



Full wwPDB EM Validation Report ⓘ

Nov 29, 2022 – 12:21 AM JST

PDB ID : 7VFB
EMDB ID : EMD-31960
Title : Human N-type voltage gated calcium channel CaV2.2-alpha2/delta1-beta1 complex, bound to PD173212
Authors : Dong, Y.; Gao, Y.; Wang, Y.; Zhao, Y.
Deposited on : 2021-09-13
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.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

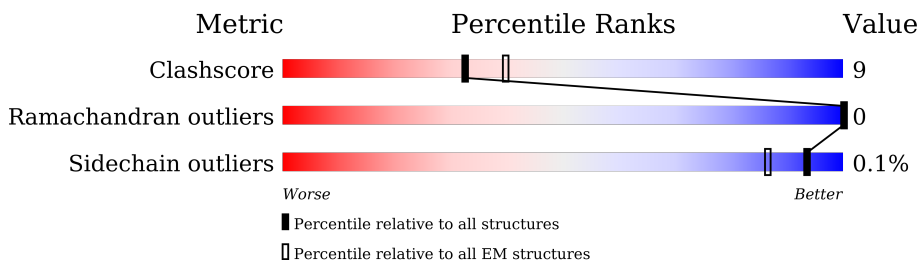
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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 ≥ 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	2339	
2	B	1103	
3	D	598	
4	C	3	
4	E	3	
5	F	3	

2 Entry composition i

There are 11 unique types of molecules in this entry. The entry contains 19776 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 Voltage-dependent N-type calcium channel subunit alpha-1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1266	Total	C	N	O	S	0	0
			10202	6715	1651	1771	65		

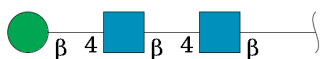
- Molecule 2 is a protein called Voltage-dependent calcium channel subunit alpha-2/delta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	955	Total	C	N	O	S	0	0
			7637	4842	1281	1483	31		

- Molecule 3 is a protein called Voltage-dependent L-type calcium channel subunit beta-1.

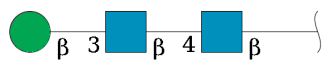
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	162	Total	C	N	O	S	0	0
			1259	805	217	232	5		

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



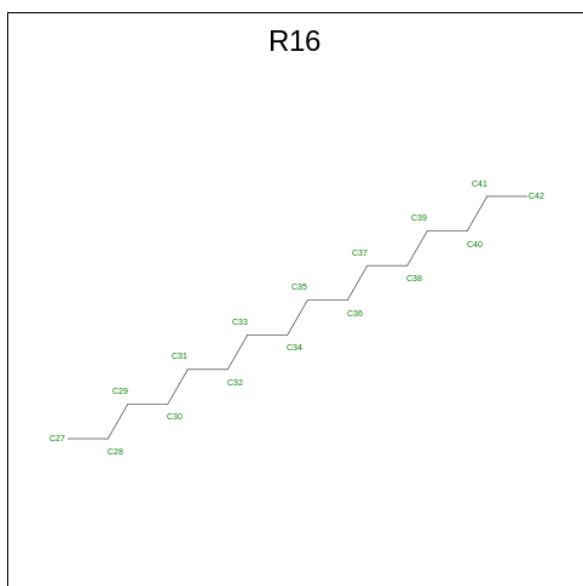
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	C	3	Total	C	N	O	0	0
			39	22	2	15		
4	E	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-3)-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
5	F	3	39	22	2	15	0	0

- Molecule 6 is HEXADECANE (three-letter code: R16) (formula: C₁₆H₃₄) (labeled as "Ligand of Interest" by depositor).



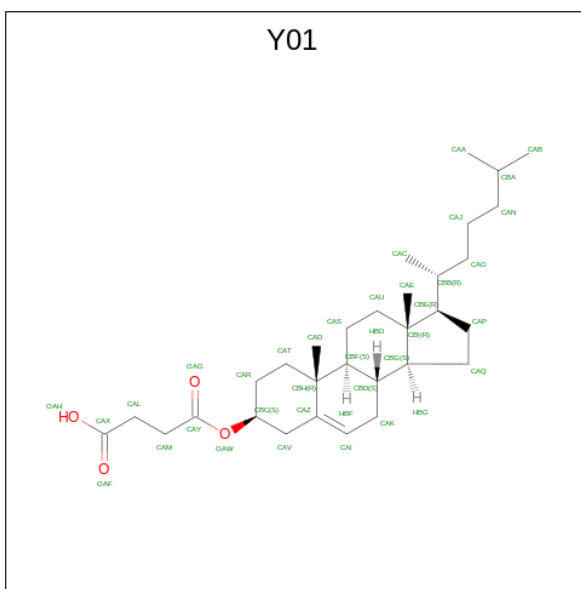
Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	C	0
			236	236	
6	A	1	Total	C	0
			236	236	
6	A	1	Total	C	0
			236	236	
6	A	1	Total	C	0
			236	236	
6	A	1	Total	C	0
			236	236	
6	A	1	Total	C	0
			236	236	
6	A	1	Total	C	0
			236	236	

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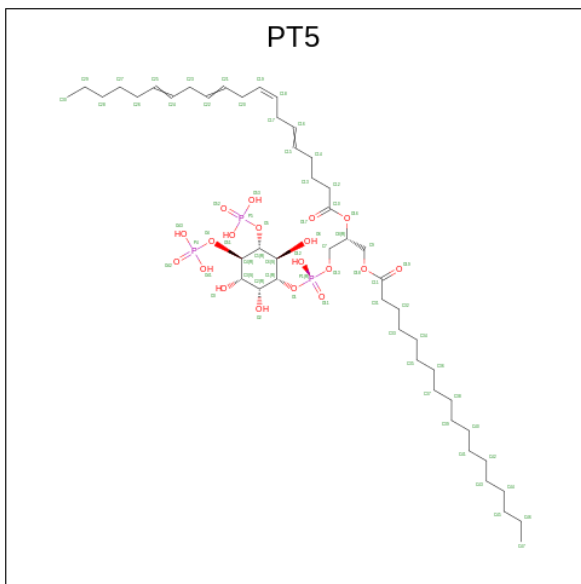
Mol	Chain	Residues	Atoms	AltConf
6	A	1	Total C 236 236	0
6	A	1	Total C 236 236	0
6	A	1	Total C 236 236	0
6	A	1	Total C 236 236	0
6	A	1	Total C 236 236	0
6	A	1	Total C 236 236	0
6	A	1	Total C 236 236	0
6	A	1	Total C 236 236	0

- Molecule 7 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: $C_{31}H_{50}O_4$) (labeled as "Ligand of Interest" by depositor).



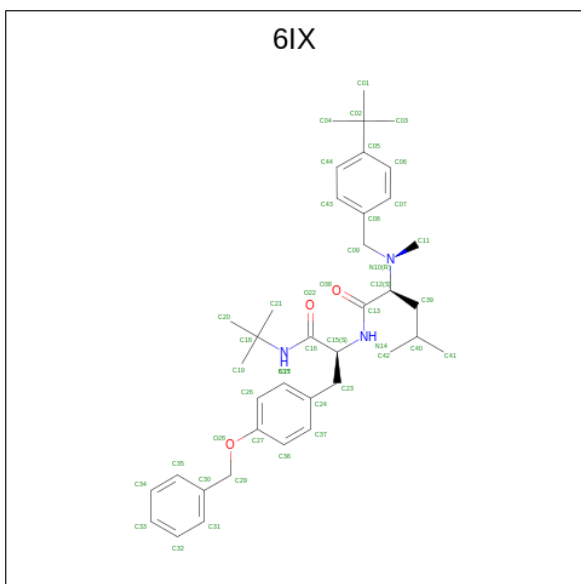
Mol	Chain	Residues	Atoms	AltConf
7	A	1	Total C O 105 93 12	0
7	A	1	Total C O 105 93 12	0
7	A	1	Total C O 105 93 12	0

- Molecule 8 is [(2R)-1-octadecanoyloxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonoxy-cyclohexyl]oxy-phosphoryloxy-propan-2-yl] (8Z)-icosa-5,8,11,14-tetraenoate (three-letter code: PT5) (formula: $C_{47}H_{85}O_{19}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf	
			Total	C	O		P
8	A	1	62	40	19	3	0

- Molecule 9 is (2 {S})- {N}-[(2 {S})-1-({tert}-butylamino)-1-oxidanylidene-3-(4-phenylmethoxyphenyl)propan-2-yl]-2-[(4- {tert}-butylphenyl)methyl-methyl-amino]-4-methyl-pentanamide (three-letter code: 6IX) (formula: $C_{38}H_{53}N_3O_3$) (labeled as "Ligand of Interest" by depositor).

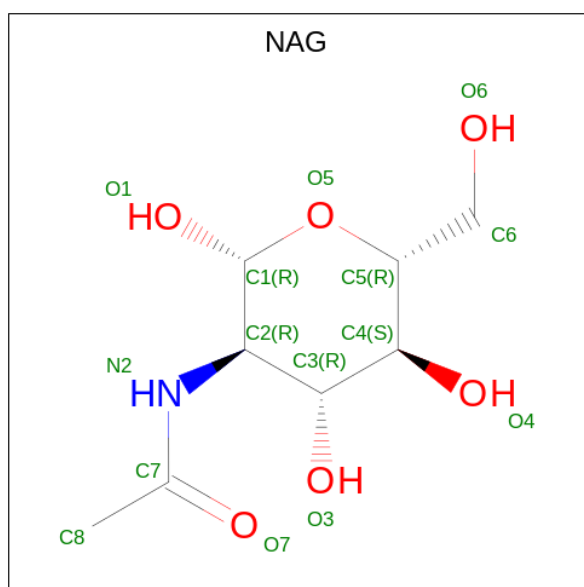


Mol	Chain	Residues	Atoms			AltConf	
			Total	C	N		O
9	A	1	44	38	3	3	0

- Molecule 10 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
10	A	1	1	1	0
10	B	1	1	1	0

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).

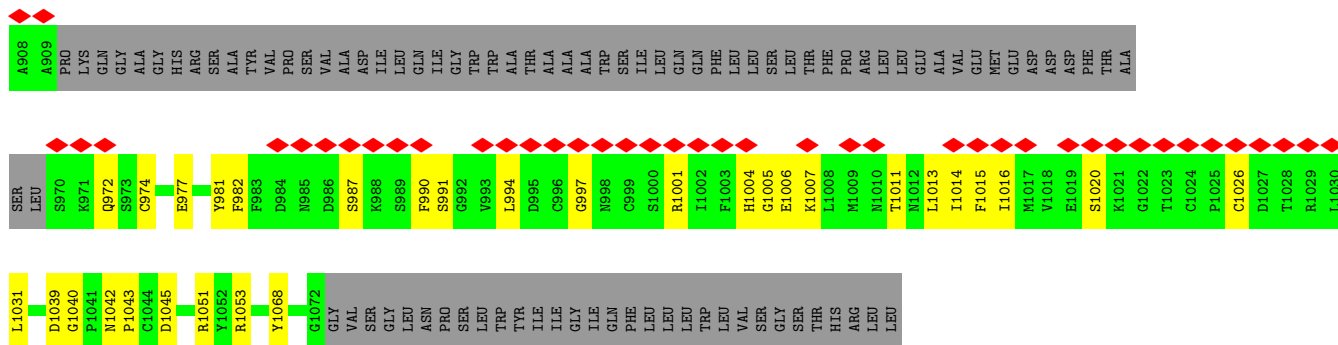


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
11	B	1	112	64	8	40	0
11	B	1	112	64	8	40	0
11	B	1	112	64	8	40	0
11	B	1	112	64	8	40	0
11	B	1	112	64	8	40	0
11	B	1	112	64	8	40	0

