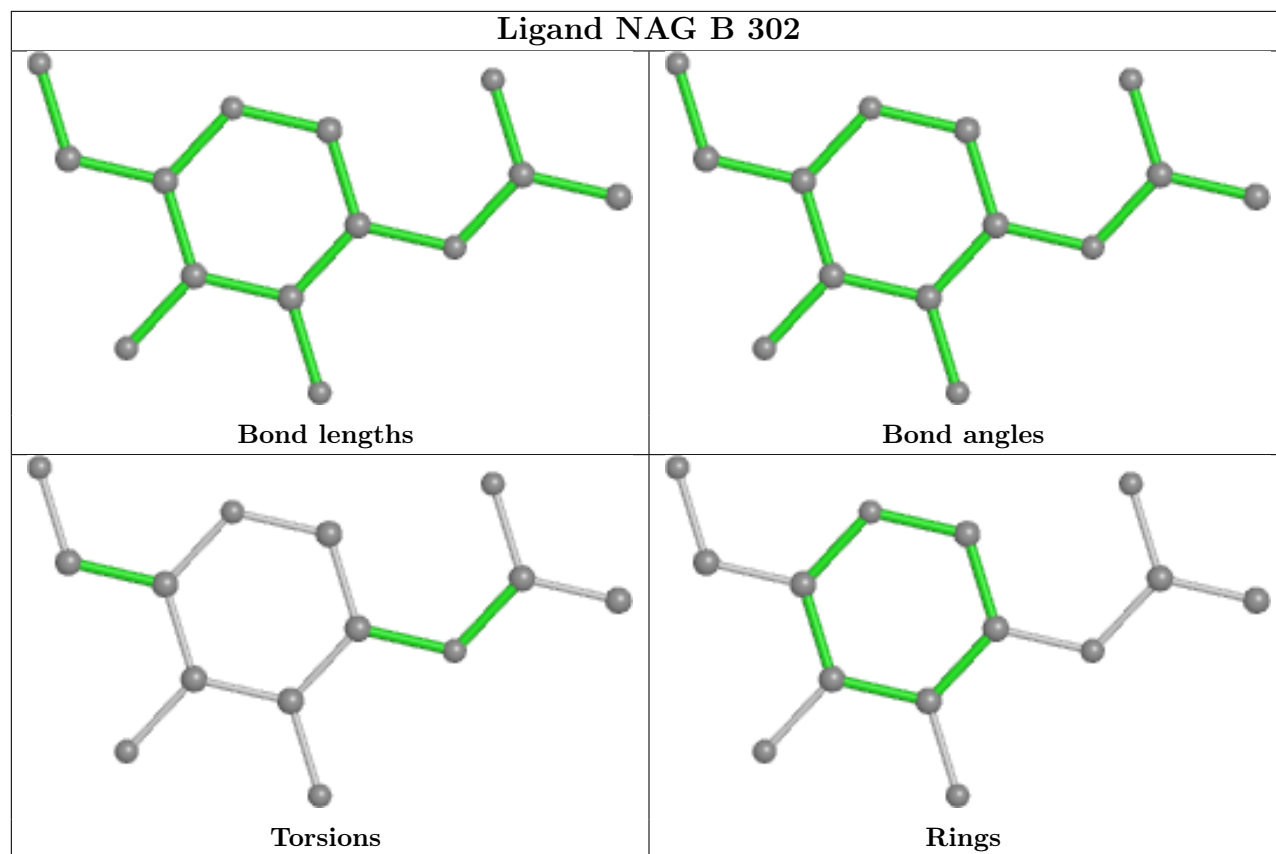
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	2008	Y01	26	0
8	A	2006	Y01	9	0
9	B	304	LPE	1	0
8	A	2005	Y01	4	0
8	A	2010	Y01	5	0
7	A	2004	P5S	4	0
8	A	2007	Y01	7	0

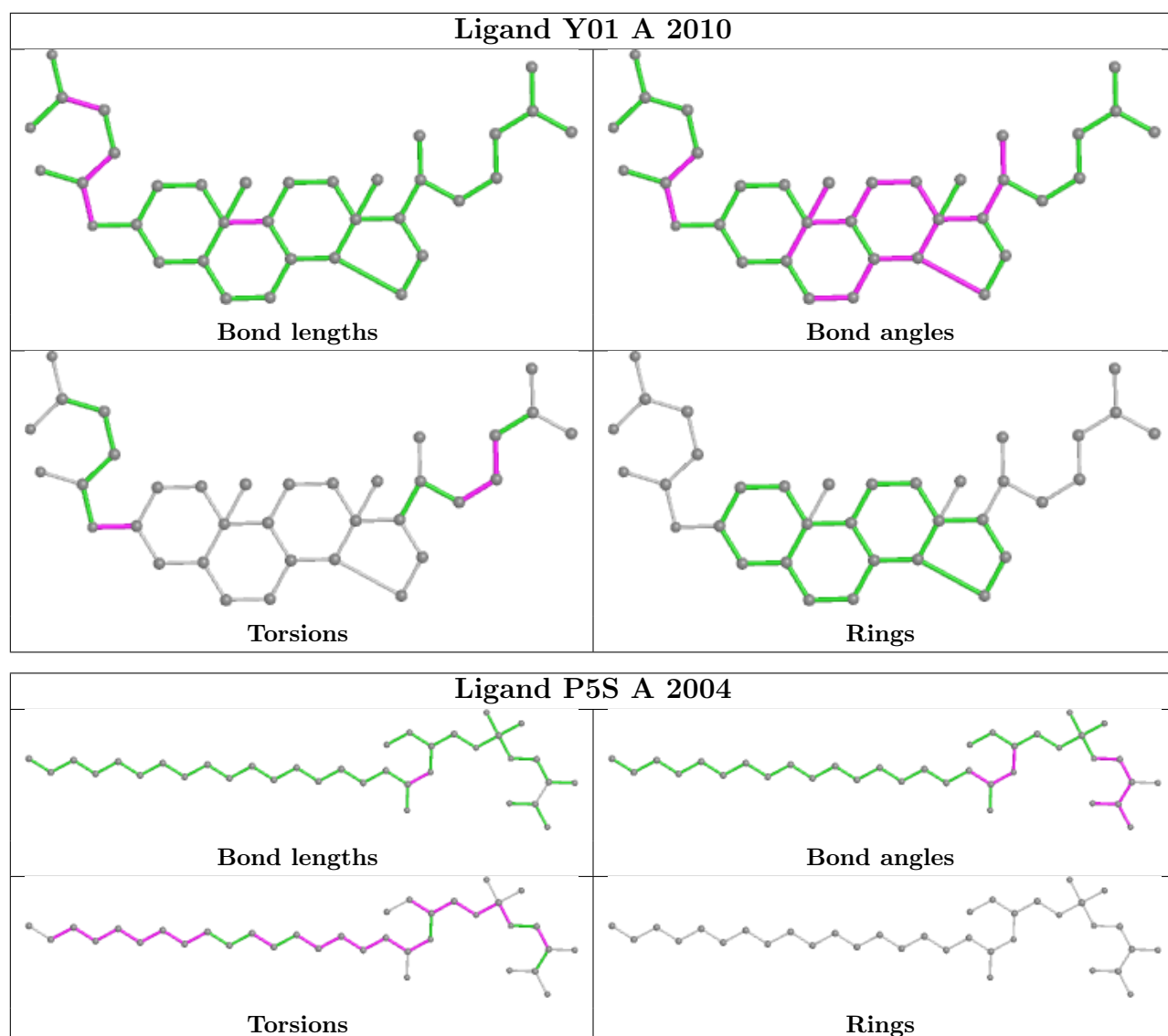
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