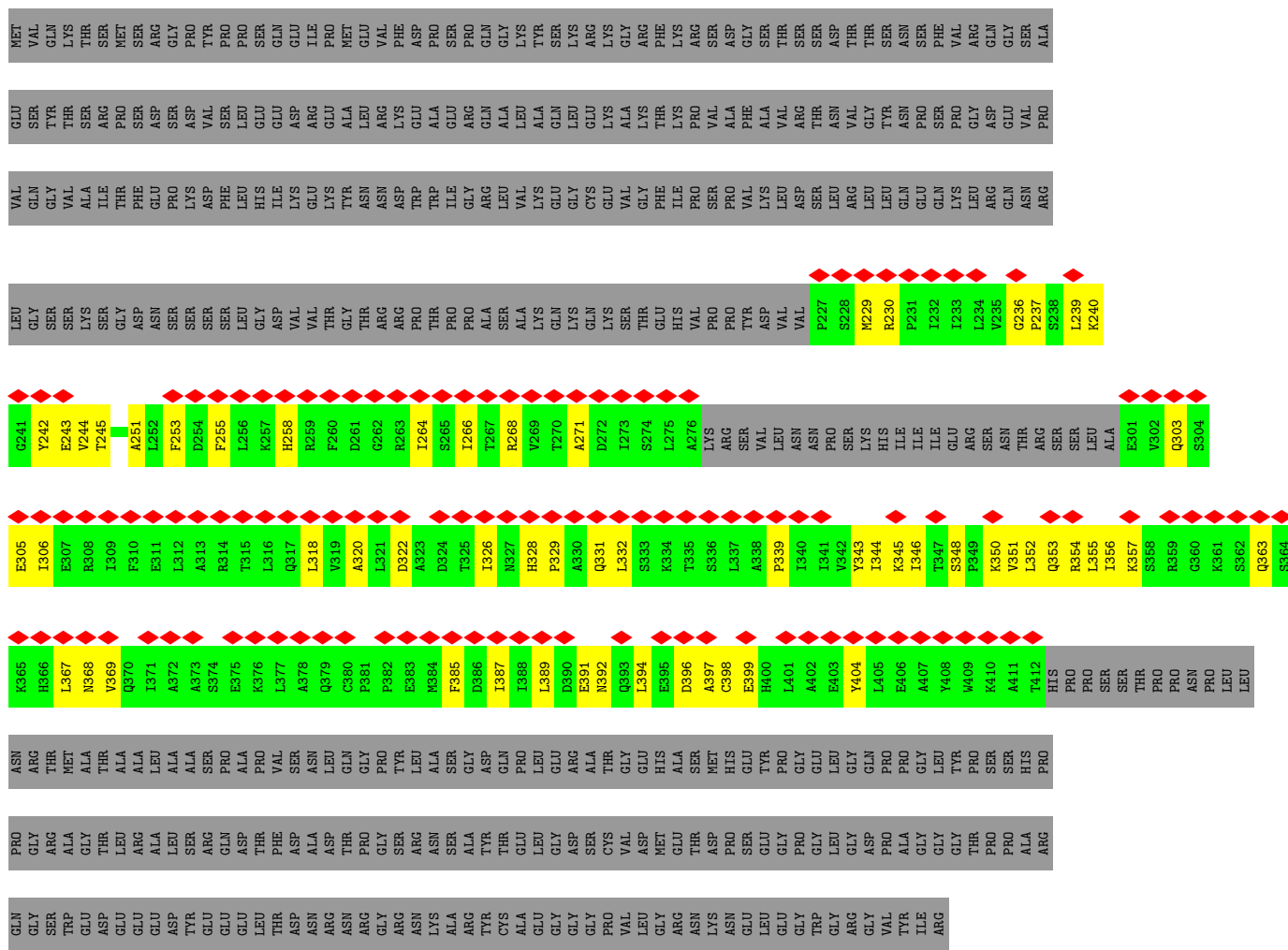
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
11	B	1	112	64	8	40	0
11	B	1	112	64	8	40	0



• Molecule 3: Voltage-dependent L-type calcium channel subunit beta-1



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





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

Chain E: 67% 33%



- Molecule 5: beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 67% 100% 33%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	224314	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	9.6	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	6.190	Depositor
Minimum map value	-3.334	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.110	Depositor
Recommended contour level	0.8	Depositor
Map size (\AA)	332.8, 332.8, 332.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.04, 1.04, 1.04	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: Y01, CA, PT5, NAG, 6IX, BMA, R16

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	0.30	0/10448	0.45	1/14152 (0.0%)
2	B	0.31	0/7799	0.48	0/10578
3	D	0.25	0/1280	0.47	0/1729
All	All	0.30	0/19527	0.46	1/26459 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	253	CYS	C-N-CA	9.44	145.29	121.70

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	10202	0	10177	174	0
2	B	7637	0	7426	147	0
3	D	1259	0	1254	45	0
4	C	39	0	34	0	0
4	E	39	0	34	2	0
5	F	39	0	34	0	0
6	A	236	0	474	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	105	0	147	8	0
8	A	62	0	63	7	0
9	A	44	0	0	1	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
11	B	112	0	104	3	0
All	All	19776	0	19747	366	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 9.