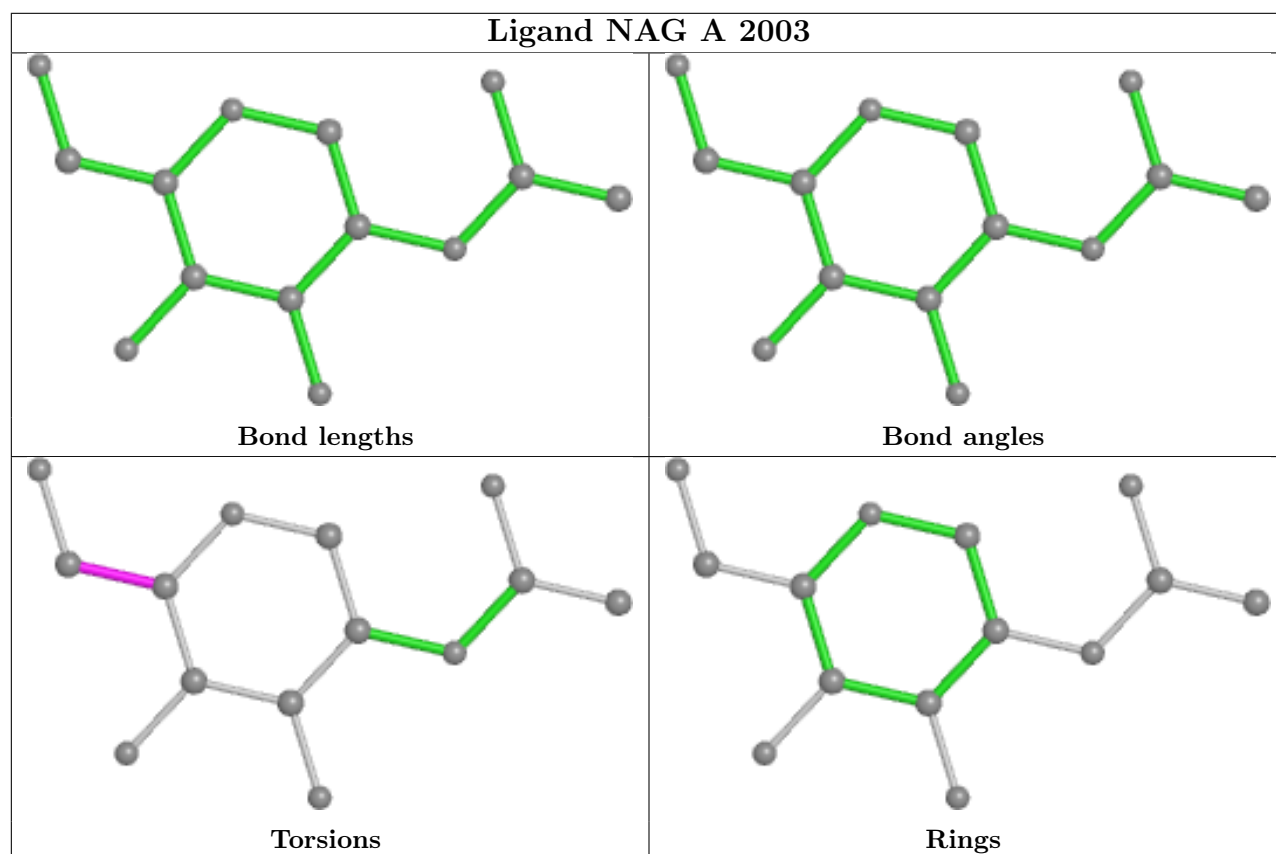
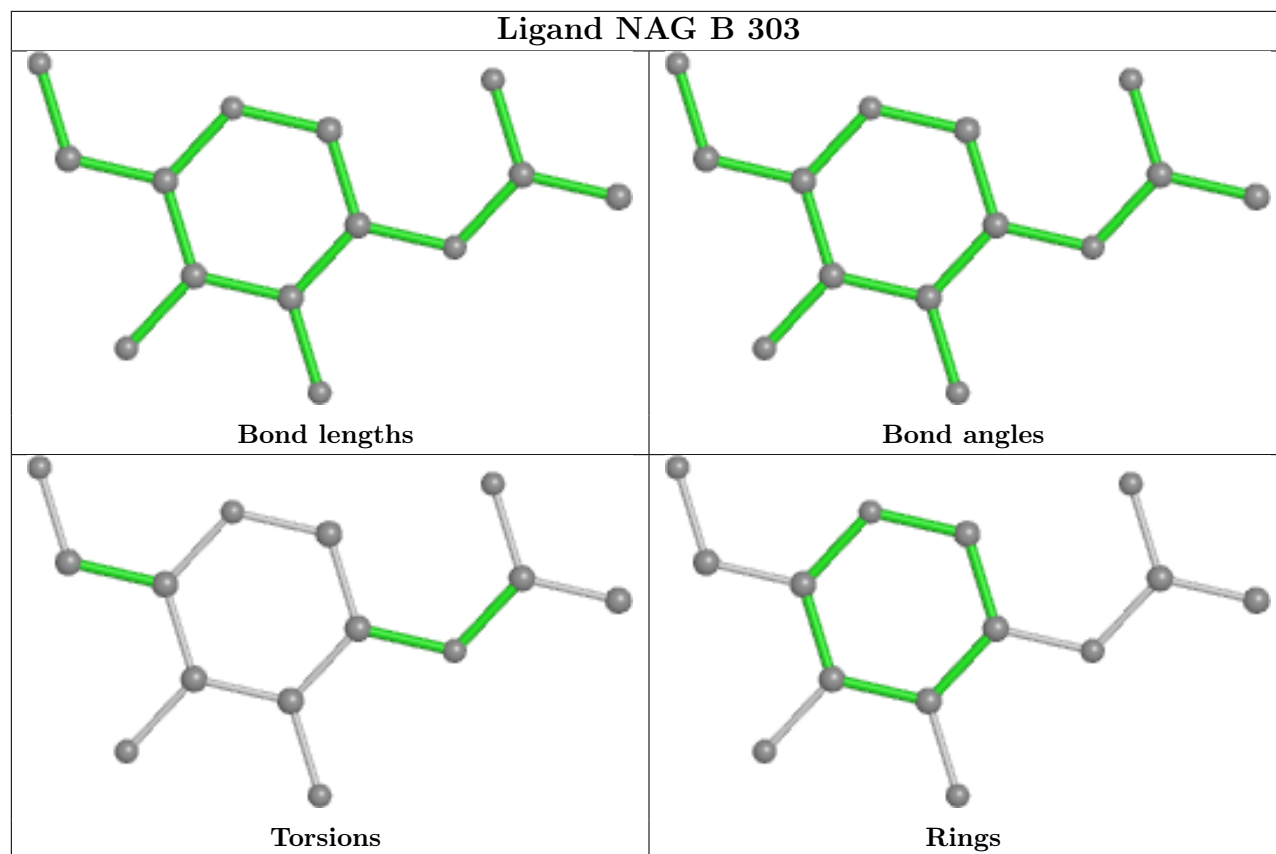