All (366) 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:1800:ARG:HD2	1:A:1821:LEU:HD11	1.58	0.85
3:D:243:GLU:H	3:D:363:GLN:HE22	1.26	0.82
2:B:85:ASP:HB3	2:B:500:LEU:HD22	1.65	0.79
2:B:994:LEU:HB3	2:B:1001:ARG:HB2	1.66	0.77
2:B:149:PHE:HB3	2:B:158:GLN:HB3	1.65	0.76
1:A:595:LEU:HB3	8:A:2420:PT5:H24	1.68	0.76
1:A:1706:VAL:O	1:A:1710:ASN:ND2	2.19	0.75
1:A:381:ILE:HD13	3:D:350:LYS:HD2	1.69	0.75
2:B:104:ALA:HB2	2:B:189:LEU:HD21	1.71	0.72
1:A:363:ARG:NH2	1:A:717:GLU:OE2	2.24	0.71
2:B:508:PRO:HG2	2:B:764:TYR:HE2	1.56	0.70
3:D:328:HIS:HB3	3:D:331:GLN:HB2	1.73	0.70
1:A:363:ARG:NH1	1:A:714:ASN:OD1	2.25	0.69
1:A:1400:PHE:HA	1:A:1404:PRO:HD2	1.74	0.69
1:A:1650:ARG:HH11	1:A:1660:ILE:HD11	1.58	0.68
3:D:240:LYS:NZ	3:D:326:ILE:O	2.27	0.68
3:D:244:VAL:HG21	3:D:356:ILE:HD13	1.76	0.68
3:D:353:GLN:HE22	3:D:357:LYS:HE2	1.59	0.68
2:B:508:PRO:HG2	2:B:764:TYR:CE2	2.29	0.67
2:B:751:ASN:O	2:B:753:GLN:NE2	2.30	0.65
2:B:644:TYR:O	2:B:647:THR:OG1	2.13	0.65
3:D:389:LEU:HD12	3:D:397:ALA:HB1	1.79	0.65
1:A:229:LEU:HB2	1:A:1585:ILE:HD11	1.78	0.65
2:B:57:LEU:HD23	2:B:798:VAL:HG11	1.78	0.65
1:A:1517:GLU:OE2	1:A:1521:LYS:NZ	2.20	0.64
3:D:229:MET:HE3	3:D:318:LEU:HA	1.79	0.64
2:B:90:LEU:HD12	2:B:615:THR:HG21	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:ASP:HA	1:A:191:LEU:HD23	1.79	0.64
2:B:423:THR:HG23	2:B:426:TYR:HE2	1.63	0.64
1:A:376:ARG:NH2	1:A:721:ASP:OD2	2.31	0.64
1:A:311:ILE:HD12	1:A:343:GLY:HA3	1.79	0.64
1:A:1262:ILE:HD11	1:A:1272:PHE:HB2	1.80	0.63
1:A:1403:PHE:HB2	1:A:1404:PRO:HD3	1.79	0.63
2:B:646:GLU:HA	2:B:649:LYS:NZ	2.13	0.63
2:B:224:VAL:HG23	2:B:225:ASP:H	1.63	0.63
1:A:1688:PHE:O	1:A:1692:ILE:HG12	1.99	0.63
1:A:1285:ILE:HG13	1:A:1414:LEU:HD11	1.81	0.63
2:B:237:ASP:OD2	2:B:424:GLN:NE2	2.32	0.63
2:B:368:ARG:HG2	2:B:398:PRO:HB3	1.80	0.63
2:B:204:LEU:HD13	2:B:456:LEU:HD13	1.81	0.62
1:A:1681:SER:HB2	6:A:2401:R16:H412	1.81	0.62
1:A:1304:PHE:HE1	1:A:1392:LEU:HD13	1.65	0.62
1:A:1613:TYR:O	1:A:1687:TYR:OH	2.16	0.61
2:B:36:TRP:HH2	2:B:829:SER:HA	1.66	0.61
1:A:119:PRO:HD2	2:B:263:SER:HA	1.82	0.61
1:A:1486:VAL:HG13	7:A:2410:Y01:HAC3	1.83	0.60
2:B:721:SER:O	2:B:724:LYS:HE3	2.01	0.60
2:B:105:GLU:OE2	2:B:442:LYS:NZ	2.33	0.60
1:A:285:GLU:OE2	1:A:1493:TYR:OH	2.18	0.60
1:A:715:ALA:O	1:A:719:THR:HG23	2.02	0.60
2:B:775:PHE:CD1	2:B:794:VAL:HG22	2.37	0.59
1:A:250:HIS:NE2	1:A:298:ASP:OD2	2.27	0.59
2:B:885:HIS:O	2:B:889:ILE:HD12	2.03	0.59
1:A:1165:ILE:HG23	7:A:2419:Y01:HAU2	1.83	0.59
1:A:108:ASN:ND2	1:A:198:ARG:HD3	2.18	0.59
1:A:596:ARG:HH21	8:A:2420:PT5:H2	1.66	0.59
1:A:1608:MET:O	1:A:1612:ILE:HG12	2.03	0.58
3:D:237:PRO:HG2	3:D:245:THR:HG23	1.85	0.58
1:A:1313:ASP:OD2	1:A:1339:ARG:NH2	2.35	0.58
1:A:135:PRO:HA	1:A:138:ILE:HG22	1.86	0.58
1:A:1752:MET:O	1:A:1756:MET:N	2.36	0.58
1:A:229:LEU:HD21	1:A:1589:LEU:HD21	1.86	0.58
1:A:1350:ASN:HD21	7:A:2404:Y01:HAR2	1.68	0.58
1:A:546:PHE:HB2	8:A:2420:PT5:H17	1.85	0.58
1:A:302:PHE:O	1:A:306:THR:HG23	2.04	0.58
1:A:485:TYR:OH	1:A:584:ARG:O	2.21	0.57
2:B:997:GLY:N	2:B:1026:CYS:SG	2.75	0.57
2:B:726:ILE:HB	2:B:729:VAL:HG22	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:LEU:O	1:A:106:ILE:HD12	2.05	0.57
2:B:128:LYS:NZ	2:B:234:ASP:OD2	2.36	0.56
1:A:85:ARG:HB3	1:A:89:LYS:NZ	2.19	0.56
2:B:57:LEU:HD13	2:B:715:LEU:HD22	1.87	0.56
2:B:713:ASN:HA	2:B:716:VAL:HG12	1.87	0.56
1:A:1161:ALA:O	1:A:1165:ILE:HG12	2.06	0.56
2:B:226:ASN:HB3	2:B:234:ASP:HB2	1.88	0.56
2:B:442:LYS:NZ	2:B:465:PRO:O	2.37	0.56
1:A:176:THR:HG21	1:A:194:VAL:HG11	1.86	0.56
1:A:1477:ILE:O	1:A:1481:ILE:HG12	2.06	0.56
1:A:529:MET:SD	1:A:554:ILE:HD11	2.47	0.55
1:A:1159:VAL:HG21	1:A:1193:VAL:HG11	1.87	0.55
1:A:1198:MET:O	1:A:1202:MET:HG2	2.06	0.55
1:A:213:LEU:HD13	1:A:615:LEU:HD13	1.88	0.55
2:B:646:GLU:HA	2:B:649:LYS:HZ3	1.70	0.55
2:B:896:LYS:HB3	2:B:977:GLU:OE2	2.06	0.55
2:B:994:LEU:N	2:B:1001:ARG:O	2.30	0.55
2:B:1042:ASN:ND2	2:B:1045:ASP:OD2	2.39	0.55
3:D:346:ILE:HD11	3:D:352:LEU:HD12	1.88	0.55
2:B:819:ASN:HA	2:B:822:ILE:HG22	1.89	0.54
1:A:285:GLU:HG3	1:A:286:TYR:H	1.72	0.54
1:A:122:ASP:HB2	2:B:262:GLY:HA3	1.90	0.54
1:A:1546:SER:OG	1:A:1574:ARG:NH1	2.39	0.54
2:B:537:PRO:HB3	2:B:972:GLN:HB2	1.89	0.54
2:B:100:LEU:HB3	2:B:488:MET:HE2	1.90	0.54
1:A:1223:ASP:OD1	1:A:1260:LYS:NZ	2.33	0.54
1:A:1228:SER:O	1:A:1232:VAL:HG23	2.07	0.54
1:A:1388:TYR:CD2	1:A:1389:ARG:HG3	2.43	0.54
1:A:566:ILE:HG22	1:A:567:LYS:HG3	1.90	0.54
2:B:884:ARG:HG3	2:B:1031:LEU:HD11	1.89	0.54
3:D:344:ILE:HA	3:D:389:LEU:HB2	1.89	0.54
1:A:292:PHE:O	1:A:679:VAL:HG11	2.07	0.54
1:A:299:ASN:HB3	1:A:302:PHE:HD2	1.73	0.53
2:B:296:SER:HA	2:B:332:ASP:HB2	1.90	0.53
2:B:604:ASN:OD1	11:B:1205:NAG:N2	2.41	0.53
3:D:268:ARG:HA	3:D:322:ASP:HB3	1.91	0.53
3:D:255:PHE:HA	3:D:258:HIS:CE1	2.43	0.53
1:A:1824:GLU:O	1:A:1828:VAL:HG22	2.09	0.53
2:B:772:ASN:HD21	2:B:1011:THR:N	2.05	0.53
2:B:128:LYS:HB3	2:B:227:SER:HA	1.91	0.53
3:D:391:GLU:HB2	3:D:397:ALA:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1248:LYS:O	1:A:1252:VAL:HG23	2.08	0.53
2:B:193:PHE:HB3	2:B:218:TYR:HB2	1.91	0.53
2:B:658:TYR:HD2	2:B:749:GLY:HA3	1.73	0.52
2:B:494:LEU:HD11	2:B:522:LEU:O	2.09	0.52
2:B:663:PRO:HD3	2:B:756:PRO:HB2	1.89	0.52
1:A:130:LEU:O	1:A:133:THR:HG22	2.09	0.52
1:A:1365:GLU:CD	1:A:1654:GLY:O	2.48	0.52
2:B:285:ASP:O	2:B:309:GLN:NE2	2.37	0.52
3:D:253:PHE:HE1	3:D:320:ALA:HB1	1.74	0.52
1:A:616:LEU:HD11	1:A:703:VAL:HG21	1.92	0.52
2:B:58:VAL:HG13	2:B:800:ILE:HG22	1.92	0.52
2:B:179:VAL:HG13	2:B:214:LEU:HD21	1.92	0.52
1:A:1650:ARG:NH1	1:A:1660:ILE:HD11	2.25	0.52
2:B:363:ASP:OD1	2:B:364:GLY:N	2.41	0.52
1:A:301:LEU:HB3	6:A:2408:R16:H322	1.92	0.52
2:B:160:SER:HB3	2:B:220:ALA:HB3	1.91	0.52
1:A:400:LEU:HD21	1:A:469:LYS:HB3	1.92	0.51
2:B:38:ASP:O	2:B:41:GLN:HG3	2.09	0.51
1:A:184:THR:OG1	1:A:187:ASP:OD2	2.28	0.51
2:B:511:TYR:OH	2:B:565:GLU:OE2	2.19	0.51
2:B:204:LEU:HD11	2:B:493:SER:HB2	1.92	0.51
2:B:407:LYS:HD2	2:B:1068:TYR:CE1	2.46	0.51
2:B:84:ARG:HG3	11:B:1206:NAG:H81	1.91	0.51
2:B:702:ILE:HA	2:B:705:VAL:HG12	1.92	0.51
2:B:74:ASN:ND2	2:B:77:GLN:OE1	2.43	0.51
2:B:562:LEU:HD12	2:B:1051:ARG:HE	1.76	0.51
2:B:59:ASP:O	2:B:63:LYS:HB2	2.10	0.51
1:A:1196:PHE:O	1:A:1200:ILE:HG12	2.11	0.50
2:B:667:CYS:HB2	2:B:670:LEU:HD13	1.93	0.50
2:B:514:ALA:HB3	2:B:522:LEU:HB3	1.92	0.50
2:B:103:GLU:HG2	2:B:192:VAL:HG21	1.92	0.50
2:B:185:TRP:HA	11:B:1209:NAG:H82	1.92	0.50
2:B:773:TYR:CE1	2:B:796:LYS:HD2	2.46	0.50
1:A:700:LEU:HD21	1:A:1405:PHE:CZ	2.47	0.50
1:A:285:GLU:HG3	1:A:286:TYR:N	2.26	0.50
1:A:1711:PHE:O	1:A:1715:THR:OG1	2.28	0.50
3:D:253:PHE:HZ	3:D:266:ILE:HG23	1.77	0.50
2:B:601:ASP:OD1	2:B:602:LYS:N	2.44	0.50
2:B:63:LYS:HD2	2:B:64:TYR:CZ	2.47	0.50
2:B:167:HIS:CE1	2:B:236:TYR:HD2	2.30	0.50
3:D:352:LEU:O	3:D:356:ILE:HG12	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:647:THR:HG21	2:B:713:ASN:HD22	1.75	0.49
3:D:391:GLU:HG2	3:D:396:ASP:HB3	1.94	0.49
2:B:592:VAL:HG11	2:B:605:ARG:HH21	1.77	0.49
1:A:1304:PHE:CE1	1:A:1392:LEU:HD13	2.47	0.49
1:A:1675:ASN:OD1	1:A:1676:ALA:N	2.46	0.49
2:B:36:TRP:O	2:B:39:LYS:HG2	2.13	0.49
2:B:631:ILE:O	2:B:704:ARG:NH1	2.46	0.49
1:A:317:THR:HG21	1:A:1650:ARG:HG3	1.93	0.49
1:A:660:LEU:O	1:A:697:ASN:ND2	2.44	0.49
3:D:253:PHE:CZ	3:D:266:ILE:HG23	2.48	0.49
3:D:387:ILE:HD11	3:D:404:TYR:CD1	2.48	0.48
2:B:709:ALA:O	2:B:742:ARG:NH1	2.45	0.48
1:A:1495:ALA:HB1	1:A:1499:TYR:HB3	1.95	0.48
1:A:1728:GLU:O	1:A:1732:VAL:HG23	2.13	0.48
2:B:66:ASP:N	2:B:66:ASP:OD1	2.45	0.48
1:A:1240:LYS:HG3	1:A:1242:LYS:H	1.79	0.48
1:A:1185:TYR:HA	1:A:1188:TYR:HD2	1.79	0.48
3:D:239:LEU:HD22	3:D:242:TYR:HE2	1.78	0.48
3:D:264:ILE:HG12	3:D:318:LEU:HB2	1.95	0.48
3:D:353:GLN:HG2	3:D:367:LEU:HD21	1.94	0.48
1:A:1255:VAL:HG12	1:A:1612:ILE:HG23	1.95	0.48
2:B:667:CYS:HA	2:B:697:CYS:CB	2.44	0.48
1:A:89:LYS:HA	1:A:92:THR:OG1	2.14	0.48
3:D:353:GLN:HG2	3:D:367:LEU:HD11	1.94	0.48
1:A:1367:TRP:N	1:A:1368:PRO:HD2	2.28	0.48
2:B:37:VAL:HG21	2:B:1006:GLU:HB3	1.94	0.48
2:B:987:SER:HB3	2:B:990:PHE:CZ	2.48	0.48
1:A:392:ILE:HD11	3:D:355:LEU:HD21	1.95	0.47
2:B:716:VAL:HG23	2:B:720:TRP:HE3	1.79	0.47
2:B:261:SER:O	2:B:327:ALA:HB1	2.14	0.47
1:A:108:ASN:HD21	1:A:198:ARG:HH11	1.62	0.47
1:A:1396:TYR:O	1:A:1400:PHE:HD2	1.97	0.47
1:A:388:TYR:CE1	3:D:392:ASN:HA	2.48	0.47
1:A:1258:PRO:O	1:A:1261:THR:HG22	2.14	0.47
1:A:1481:ILE:O	1:A:1485:THR:HG23	2.15	0.47
1:A:1538:PHE:O	1:A:1542:THR:HG23	2.14	0.47
2:B:109:ALA:HB2	2:B:469:ILE:HG23	1.95	0.47
1:A:1255:VAL:O	1:A:1258:PRO:HD2	2.14	0.47
1:A:584:ARG:NH2	8:A:2420:PT5:O53	2.44	0.47
2:B:481:ASN:OD1	4:E:1:NAG:O6	2.28	0.47
2:B:507:CYS:HG	2:B:626:TYR:HE1	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:147:PRO:HB3	2:B:163:HIS:NE2	2.29	0.47
1:A:591:TYR:HB3	1:A:1284:ASN:ND2	2.31	0.47
2:B:295:ASN:ND2	2:B:328:LYS:O	2.30	0.47
2:B:396:ARG:O	2:B:400:GLN:HG3	2.15	0.46
3:D:368:ASN:OD1	3:D:369:VAL:N	2.45	0.46
1:A:1247:ILE:O	1:A:1251:ARG:HG2	2.14	0.46
2:B:224:VAL:HG23	2:B:225:ASP:N	2.30	0.46
1:A:599:VAL:HG11	8:A:2420:PT5:H15	1.97	0.46
2:B:157:ARG:NH2	2:B:222:PRO:O	2.49	0.46
2:B:218:TYR:HB3	2:B:219:PRO:HD3	1.97	0.46
2:B:352:ALA:O	2:B:354:CYS:N	2.49	0.46
1:A:294:ILE:HG12	1:A:679:VAL:HG12	1.96	0.46
2:B:280:LEU:HA	2:B:283:LEU:HD12	1.97	0.46
2:B:508:PRO:HG3	2:B:759:TYR:CD1	2.50	0.46
3:D:332:LEU:HD23	3:D:332:LEU:O	2.15	0.46
1:A:1481:ILE:HD13	1:A:1514:PHE:CZ	2.51	0.46
2:B:114:ARG:NH1	2:B:116:ASP:O	2.49	0.46
2:B:710:GLY:O	2:B:714:GLU:HG3	2.15	0.46
2:B:193:PHE:HB3	2:B:218:TYR:CG	2.51	0.46
7:A:2419:Y01:HAS2	7:A:2419:Y01:HAE1	1.82	0.45
3:D:348:SER:O	3:D:351:VAL:HG22	2.16	0.45
1:A:546:PHE:HZ	1:A:581:ARG:HA	1.81	0.45
1:A:1173:VAL:HG13	1:A:1174:ARG:HG3	1.98	0.45
1:A:1628:ASP:OD2	1:A:1634:ARG:NH2	2.49	0.45
2:B:667:CYS:HA	2:B:697:CYS:HB2	1.98	0.45
1:A:395:ALA:HB2	3:D:251:ALA:HB2	1.97	0.45
1:A:465:ARG:O	1:A:468:GLU:HG3	2.16	0.45
2:B:596:ASP:OD1	2:B:596:ASP:N	2.50	0.45
2:B:881:SER:OG	2:B:1026:CYS:O	2.34	0.45
1:A:307:VAL:O	1:A:311:ILE:HG12	2.17	0.45
1:A:683:MET:HB3	6:A:2408:R16:H332	1.99	0.45
1:A:1717:ASP:OD1	1:A:1718:SER:N	2.50	0.45
7:A:2410:Y01:HAE2	6:A:2411:R16:H322	1.98	0.45
1:A:1219:TRP:HE1	1:A:1269:LYS:HE3	1.82	0.45
1:A:299:ASN:OD1	1:A:300:ILE:N	2.47	0.45
1:A:1402:VAL:O	1:A:1406:PHE:HB3	2.17	0.45
2:B:50:THR:O	2:B:719:TYR:OH	2.29	0.45
1:A:1595:SER:CB	1:A:1710:ASN:HD21	2.30	0.45
1:A:1297:ALA:O	1:A:1301:VAL:HG23	2.17	0.45
1:A:252:ALA:HB2	1:A:287:TRP:CE3	2.52	0.44
1:A:377:ARG:HA	1:A:377:ARG:HD2	1.84	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:673:ILE:HD11	1:A:686:SER:HB3	2.00	0.44
2:B:398:PRO:O	2:B:402:MET:HG3	2.17	0.44
2:B:423:THR:CG2	2:B:426:TYR:HE2	2.28	0.44
2:B:860:LEU:HD12	2:B:860:LEU:HA	1.87	0.44
2:B:1001:ARG:HE	2:B:1020:SER:HB3	1.82	0.44
1:A:660:LEU:HD22	1:A:696:GLY:HA3	1.97	0.44
7:A:2404:Y01:HAP1	7:A:2404:Y01:HAO2	1.61	0.44
2:B:569:ASP:O	2:B:573:GLU:HG3	2.17	0.44
1:A:218:LYS:HB3	1:A:218:LYS:HE3	1.72	0.44
1:A:337:ILE:HD13	6:A:2415:R16:H301	1.98	0.44
2:B:112:GLN:OE1	2:B:112:GLN:N	2.46	0.44
2:B:1007:LYS:HA	2:B:1014:ILE:HA	1.99	0.44
1:A:1405:PHE:O	1:A:1409:ASN:ND2	2.48	0.44
1:A:1519:VAL:O	1:A:1522:ILE:HG22	2.18	0.44
2:B:660:PHE:HB2	2:B:741:THR:CG2	2.48	0.44
2:B:735:VAL:HG22	2:B:741:THR:OG1	2.17	0.44
1:A:181:THR:O	1:A:181:THR:HG22	2.18	0.44
1:A:720:LYS:HD2	1:A:769:GLU:OE2	2.18	0.44
2:B:494:LEU:HD12	2:B:494:LEU:HA	1.85	0.44
1:A:108:ASN:HD21	1:A:198:ARG:NH1	2.16	0.44
1:A:640:GLU:HG2	1:A:641:THR:N	2.33	0.44
1:A:1721:LEU:H	1:A:1721:LEU:HD23	1.83	0.44
1:A:85:ARG:HB3	1:A:89:LYS:HZ3	1.81	0.43
1:A:616:LEU:O	1:A:620:ILE:HG13	2.18	0.43
2:B:780:PHE:CE1	2:B:870:GLN:HA	2.53	0.43
1:A:294:ILE:CG1	1:A:679:VAL:HG12	2.48	0.43
2:B:828:THR:HG22	2:B:831:ARG:HH21	1.82	0.43
3:D:271:ALA:HB3	3:D:305:GLU:OE2	2.18	0.43
1:A:154:PHE:HD1	1:A:155:VAL:HG13	1.83	0.43
1:A:399:MET:HG2	1:A:403:GLU:OE1	2.18	0.43
2:B:753:GLN:NE2	2:B:785:PRO:HG2	2.33	0.43
2:B:1039:ASP:OD1	2:B:1040:GLY:N	2.51	0.43
3:D:255:PHE:CE2	3:D:398:CYS:HB3	2.53	0.43
1:A:1519:VAL:O	1:A:1523:ILE:HG12	2.18	0.43
6:A:2401:R16:H411	6:A:2401:R16:H382	1.80	0.43
1:A:1289:TYR:CE1	1:A:1403:PHE:HD2	2.35	0.43
1:A:1496:PRO:O	1:A:1497:TYR:HB3	2.18	0.43
2:B:882:LEU:HD21	2:B:1016:ILE:HG21	2.00	0.43
1:A:496:THR:HA	1:A:499:VAL:HG22	1.99	0.43
1:A:657:PHE:O	1:A:661:THR:HG23	2.18	0.43
1:A:1359:PHE:O	1:A:1363:THR:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:432:ARG:HB2	2:B:433:PRO:HD3	2.01	0.43
2:B:470:THR:HG21	4:E:1:NAG:H5	2.00	0.43
2:B:635:LEU:HD23	2:B:635:LEU:HA	1.87	0.43
2:B:798:VAL:HG23	2:B:809:PRO:HD2	2.00	0.43
1:A:119:PRO:HG3	1:A:636:ASN:OD1	2.19	0.43
1:A:391:TRP:NE1	3:D:394:LEU:HD13	2.33	0.43
1:A:594:SER:HA	1:A:719:THR:HG21	2.00	0.43
1:A:1609:LEU:HD22	1:A:1698:LEU:HD22	2.00	0.43
2:B:392:HIS:HE1	2:B:396:ARG:HE	1.67	0.43
1:A:112:LEU:HD21	1:A:195:ARG:NE	2.34	0.43
3:D:230:ARG:NH2	3:D:339:PRO:O	2.52	0.43
1:A:484:PHE:HA	1:A:487:VAL:HG12	2.00	0.43
2:B:892:TYR:HA	2:B:982:PHE:O	2.19	0.43
2:B:994:LEU:HD22	2:B:1001:ARG:HD3	2.00	0.42
3:D:353:GLN:NE2	3:D:357:LYS:HE2	2.31	0.42
1:A:1457:ARG:HA	1:A:1462:TYR:HB2	2.01	0.42
1:A:1519:VAL:HA	1:A:1522:ILE:HG22	2.00	0.42
2:B:261:SER:O	2:B:264:VAL:HG22	2.19	0.42
1:A:1591:THR:HG22	1:A:1710:ASN:OD1	2.19	0.42
2:B:860:LEU:HD22	2:B:1013:LEU:HD21	2.02	0.42
3:D:387:ILE:HD11	3:D:404:TYR:CE1	2.54	0.42
7:A:2419:Y01:HAC3	7:A:2419:Y01:HAJ2	1.90	0.42
2:B:208:PHE:HD1	2:B:488:MET:SD	2.41	0.42
1:A:1515:SER:O	1:A:1519:VAL:HG23	2.20	0.42
1:A:1840:LEU:O	1:A:1844:HIS:N	2.48	0.42
6:A:2401:R16:H352	6:A:2403:R16:H362	2.01	0.42
2:B:37:VAL:HA	2:B:40:MET:HG2	2.01	0.42
2:B:537:PRO:HD3	2:B:974:CYS:HB3	2.00	0.42
3:D:354:ARG:HE	3:D:354:ARG:HB3	1.71	0.42
1:A:176:THR:CG2	1:A:194:VAL:HG11	2.50	0.42
2:B:241:ARG:HD2	2:B:241:ARG:HA	1.80	0.42
2:B:991:SER:HB3	2:B:1004:HIS:ND1	2.35	0.42
1:A:650:PRO:O	1:A:653:ILE:HG22	2.19	0.42
8:A:2420:PT5:H52	8:A:2420:PT5:H18	1.75	0.42
2:B:306:HIS:CG	2:B:349:VAL:HG11	2.54	0.42
1:A:229:LEU:HD22	1:A:1585:ILE:HD11	2.02	0.42
1:A:314:GLU:HG3	1:A:665:TRP:CD1	2.55	0.42
1:A:723:GLU:O	1:A:727:GLU:OE1	2.37	0.42
3:D:303:GLN:HA	3:D:306:ILE:HD13	2.01	0.42
1:A:157:HIS:C	1:A:159:GLY:H	2.23	0.42
1:A:712:LEU:HD12	1:A:1413:ALA:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:771:ARG:HA	1:A:771:ARG:HD2	1.87	0.42
3:D:236:GLY:N	3:D:237:PRO:HD2	2.35	0.42
1:A:132:ASP:O	1:A:135:PRO:HD2	2.20	0.42
1:A:176:THR:HG23	1:A:191:LEU:HD12	2.01	0.42
1:A:262:PRO:HG3	1:A:287:TRP:CD1	2.55	0.42
2:B:93:ARG:HB2	2:B:446:TRP:HH2	1.85	0.42
1:A:1156:ILE:HD13	1:A:1156:ILE:HA	1.93	0.41
7:A:2410:Y01:HAS2	7:A:2410:Y01:HAE1	1.87	0.41
2:B:52:SER:OG	2:B:814:ILE:HG12	2.20	0.41
2:B:258:VAL:HG12	2:B:260:VAL:HG13	2.01	0.41
2:B:645:SER:HB3	2:B:687:ILE:HG21	2.02	0.41
1:A:1646:MET:HB2	6:A:2415:R16:H341	2.01	0.41
2:B:671:LYS:HD3	2:B:671:LYS:HA	1.82	0.41
3:D:343:TYR:CE2	3:D:345:LYS:HD2	2.56	0.41
2:B:193:PHE:CG	2:B:218:TYR:HB2	2.55	0.41
2:B:396:ARG:HD3	2:B:410:TYR:OH	2.21	0.41
2:B:735:VAL:HB	2:B:811:VAL:HG12	2.02	0.41
3:D:306:ILE:H	3:D:306:ILE:HD12	1.85	0.41
3:D:396:ASP:O	3:D:399:GLU:HG3	2.21	0.41
1:A:1565:SER:HB3	1:A:1568:ARG:HH11	1.85	0.41
1:A:1672:GLU:OE1	1:A:1672:GLU:N	2.49	0.41
2:B:752:TRP:NE1	2:B:754:GLU:HB2	2.35	0.41
3:D:329:PRO:HG3	3:D:385:PHE:CZ	2.56	0.41
1:A:676:GLN:HB3	6:A:2407:R16:H382	2.01	0.41
2:B:33:ILE:HA	2:B:36:TRP:HB3	2.02	0.41
2:B:168:ILE:HG12	2:B:214:LEU:CD2	2.50	0.41
1:A:207:PRO:HA	1:A:210:GLN:HG3	2.03	0.41
1:A:1222:LEU:HA	1:A:1225:ILE:HG12	2.03	0.41
2:B:472:GLN:O	2:B:473:PHE:HB2	2.21	0.41
1:A:591:TYR:HB3	1:A:1284:ASN:HD21	1.85	0.41
1:A:1487:VAL:HG21	1:A:1510:PHE:HE2	1.85	0.41
1:A:1721:LEU:HD22	1:A:1802:ALA:HB1	2.02	0.41
2:B:289:VAL:HG12	2:B:310:ALA:HB2	2.03	0.41
2:B:317:VAL:HG21	2:B:1043:PRO:HG2	2.03	0.41
2:B:856:GLY:HA2	2:B:981:TYR:HB2	2.02	0.41
1:A:108:ASN:HD21	1:A:198:ARG:HD3	1.85	0.41
1:A:1583:TYR:O	1:A:1587:ILE:HG12	2.21	0.41
1:A:1818:ASP:HA	1:A:1821:LEU:HD12	2.02	0.41
1:A:493:ALA:HB2	1:A:582:LEU:HD21	2.03	0.40
1:A:1181:ASN:O	1:A:1184:LYS:HG2	2.21	0.40
2:B:653:PHE:CZ	2:B:659:THR:HB	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1005:GLY:HA2	2:B:1015:PHE:O	2.20	0.40
1:A:295:THR:HA	1:A:306:THR:HG22	2.03	0.40
1:A:391:TRP:CD1	3:D:394:LEU:HD13	2.57	0.40
2:B:186:THR:HG22	2:B:189:LEU:HD12	2.03	0.40
2:B:421:ILE:O	2:B:425:GLU:HG3	2.22	0.40
3:D:387:ILE:HD13	3:D:387:ILE:HA	1.88	0.40
1:A:1289:TYR:CE1	9:A:2421:6IX:C33	3.03	0.40
1:A:1367:TRP:CD1	1:A:1368:PRO:HD3	2.57	0.40
1:A:1406:PHE:CD1	8:A:2420:PT5:H47	2.57	0.40
1:A:1305:LYS:HE2	1:A:1305:LYS:HB3	1.92	0.40
1:A:1473:PHE:O	1:A:1477:ILE:HG12	2.21	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	1248/2339 (53%)	1192 (96%)	56 (4%)	0	100	100
2	B	947/1103 (86%)	898 (95%)	49 (5%)	0	100	100
3	D	158/598 (26%)	152 (96%)	6 (4%)	0	100	100
All	All	2353/4040 (58%)	2242 (95%)	111 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1089/1991 (55%)	1087 (100%)	2 (0%)	93	98
2	B	846/971 (87%)	845 (100%)	1 (0%)	93	98
3	D	131/510 (26%)	131 (100%)	0	100	100
All	All	2066/3472 (60%)	2063 (100%)	3 (0%)	93	98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	495	ASN
1	A	1484	ASN
2	B	1053	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
2	B	392	HIS
3	D	328	HIS
3	D	353	GLN
3	D	363	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](#)

9 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	C	1	4,2	14,14,15	0.33	0	17,19,21	0.52	0
4	NAG	C	2	4	14,14,15	0.19	0	17,19,21	0.45	0
4	BMA	C	3	4	11,11,12	0.60	0	15,15,17	0.75	0
4	NAG	E	1	4,2	14,14,15	0.42	0	17,19,21	0.48	0
4	NAG	E	2	4	14,14,15	0.19	0	17,19,21	0.54	0
4	BMA	E	3	4	11,11,12	0.58	0	15,15,17	0.68	0
5	NAG	F	1	5,2	14,14,15	0.79	1 (7%)	17,19,21	0.99	1 (5%)
5	NAG	F	2	5	14,14,15	0.29	0	17,19,21	0.45	0
5	BMA	F	3	5	11,11,12	0.63	0	15,15,17	0.80	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	C	1	4,2	-	2/6/23/26	0/1/1/1
4	NAG	C	2	4	-	0/6/23/26	0/1/1/1
4	BMA	C	3	4	-	0/2/19/22	0/1/1/1
4	NAG	E	1	4,2	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	BMA	E	3	4	-	2/2/19/22	0/1/1/1
5	NAG	F	1	5,2	-	2/6/23/26	0/1/1/1
5	NAG	F	2	5	-	1/6/23/26	0/1/1/1
5	BMA	F	3	5	-	1/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	1	NAG	O5-C1	2.71	1.48	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	1	NAG	C1-O5-C5	3.84	117.40	112.19