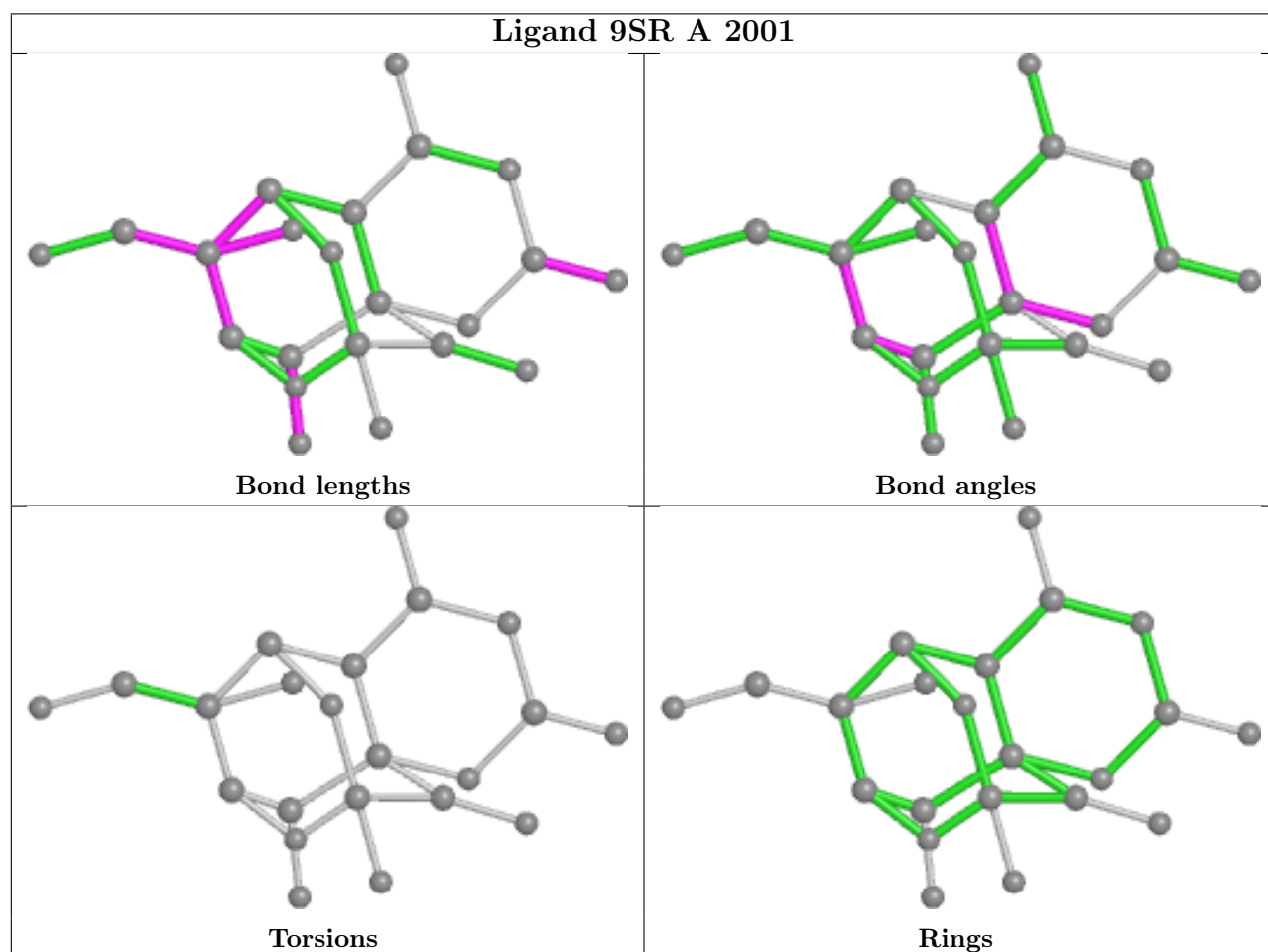
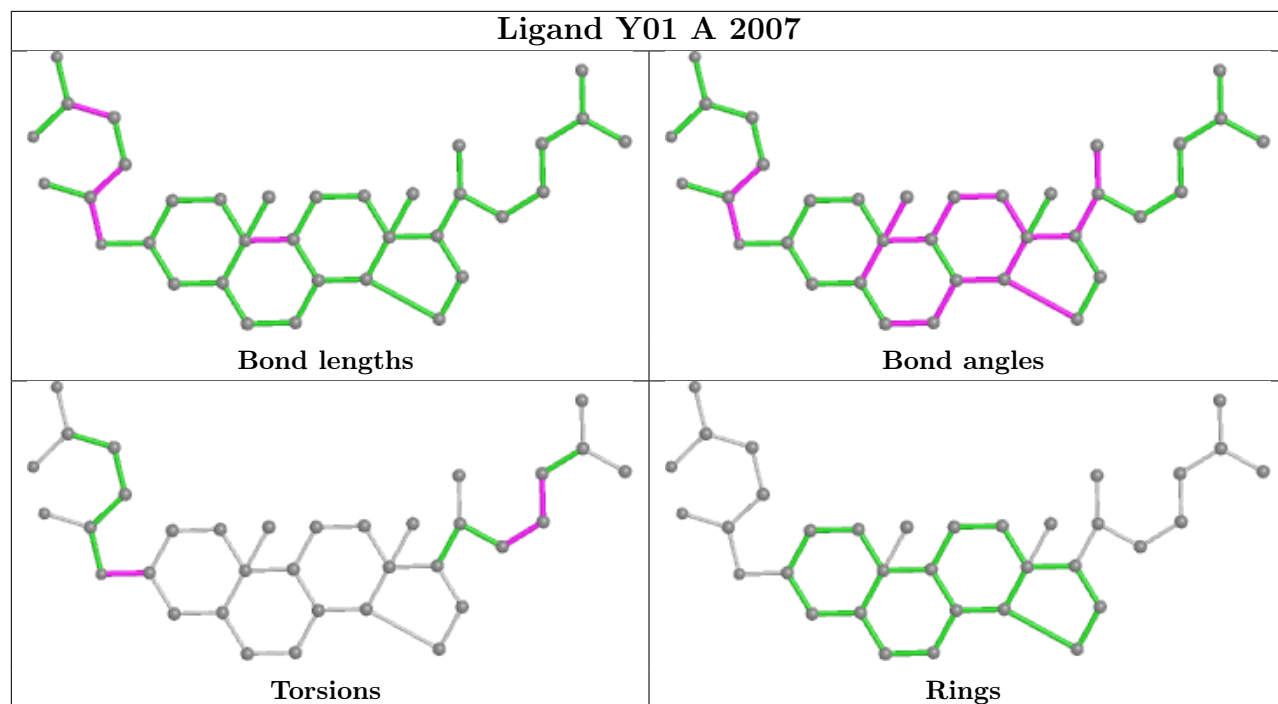