There are no chirality outliers.

All (12) torsion outliers are listed below:

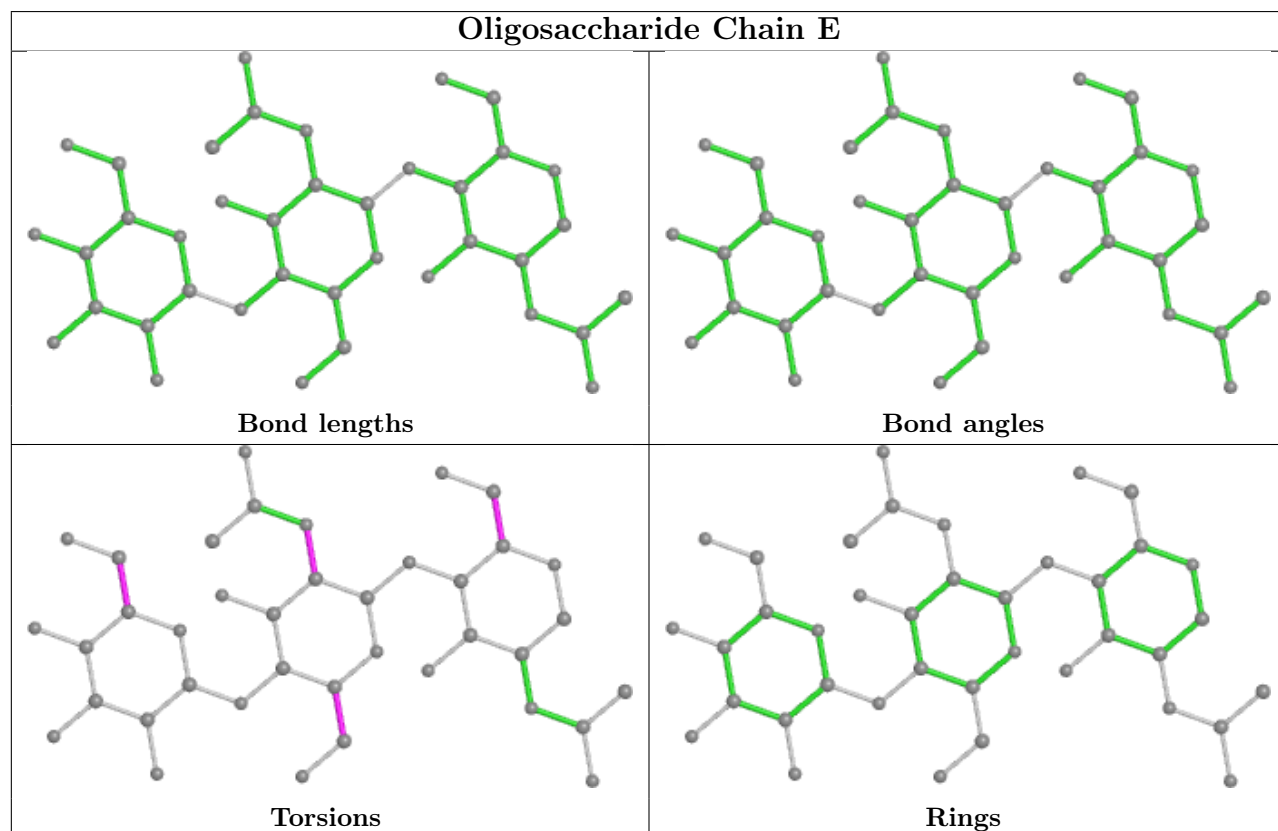
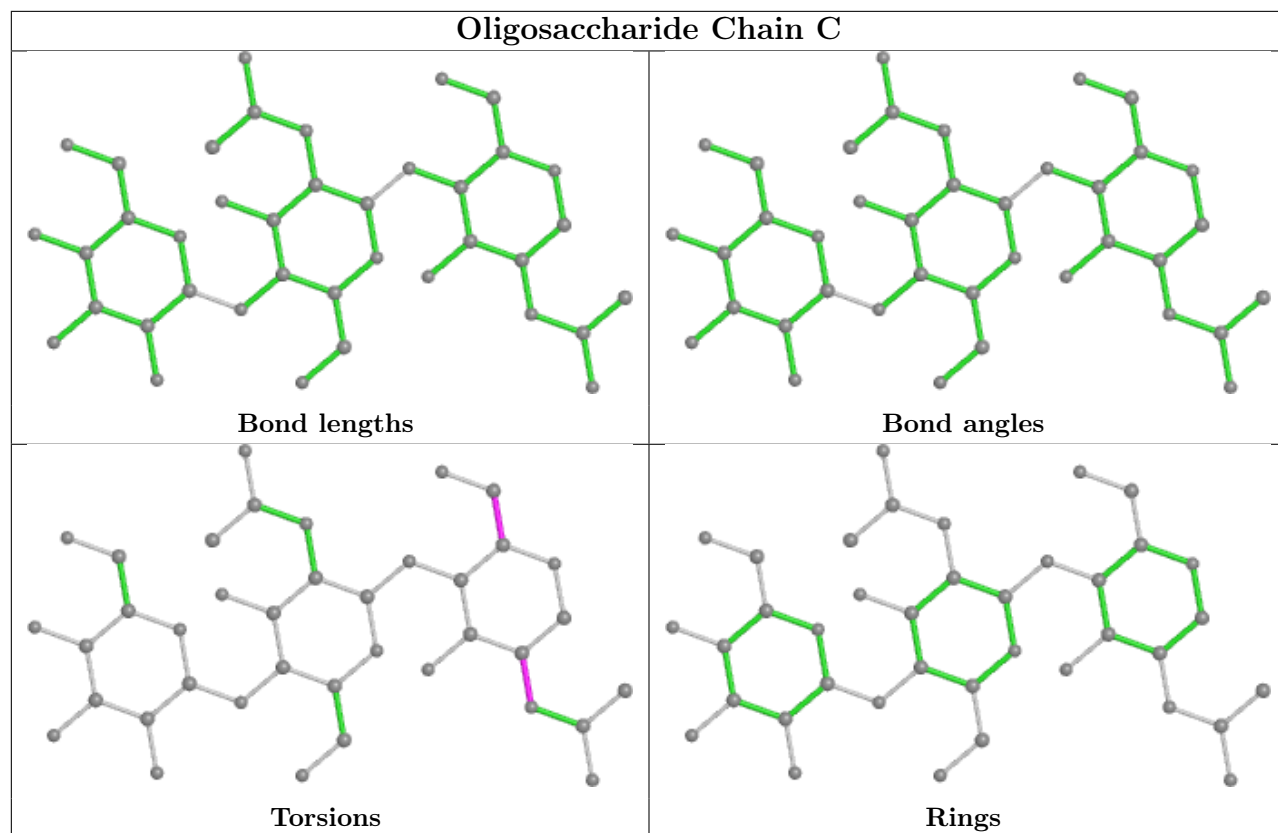
Mol	Chain	Res	Type	Atoms
4	E	1	NAG	O5-C5-C6-O6
5	F	1	NAG	O5-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
4	E	3	BMA	O5-C5-C6-O6
5	F	1	NAG	C4-C5-C6-O6
4	E	3	BMA	C4-C5-C6-O6
4	C	1	NAG	O5-C5-C6-O6
5	F	3	BMA	O5-C5-C6-O6
5	F	2	NAG	O5-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
4	E	2	NAG	C3-C2-N2-C7
4	C	1	NAG	C3-C2-N2-C7

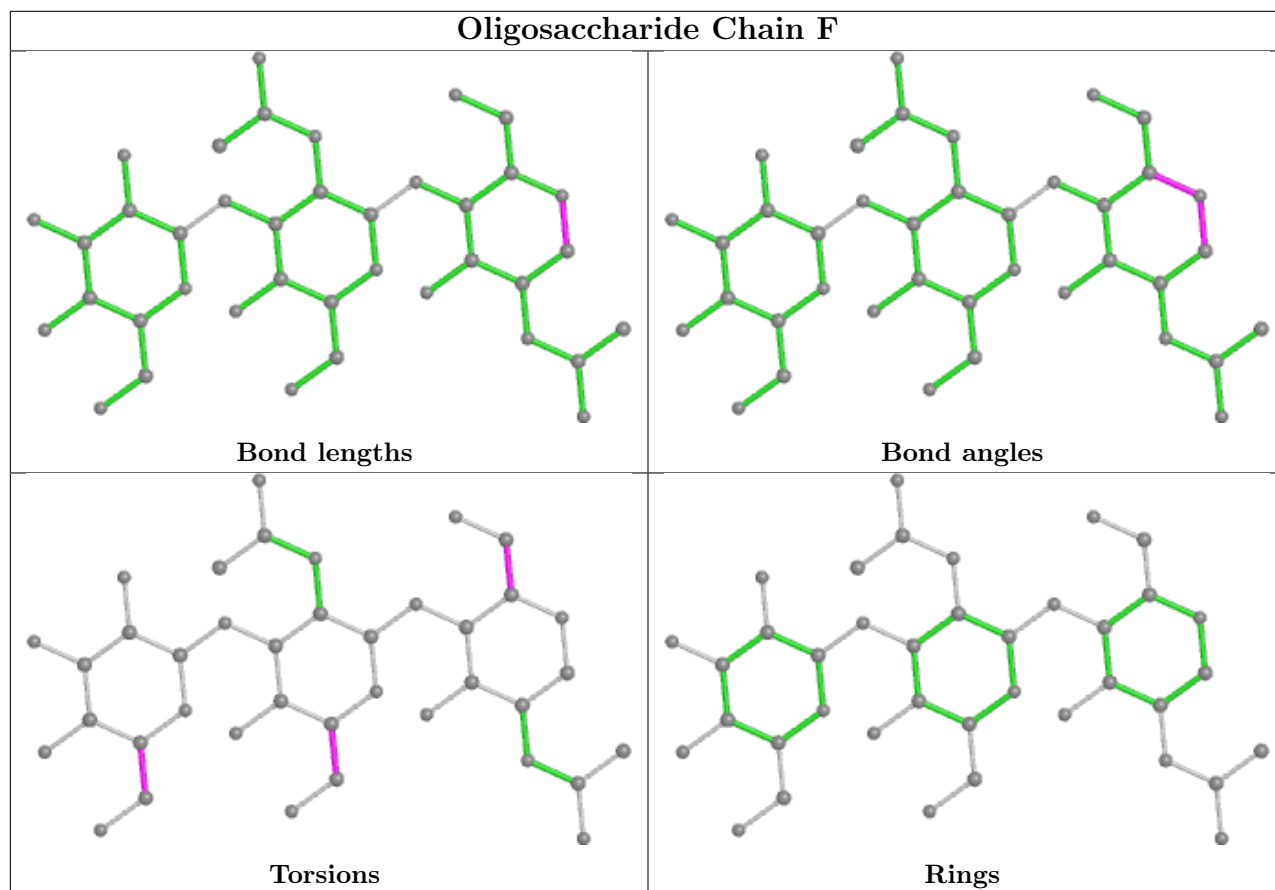
There are no ring outliers.

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](#)

Of 31 ligands modelled in this entry, 2 are monoatomic - leaving 29 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	$\# Z > 2$
6	R16	A	2401	-	15,15,15	0.11	0	14,14,14	0.20	0
11	NAG	B	1209	2	14,14,15	0.21	0	17,19,21	0.50	0
6	R16	A	2406	-	15,15,15	0.12	0	14,14,14	0.17	0
6	R16	A	2417	-	15,15,15	0.12	0	14,14,14	0.19	0
7	Y01	A	2404	-	38,38,38	4.00	12 (31%)	57,57,57	2.12	19 (33%)
11	NAG	B	1207	2	14,14,15	0.20	0	17,19,21	0.40	0
11	NAG	B	1208	2	14,14,15	0.24	0	17,19,21	0.53	0
7	Y01	A	2419	-	38,38,38	4.00	12 (31%)	57,57,57	2.12	17 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	R16	A	2415	-	14,14,15	0.11	0	13,13,14	0.25	0
6	R16	A	2416	-	12,12,15	0.11	0	11,11,14	0.20	0
11	NAG	B	1202	2	14,14,15	0.22	0	17,19,21	0.48	0
9	6IX	A	2421	1	45,46,46	1.99	6 (13%)	61,65,65	0.89	2 (3%)
6	R16	A	2403	-	15,15,15	0.10	0	14,14,14	0.17	0
6	R16	A	2418	-	15,15,15	0.11	0	14,14,14	0.20	0
6	R16	A	2402	-	15,15,15	0.11	0	14,14,14	0.20	0
6	R16	A	2408	-	15,15,15	0.10	0	14,14,14	0.20	0
6	R16	A	2412	-	14,14,15	0.11	0	13,13,14	0.18	0
6	R16	A	2413	-	12,12,15	0.10	0	11,11,14	0.20	0
6	R16	A	2409	-	10,10,15	0.10	0	9,9,14	0.20	0
11	NAG	B	1205	2	14,14,15	0.34	0	17,19,21	0.49	0
6	R16	A	2411	-	12,12,15	0.09	0	11,11,14	0.18	0
8	PT5	A	2420	-	62,62,69	1.46	10 (16%)	76,80,87	0.92	2 (2%)
11	NAG	B	1204	2	14,14,15	0.24	0	17,19,21	0.55	0
11	NAG	B	1206	2	14,14,15	0.18	0	17,19,21	0.40	0
11	NAG	B	1203	2	14,14,15	0.25	0	17,19,21	0.45	0
6	R16	A	2407	-	15,15,15	0.10	0	14,14,14	0.14	0
6	R16	A	2405	-	15,15,15	0.11	0	14,14,14	0.17	0
7	Y01	A	2410	-	38,38,38	4.00	12 (31%)	57,57,57	2.10	17 (29%)
6	R16	A	2414	-	11,11,15	0.10	0	10,10,14	0.19	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
6	R16	A	2401	-	-	5/13/13/13	-
11	NAG	B	1209	2	-	0/6/23/26	0/1/1/1
6	R16	A	2406	-	-	6/13/13/13	-
6	R16	A	2417	-	-	7/13/13/13	-
7	Y01	A	2404	-	-	12/19/77/77	0/4/4/4
11	NAG	B	1207	2	-	0/6/23/26	0/1/1/1
11	NAG	B	1208	2	-	3/6/23/26	0/1/1/1
7	Y01	A	2419	-	-	16/19/77/77	0/4/4/4
6	R16	A	2415	-	-	4/12/12/13	-
6	R16	A	2416	-	-	2/10/10/13	-
11	NAG	B	1202	2	-	2/6/23/26	0/1/1/1
9	6IX	A	2421	1	-	11/44/44/44	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	R16	A	2403	-	-	6/13/13/13	-
6	R16	A	2418	-	-	3/13/13/13	-
6	R16	A	2402	-	-	5/13/13/13	-
6	R16	A	2408	-	-	6/13/13/13	-
6	R16	A	2412	-	-	4/12/12/13	-
6	R16	A	2413	-	-	1/10/10/13	-
6	R16	A	2409	-	-	3/8/8/13	-
11	NAG	B	1205	2	-	3/6/23/26	0/1/1/1
6	R16	A	2411	-	-	5/10/10/13	-
8	PT5	A	2420	-	-	25/59/83/90	0/1/1/1
11	NAG	B	1204	2	-	3/6/23/26	0/1/1/1
11	NAG	B	1206	2	-	2/6/23/26	0/1/1/1
11	NAG	B	1203	2	-	0/6/23/26	0/1/1/1
6	R16	A	2407	-	-	3/13/13/13	-
6	R16	A	2405	-	-	6/13/13/13	-
7	Y01	A	2410	-	-	9/19/77/77	0/4/4/4
6	R16	A	2414	-	-	4/9/9/13	-

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	2404	Y01	CAI-CAZ	16.46	1.69	1.33
7	A	2419	Y01	CAI-CAZ	16.36	1.69	1.33
7	A	2410	Y01	CAI-CAZ	16.33	1.69	1.33
9	A	2421	6IX	C13-N14	7.20	1.49	1.34
7	A	2404	Y01	CAU-CBI	-7.13	1.41	1.54
7	A	2419	Y01	CAU-CBI	-7.10	1.41	1.54
7	A	2419	Y01	CAQ-CAP	6.99	1.73	1.54
7	A	2410	Y01	CAU-CBI	-6.98	1.41	1.54
9	A	2421	6IX	C16-N17	6.98	1.48	1.34
7	A	2410	Y01	CBH-CBF	6.93	1.67	1.56
7	A	2419	Y01	CBH-CBF	6.89	1.67	1.56
7	A	2404	Y01	CAQ-CAP	6.87	1.72	1.54
7	A	2410	Y01	CAQ-CAP	6.86	1.72	1.54
7	A	2404	Y01	CBH-CBF	6.68	1.67	1.56
7	A	2404	Y01	CAK-CBD	6.14	1.63	1.53
7	A	2419	Y01	CAK-CBD	6.08	1.63	1.53
7	A	2410	Y01	CAK-CBD	6.00	1.63	1.53
7	A	2410	Y01	CAU-CAS	5.89	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	2404	Y01	CAU-CAS	5.86	1.65	1.53
7	A	2419	Y01	CAU-CAS	5.83	1.65	1.53
7	A	2410	Y01	CBI-CBE	5.50	1.65	1.55
7	A	2404	Y01	CBI-CBE	5.46	1.65	1.55
7	A	2419	Y01	CBI-CBE	5.44	1.65	1.55
7	A	2410	Y01	CBB-CBE	-5.16	1.45	1.54
7	A	2410	Y01	CAQ-CBG	5.09	1.64	1.54
7	A	2419	Y01	CAQ-CBG	5.08	1.64	1.54
7	A	2404	Y01	CAQ-CBG	5.04	1.64	1.54
7	A	2404	Y01	CBB-CBE	-4.89	1.45	1.54
7	A	2419	Y01	CBB-CBE	-4.84	1.45	1.54
9	A	2421	6IX	C09-C08	4.30	1.59	1.51
8	A	2420	PT5	C19-C18	3.93	1.54	1.31
8	A	2420	PT5	C16-C15	3.84	1.54	1.31
8	A	2420	PT5	C22-C21	3.81	1.53	1.31
8	A	2420	PT5	C25-C24	3.70	1.53	1.31
9	A	2421	6IX	O28-C27	3.44	1.45	1.37
8	A	2420	PT5	P4-O4	3.43	1.65	1.59
8	A	2420	PT5	P5-O5	3.35	1.65	1.59
7	A	2419	Y01	OAW-CAY	3.03	1.42	1.34
7	A	2410	Y01	OAW-CAY	2.99	1.42	1.34
7	A	2404	Y01	OAW-CAY	2.97	1.42	1.34
7	A	2404	Y01	CAO-CBB	2.91	1.61	1.54
7	A	2419	Y01	CAO-CBB	2.87	1.61	1.54
8	A	2420	PT5	O18-C11	2.75	1.41	1.33
7	A	2410	Y01	CAO-CBB	2.74	1.61	1.54
9	A	2421	6IX	O22-C16	-2.66	1.18	1.23
9	A	2421	6IX	O38-C13	-2.53	1.18	1.23
7	A	2410	Y01	CBH-CAZ	-2.51	1.47	1.52
8	A	2420	PT5	O16-C10	2.46	1.41	1.34
7	A	2404	Y01	CBH-CAZ	-2.25	1.48	1.52
8	A	2420	PT5	O16-C8	-2.13	1.41	1.46
8	A	2420	PT5	P1-O1	2.13	1.66	1.60
7	A	2419	Y01	CBH-CAZ	-2.05	1.48	1.52