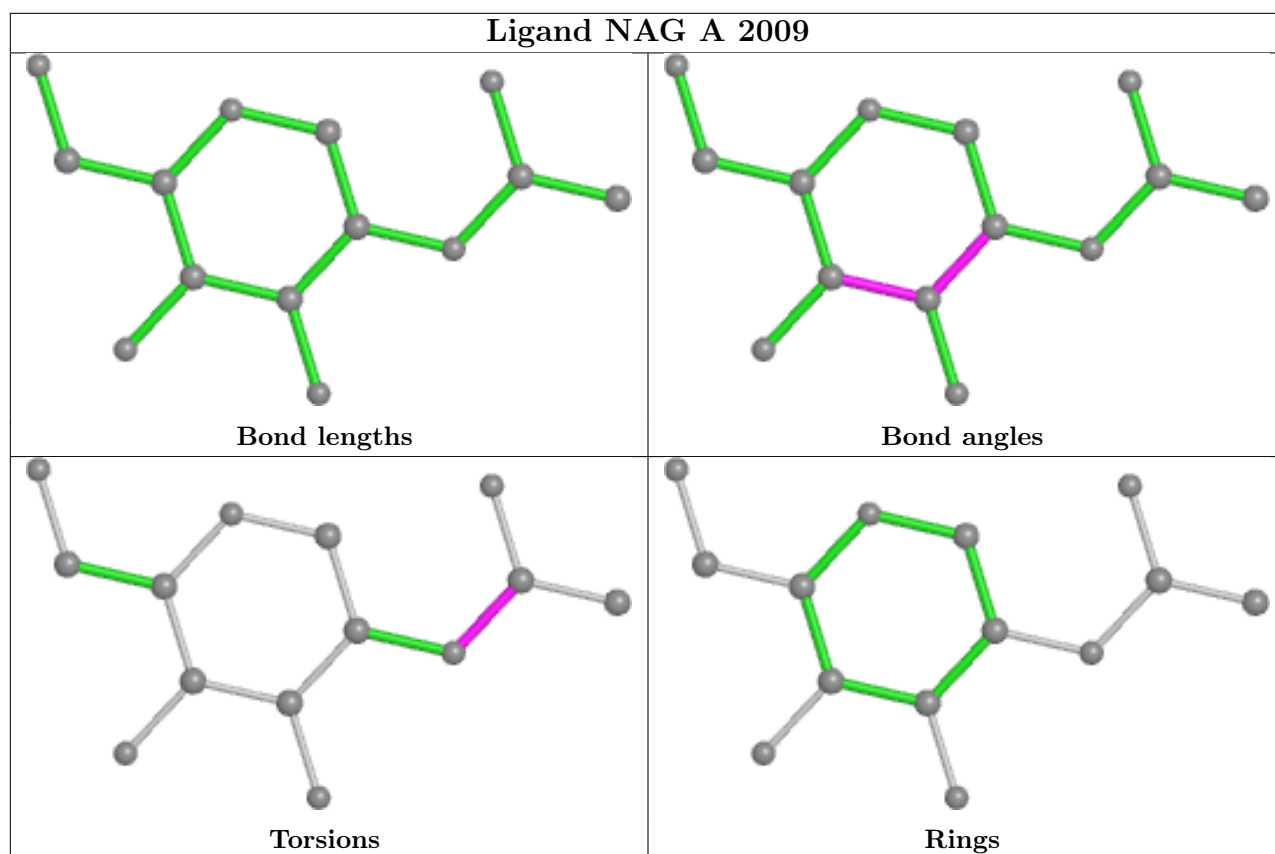
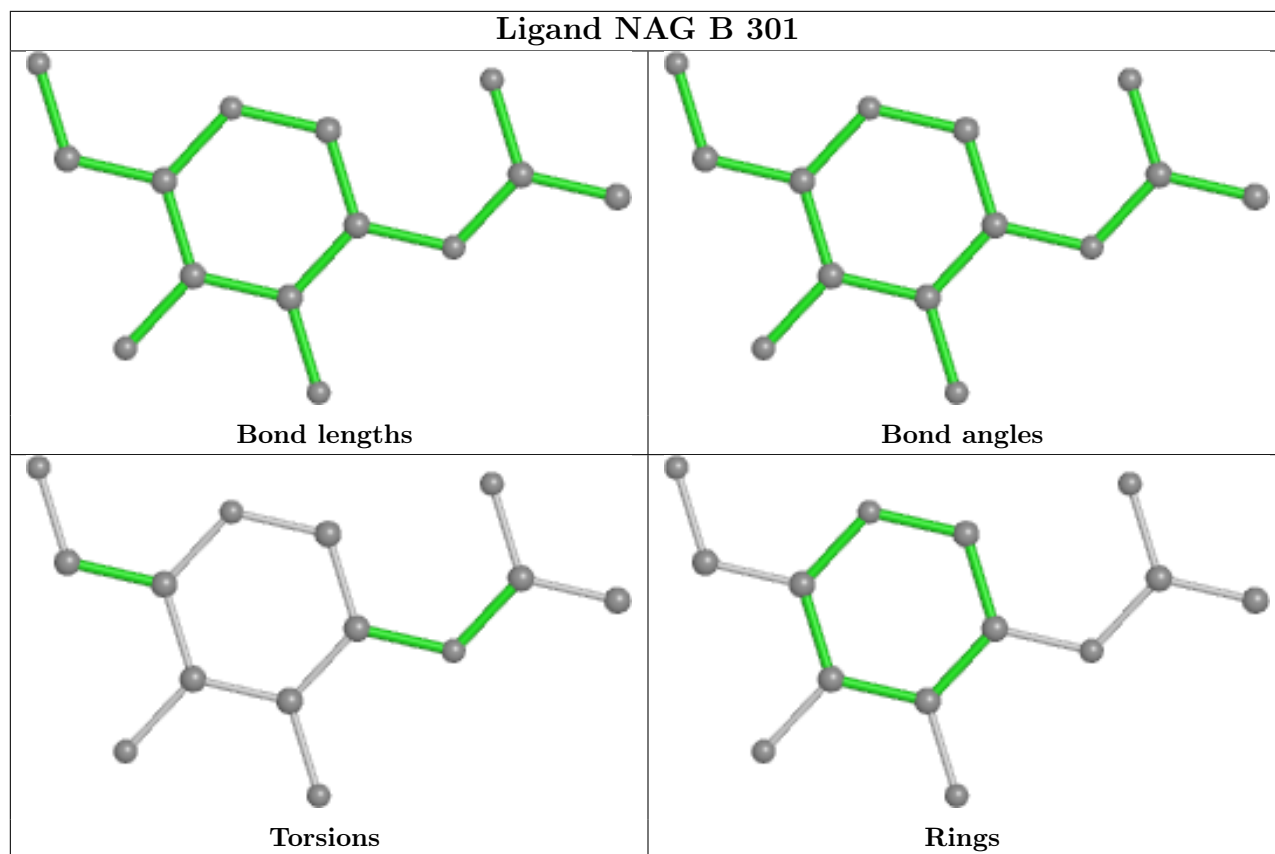












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



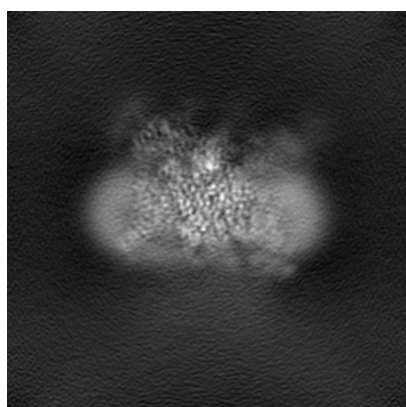
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32370. These allow visual inspection of the internal detail of the map and identification of artifacts.

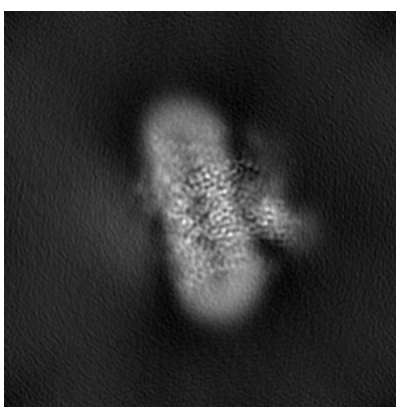
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

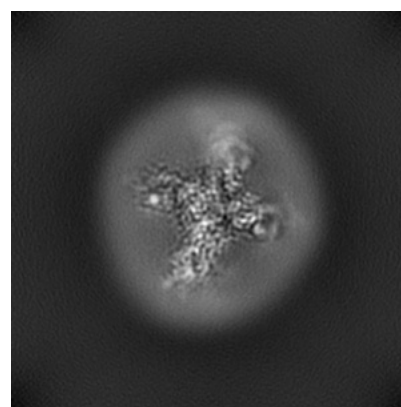
#### 6.1.1 Primary map



X



Y

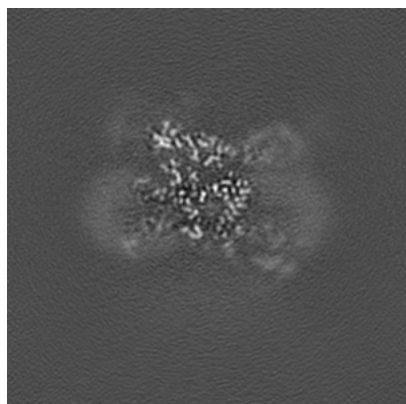


Z

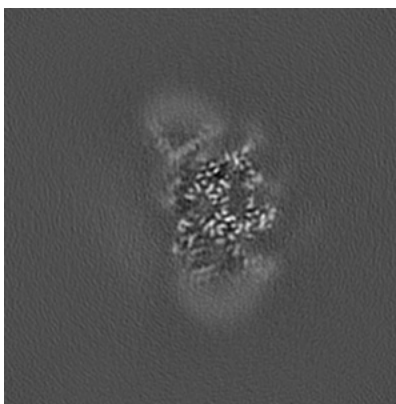
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

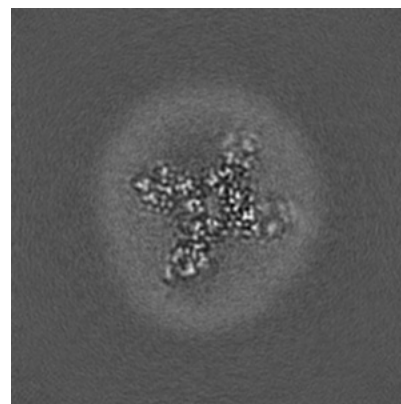
#### 6.2.1 Primary map



X Index: 120



Y Index: 120

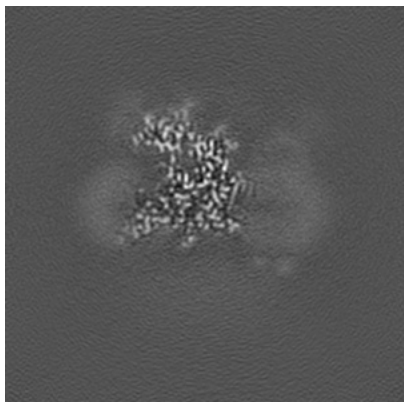


Z Index: 120

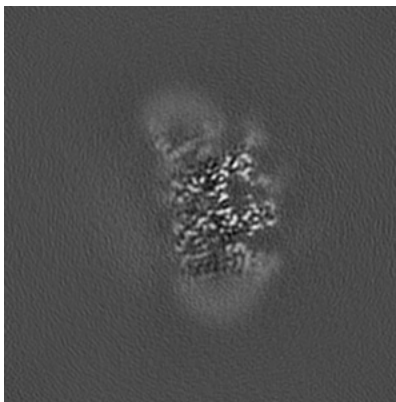
The images above show central slices of the map in three orthogonal directions.