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	2404	Y01	CAD-CBH-CBF	-5.37	105.27	111.68
7	A	2410	Y01	CAK-CAI-CAZ	-5.23	115.42	125.06
7	A	2419	Y01	CAK-CAI-CAZ	-5.21	115.45	125.06
7	A	2419	Y01	CBH-CAZ-CAI	-4.96	115.31	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	2419	Y01	CAU-CBI-CBE	4.78	123.72	116.57
7	A	2419	Y01	CAD-CBH-CBF	-4.75	106.02	111.68
7	A	2410	Y01	CAU-CBI-CBE	4.66	123.55	116.57
7	A	2410	Y01	CAD-CBH-CBF	-4.61	106.19	111.68
7	A	2404	Y01	CAU-CBI-CBE	4.54	123.37	116.57
7	A	2404	Y01	CAK-CAI-CAZ	-4.52	116.72	125.06
7	A	2404	Y01	OAW-CAY-CAM	4.19	120.53	111.50
7	A	2404	Y01	CBG-CBI-CBE	4.17	105.01	100.07
7	A	2410	Y01	OAW-CAY-CAM	4.16	120.46	111.50
7	A	2419	Y01	OAW-CAY-CAM	4.10	120.33	111.50
8	A	2420	PT5	O16-C10-C12	4.07	120.27	111.50
7	A	2404	Y01	CBH-CAZ-CAI	-4.00	116.79	122.90
7	A	2410	Y01	CBH-CAZ-CAI	-3.96	116.84	122.90
7	A	2410	Y01	CAE-CBI-CBG	-3.76	104.70	111.71
7	A	2419	Y01	CAU-CBI-CBG	3.54	112.76	107.27
7	A	2419	Y01	CBF-CBD-CBG	3.51	113.79	109.09
7	A	2419	Y01	CAE-CBI-CBG	-3.49	105.21	111.71
7	A	2404	Y01	CAE-CBI-CAU	-3.48	105.09	110.59
7	A	2410	Y01	CBI-CBE-CBB	-3.46	114.06	119.49
7	A	2404	Y01	CBI-CBE-CBB	-3.46	114.06	119.49
7	A	2404	Y01	CAE-CBI-CBG	-3.45	105.29	111.71
7	A	2410	Y01	CAE-CBI-CBE	-3.42	105.34	111.71
7	A	2410	Y01	CBG-CBI-CBE	3.36	104.06	100.07
7	A	2410	Y01	CAT-CAR-CBC	3.33	116.00	110.33
7	A	2419	Y01	CAE-CBI-CAU	-3.29	105.40	110.59
7	A	2419	Y01	CAE-CBI-CBE	-3.27	105.62	111.71
7	A	2404	Y01	CAE-CBI-CBE	-3.19	105.77	111.71
7	A	2410	Y01	CBF-CBD-CBG	3.06	113.18	109.09
7	A	2419	Y01	CBI-CBE-CBB	-3.03	114.73	119.49
7	A	2410	Y01	CAE-CBI-CAU	-2.98	105.89	110.59
7	A	2419	Y01	CAC-CBB-CBE	-2.93	108.43	112.92
7	A	2410	Y01	CAU-CBI-CBG	2.89	111.75	107.27
7	A	2419	Y01	CAO-CBB-CBE	2.85	116.18	110.28
7	A	2404	Y01	CAO-CBB-CBE	2.84	116.16	110.28
7	A	2404	Y01	CAC-CBB-CBE	-2.77	108.67	112.92
7	A	2419	Y01	CAT-CBH-CAZ	2.75	113.80	108.75
7	A	2404	Y01	CAS-CBF-CBH	-2.71	109.51	113.08
8	A	2420	PT5	O18-C11-C31	2.62	120.12	111.91
7	A	2410	Y01	CAC-CBB-CBE	-2.50	109.09	112.92
9	A	2421	6IX	C23-C15-N14	-2.45	105.63	110.79
7	A	2404	Y01	CAU-CBI-CBG	2.36	110.93	107.27
7	A	2410	Y01	CBF-CBH-CAZ	2.33	113.31	109.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	2404	Y01	CAL-CAM-CAY	-2.32	106.69	113.43
7	A	2404	Y01	CAT-CBH-CAZ	2.30	112.96	108.75
7	A	2419	Y01	CAK-CBD-CBG	-2.28	107.60	110.91
7	A	2410	Y01	CAO-CBB-CBE	2.26	114.96	110.28
7	A	2404	Y01	CBF-CBH-CAZ	2.22	113.13	109.65
7	A	2419	Y01	CBG-CBI-CBE	2.18	102.65	100.07
9	A	2421	6IX	C24-C23-C15	-2.14	107.47	113.39
7	A	2404	Y01	CAK-CBD-CBF	2.13	112.29	109.71
7	A	2419	Y01	CAL-CAM-CAY	-2.05	107.48	113.43
7	A	2410	Y01	CAV-CAZ-CBH	-2.03	113.72	116.42
7	A	2404	Y01	CBF-CBD-CBG	2.03	111.81	109.09

There are no chirality outliers.

All (156) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	2404	Y01	CAO-CBB-CBE-CAP
7	A	2404	Y01	CAC-CBB-CBE-CAP
7	A	2419	Y01	CAO-CBB-CBE-CAP
7	A	2419	Y01	CAO-CBB-CBE-CBI
7	A	2419	Y01	CAC-CBB-CBE-CBI
7	A	2419	Y01	CAV-CBC-OAW-CAY
8	A	2420	PT5	C7-O13-P1-O12
8	A	2420	PT5	C7-O13-P1-O11
8	A	2420	PT5	C7-O13-P1-O1
8	A	2420	PT5	C5-O5-P5-O51
8	A	2420	PT5	C12-C10-O16-C8
9	A	2421	6IX	C39-C12-N10-C09
8	A	2420	PT5	O19-C11-O18-C9
8	A	2420	PT5	C31-C11-O18-C9
7	A	2419	Y01	CAC-CBB-CBE-CAP
7	A	2404	Y01	CAC-CBB-CBE-CBI
7	A	2404	Y01	CAO-CBB-CBE-CBI
8	A	2420	PT5	O17-C10-O16-C8
7	A	2404	Y01	CAJ-CAO-CBB-CAC
7	A	2419	Y01	CAJ-CAO-CBB-CAC
11	B	1208	NAG	O5-C5-C6-O6
7	A	2410	Y01	CAX-CAL-CAM-CAY
8	A	2420	PT5	C14-C15-C16-C17
7	A	2419	Y01	OAG-CAY-OAW-CBC
11	B	1206	NAG	O5-C5-C6-O6
11	B	1202	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
11	B	1205	NAG	O5-C5-C6-O6
11	B	1208	NAG	C4-C5-C6-O6
7	A	2419	Y01	CAM-CAY-OAW-CBC
11	B	1204	NAG	O5-C5-C6-O6
7	A	2419	Y01	CAJ-CAO-CBB-CBE
11	B	1205	NAG	C4-C5-C6-O6
11	B	1202	NAG	C4-C5-C6-O6
9	A	2421	6IX	C36-C27-O28-C29
9	A	2421	6IX	C39-C12-N10-C11
9	A	2421	6IX	C26-C27-O28-C29
11	B	1204	NAG	C4-C5-C6-O6
7	A	2404	Y01	CAX-CAL-CAM-CAY
11	B	1206	NAG	C4-C5-C6-O6
6	A	2418	R16	C35-C36-C37-C38
7	A	2404	Y01	CAJ-CAO-CBB-CBE
8	A	2420	PT5	C17-C18-C19-C20
6	A	2401	R16	C28-C29-C30-C31
6	A	2406	R16	C28-C29-C30-C31
6	A	2416	R16	C34-C35-C36-C37
6	A	2417	R16	C37-C38-C39-C40
6	A	2407	R16	C34-C35-C36-C37
6	A	2408	R16	C33-C34-C35-C36
6	A	2414	R16	C35-C36-C37-C38
8	A	2420	PT5	C36-C37-C38-C39
6	A	2402	R16	C35-C36-C37-C38
6	A	2403	R16	C30-C31-C32-C33
8	A	2420	PT5	C31-C32-C33-C34
7	A	2410	Y01	CAJ-CAN-CBA-CAA
6	A	2409	R16	C33-C34-C35-C36
6	A	2412	R16	C37-C38-C39-C40
6	A	2412	R16	C31-C32-C33-C34
6	A	2418	R16	C32-C33-C34-C35
6	A	2409	R16	C36-C37-C38-C39
6	A	2411	R16	C37-C38-C39-C40
6	A	2412	R16	C28-C29-C30-C31
6	A	2406	R16	C33-C34-C35-C36
6	A	2401	R16	C37-C38-C39-C40
7	A	2410	Y01	CAJ-CAN-CBA-CAB
7	A	2419	Y01	CAX-CAL-CAM-CAY
7	A	2410	Y01	CAC-CBB-CBE-CBI
6	A	2415	R16	C35-C36-C37-C38
8	A	2420	PT5	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
7	A	2410	Y01	CAO-CBB-CBE-CBI
6	A	2415	R16	C37-C38-C39-C40
6	A	2406	R16	C29-C30-C31-C32
8	A	2420	PT5	C27-C28-C29-C30
7	A	2410	Y01	CAJ-CAO-CBB-CBE
6	A	2414	R16	C34-C35-C36-C37
6	A	2411	R16	C34-C35-C36-C37
6	A	2416	R16	C37-C38-C39-C40
7	A	2404	Y01	CAO-CAJ-CAN-CBA
6	A	2418	R16	C37-C38-C39-C40
8	A	2420	PT5	C25-C26-C27-C28
6	A	2414	R16	C36-C37-C38-C39
6	A	2417	R16	C27-C28-C29-C30
6	A	2405	R16	C28-C29-C30-C31
7	A	2419	Y01	CAN-CAJ-CAO-CBB
6	A	2405	R16	C32-C33-C34-C35
6	A	2405	R16	C38-C39-C40-C41
6	A	2408	R16	C29-C30-C31-C32
6	A	2408	R16	C32-C33-C34-C35
6	A	2417	R16	C32-C33-C34-C35
6	A	2417	R16	C28-C29-C30-C31
6	A	2402	R16	C32-C33-C34-C35
6	A	2401	R16	C34-C35-C36-C37
6	A	2403	R16	C33-C34-C35-C36
8	A	2420	PT5	O13-C7-C8-O16
7	A	2410	Y01	CAC-CBB-CBE-CAP
8	A	2420	PT5	C8-C7-O13-P1
6	A	2406	R16	C34-C35-C36-C37
6	A	2406	R16	C38-C39-C40-C41
9	A	2421	6IX	N14-C15-C16-O22
7	A	2419	Y01	CAJ-CAN-CBA-CAB
9	A	2421	6IX	N14-C15-C16-N17
7	A	2404	Y01	CAM-CAY-OAW-CBC
8	A	2420	PT5	C5-O5-P5-O52
6	A	2403	R16	C29-C30-C31-C32
6	A	2403	R16	C39-C40-C41-C42
6	A	2405	R16	C30-C31-C32-C33
7	A	2404	Y01	OAG-CAY-OAW-CBC
6	A	2401	R16	C27-C28-C29-C30
6	A	2415	R16	C28-C29-C30-C31
9	A	2421	6IX	C13-C12-N10-C09
6	A	2408	R16	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
6	A	2401	R16	C38-C39-C40-C41
6	A	2402	R16	C39-C40-C41-C42
6	A	2403	R16	C28-C29-C30-C31
7	A	2419	Y01	CAJ-CAN-CBA-CAA
6	A	2408	R16	C37-C38-C39-C40
7	A	2410	Y01	CAO-CBB-CBE-CAP
6	A	2406	R16	C35-C36-C37-C38
6	A	2407	R16	C30-C31-C32-C33
8	A	2420	PT5	C9-C8-O16-C10
8	A	2420	PT5	C33-C34-C35-C36
7	A	2410	Y01	CAJ-CAO-CBB-CAC
8	A	2420	PT5	C37-C38-C39-C40
6	A	2414	R16	C37-C38-C39-C40
6	A	2413	R16	C33-C34-C35-C36
11	B	1208	NAG	C3-C2-N2-C7
6	A	2405	R16	C29-C30-C31-C32
6	A	2411	R16	C30-C31-C32-C33
6	A	2408	R16	C39-C40-C41-C42
6	A	2402	R16	C36-C37-C38-C39
6	A	2409	R16	C32-C33-C34-C35
6	A	2411	R16	C38-C39-C40-C41
8	A	2420	PT5	C15-C16-C17-C18
11	B	1205	NAG	C1-C2-N2-C7
8	A	2420	PT5	O13-C7-C8-C9
6	A	2417	R16	C34-C35-C36-C37
6	A	2412	R16	C36-C37-C38-C39
6	A	2417	R16	C39-C40-C41-C42
6	A	2402	R16	C37-C38-C39-C40
6	A	2405	R16	C31-C32-C33-C34
6	A	2417	R16	C36-C37-C38-C39
9	A	2421	6IX	C23-C15-C16-O22
6	A	2403	R16	C34-C35-C36-C37
7	A	2404	Y01	CAM-CAL-CAX-OAF
7	A	2404	Y01	CAM-CAL-CAX-OAH
8	A	2420	PT5	C4-O4-P4-O43
6	A	2407	R16	C35-C36-C37-C38
6	A	2411	R16	C32-C33-C34-C35
6	A	2415	R16	C29-C30-C31-C32
11	B	1204	NAG	C3-C2-N2-C7
7	A	2419	Y01	CAL-CAM-CAY-OAW
7	A	2419	Y01	CAM-CAL-CAX-OAH
9	A	2421	6IX	C04-C02-C05-C44