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

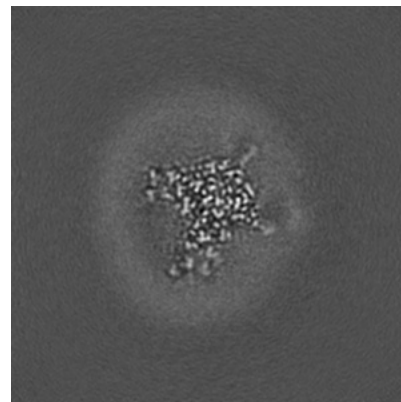
### 6.3.1 Primary map



X Index: 112



Y Index: 122



Z Index: 130

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

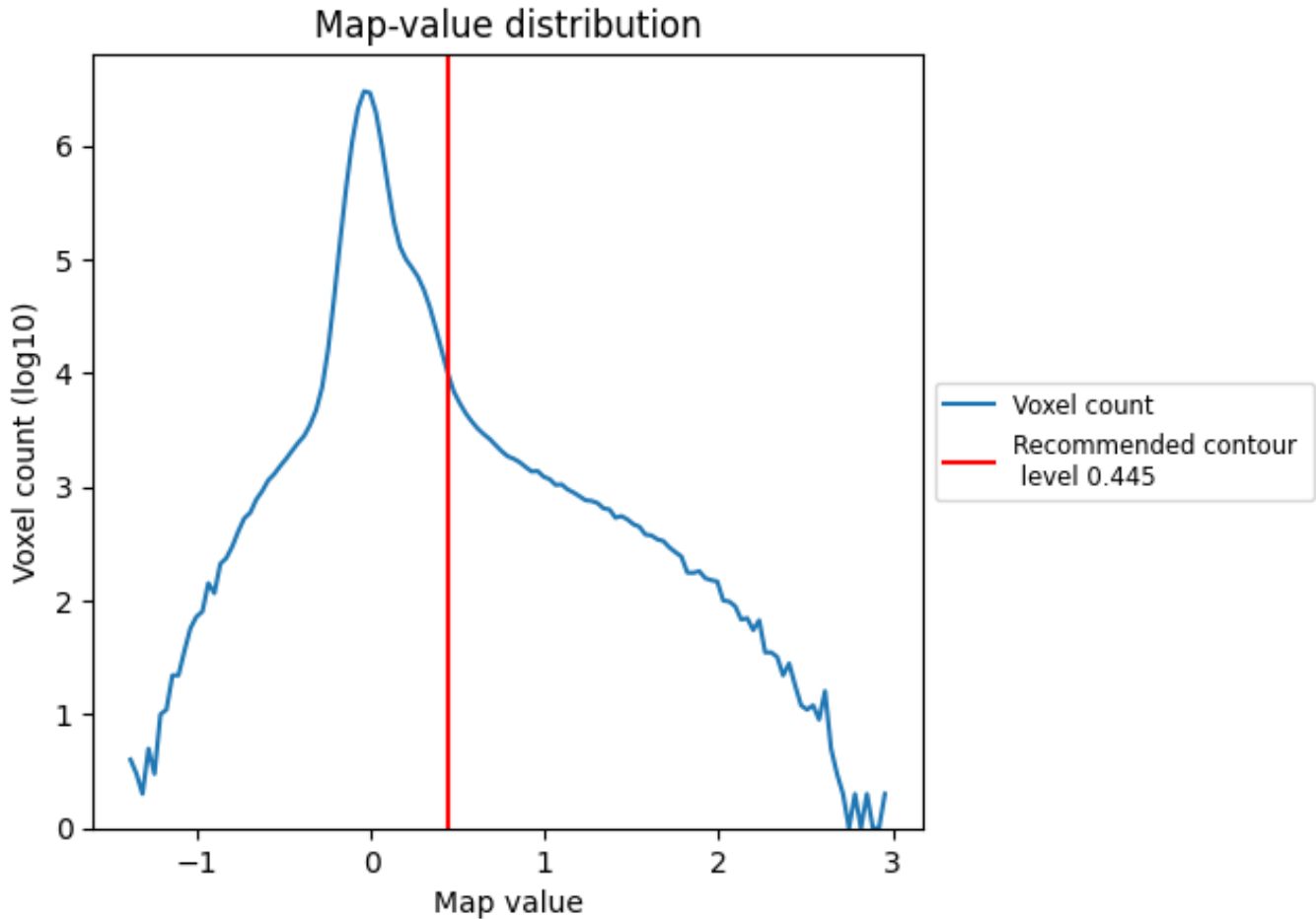
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

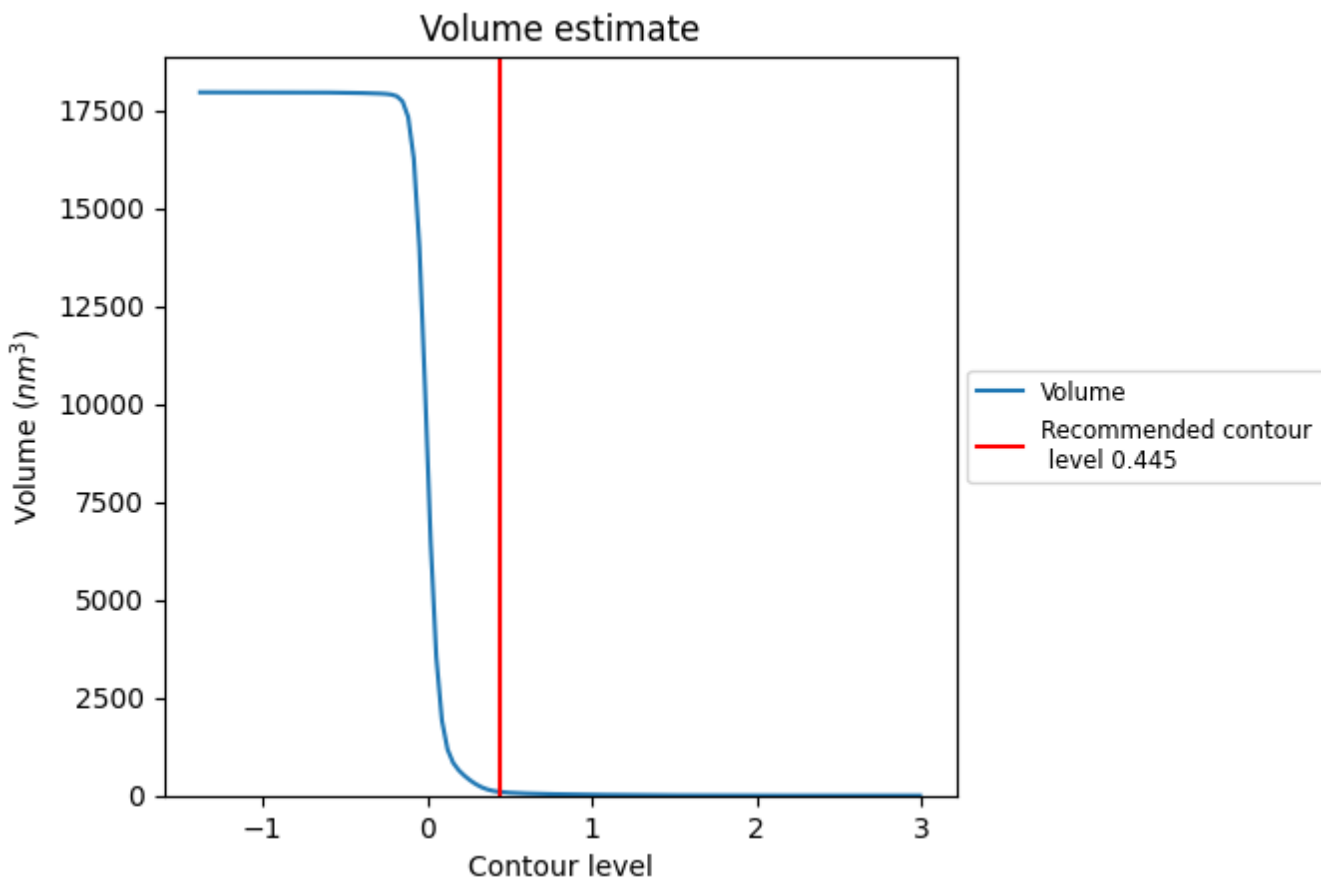
This section contains the results of statistical analysis of the map.

### 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.

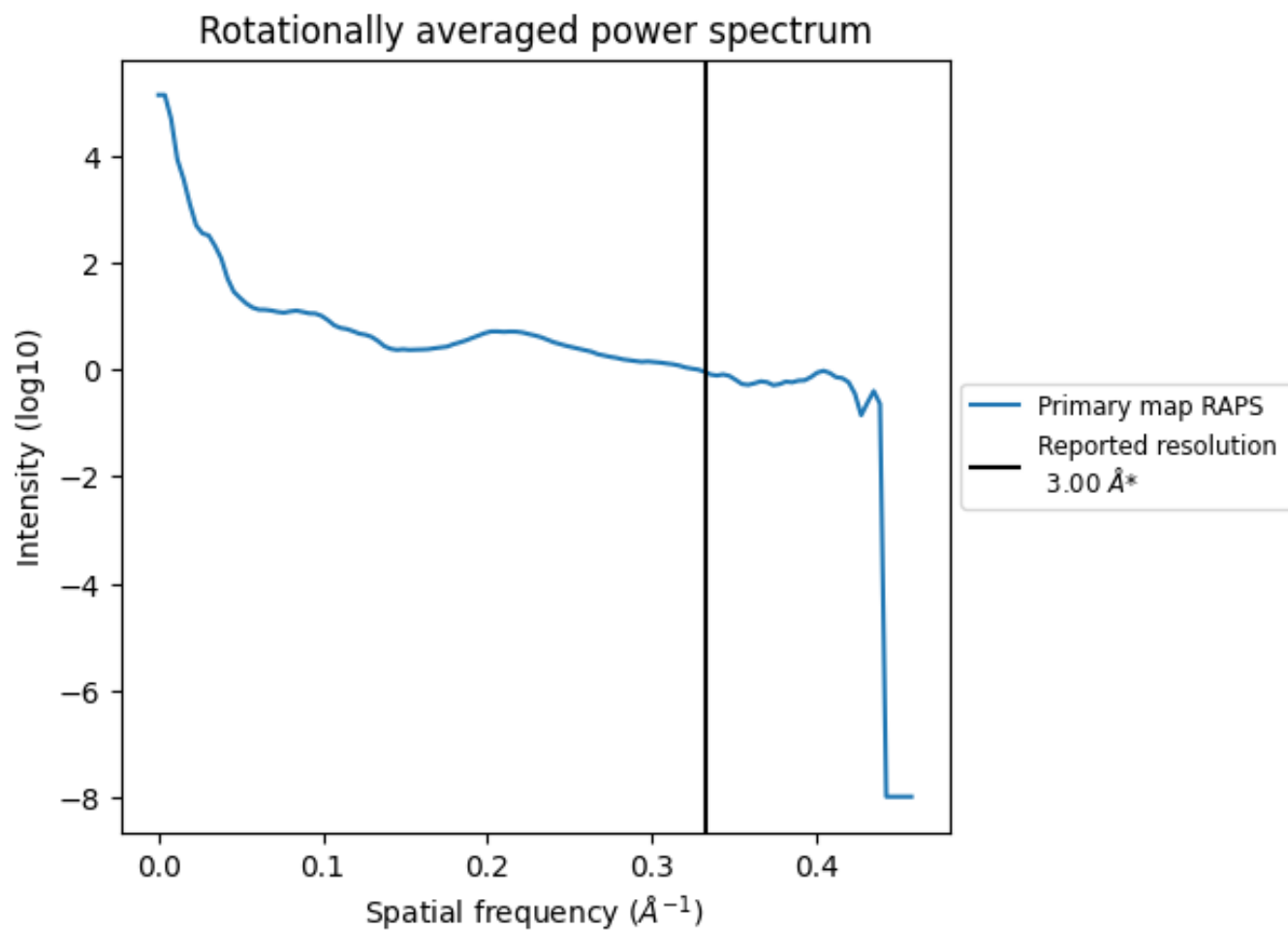
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 91 nm<sup>3</sup>; this corresponds to an approximate mass of 82 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 0.333 Å<sup>-1</sup>

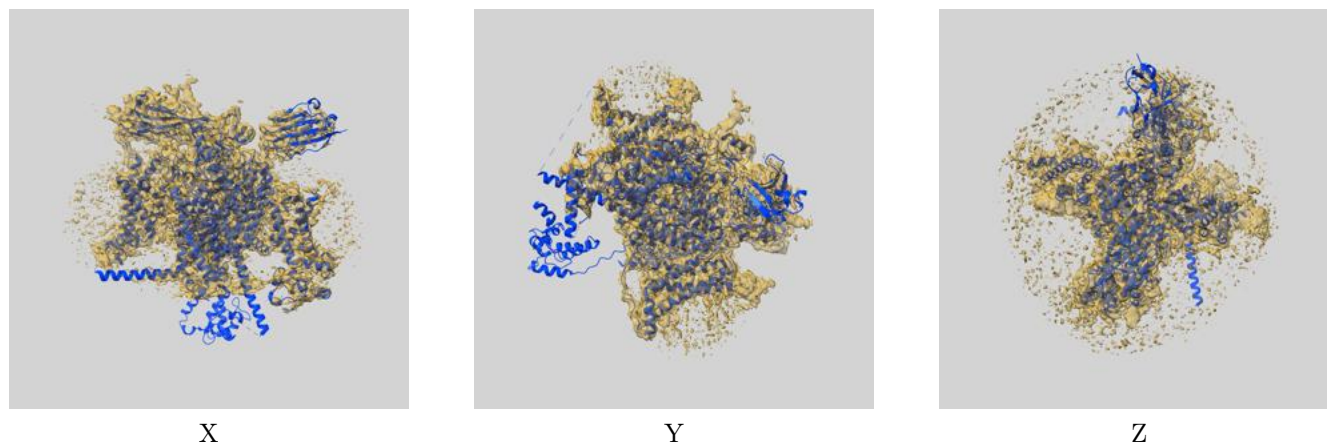
## 8 Fourier-Shell correlation

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-32370 and PDB model 7W9M. Per-residue inclusion information can be found in section [3](#) on page [10](#).

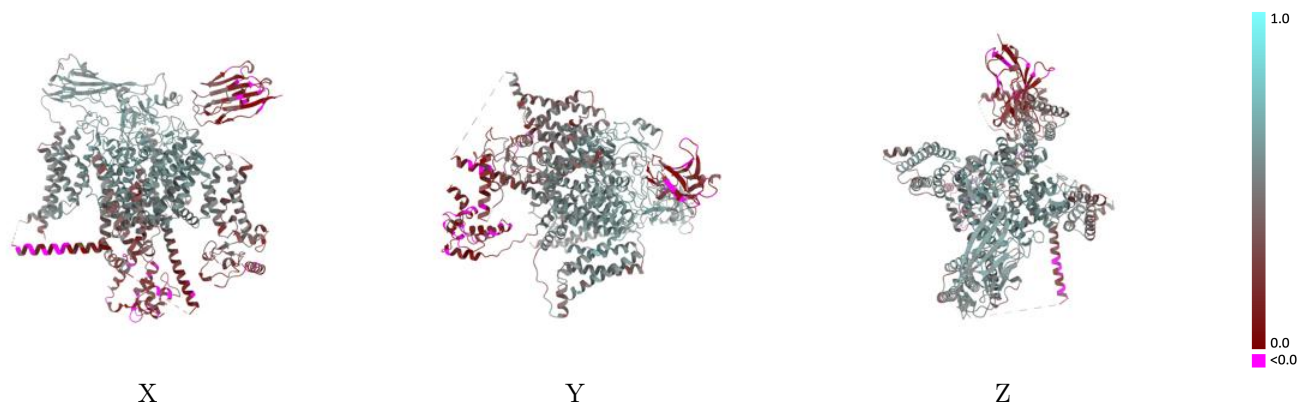
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.445 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.

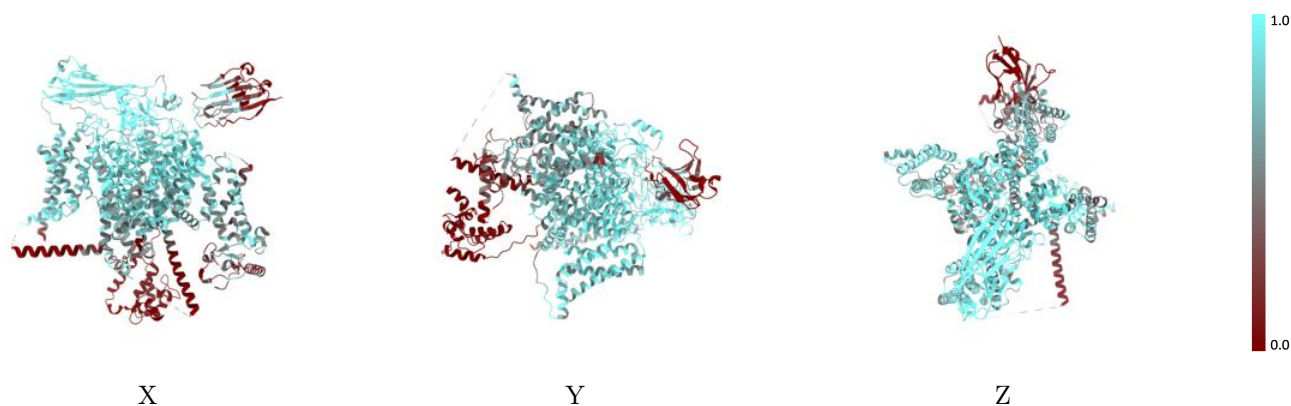


## 9.2 Q-score mapped to coordinate model [i](#)



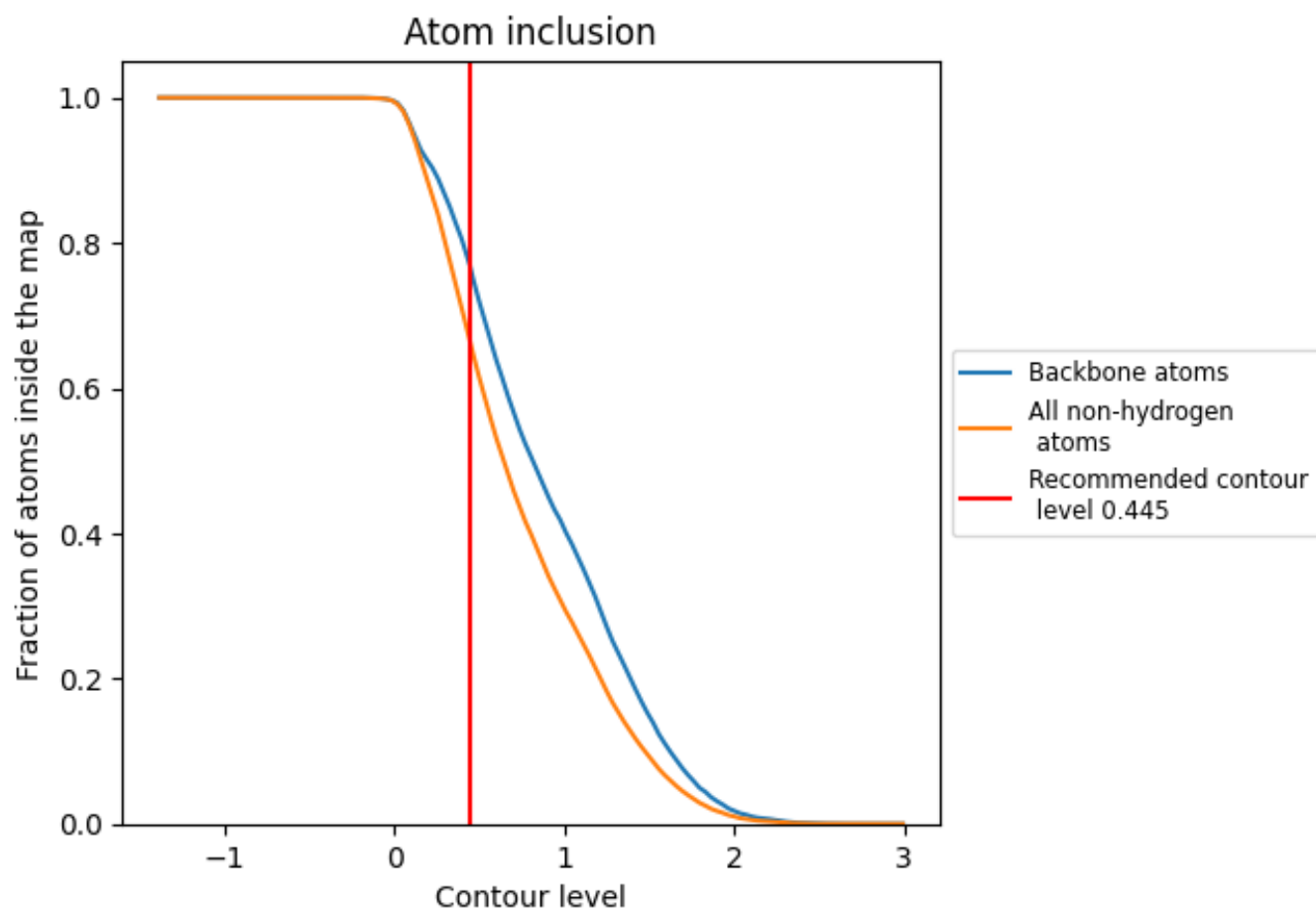
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.445).













## 9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 67% 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 (0.445) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6652	 0.4370
A	 0.6747	 0.4490
B	 0.8456	 0.5120
C	 0.2702	 0.1760
D	 0.6786	 0.4410
E	 0.8214	 0.3130