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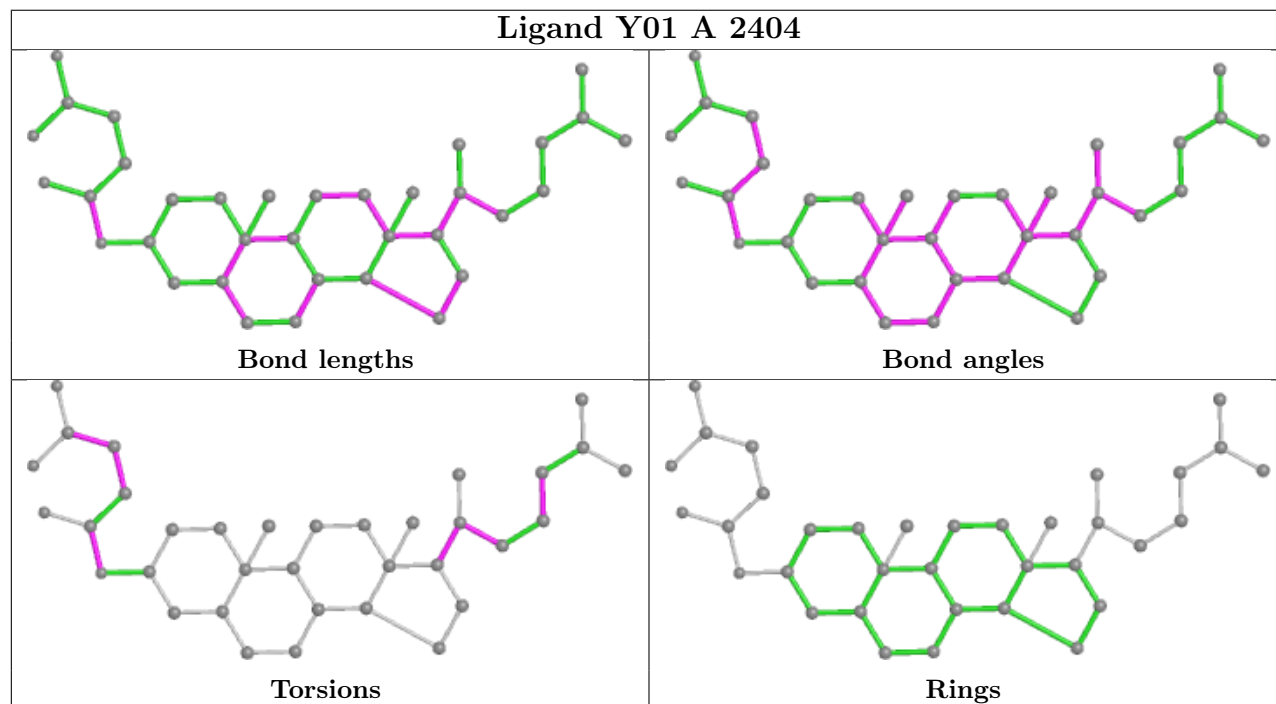
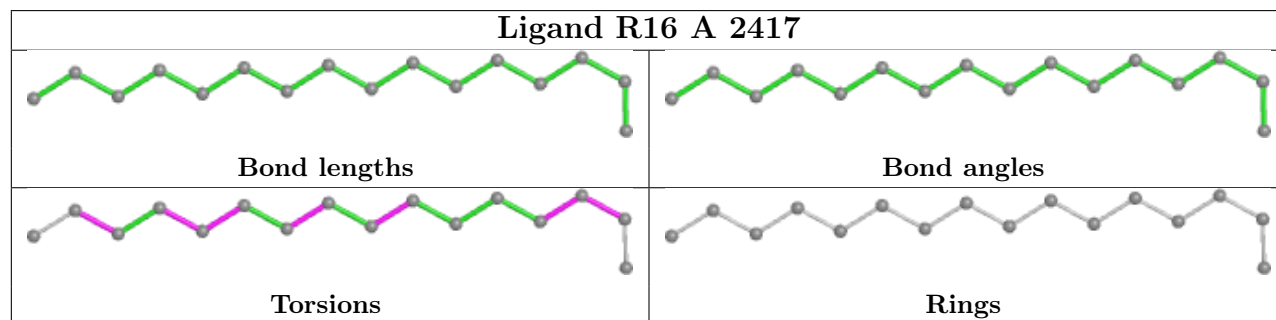
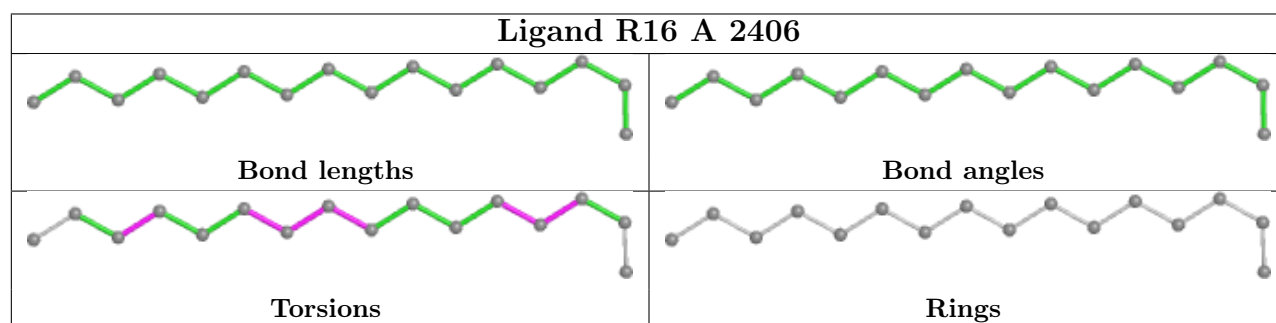
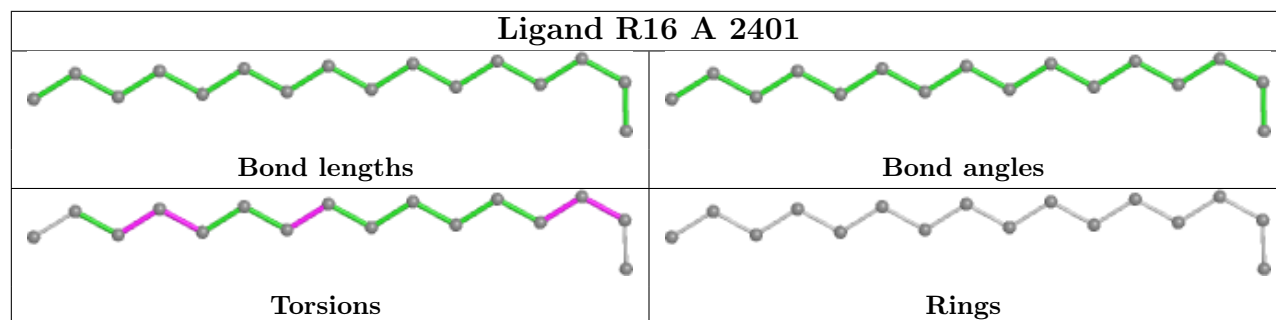
Mol	Chain	Res	Type	Atoms
7	A	2419	Y01	CAM-CAL-CAX-OAF
9	A	2421	6IX	C23-C15-C16-N17
8	A	2420	PT5	C34-C35-C36-C37
9	A	2421	6IX	C04-C02-C05-C06

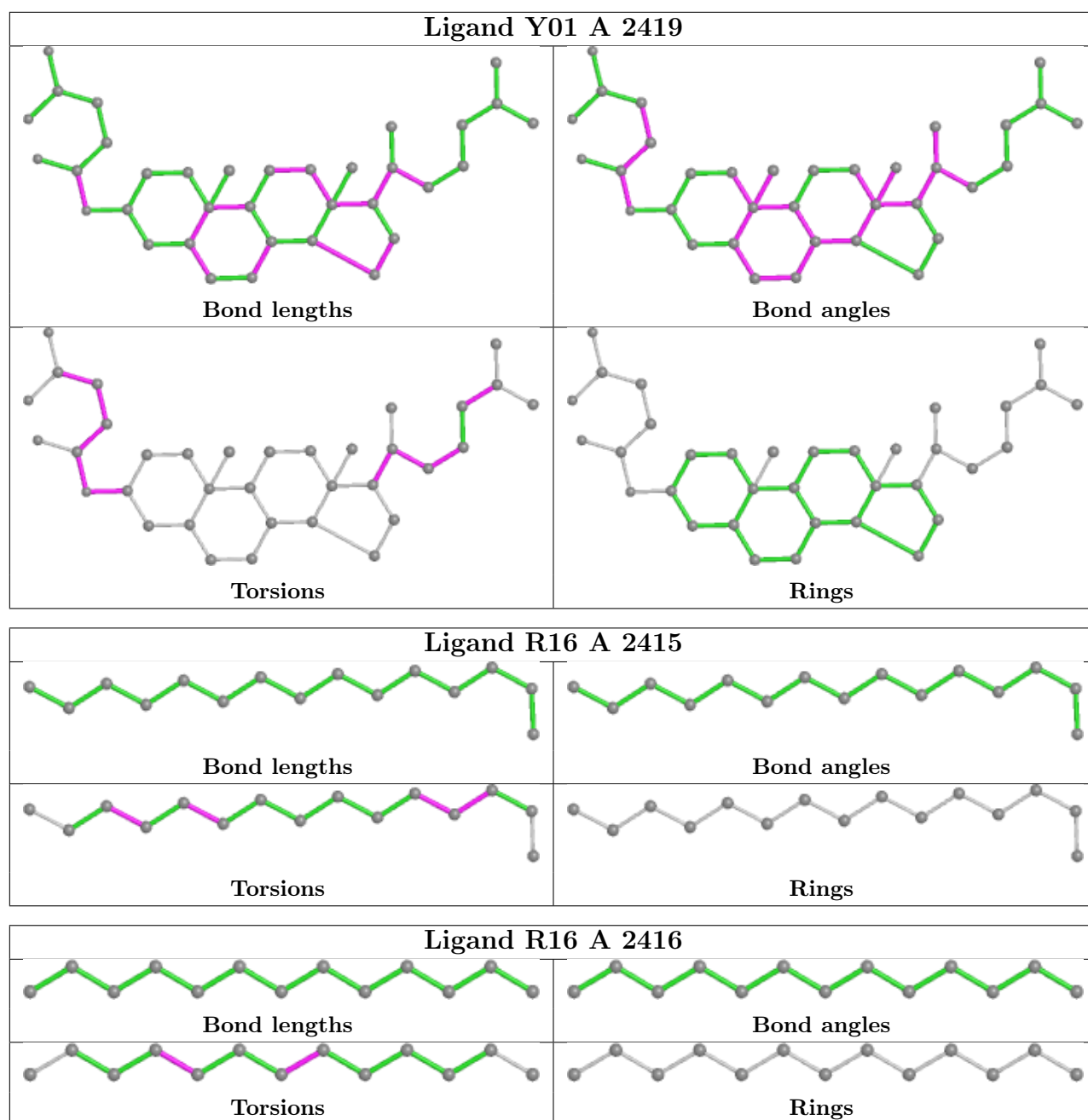
There are no ring outliers.

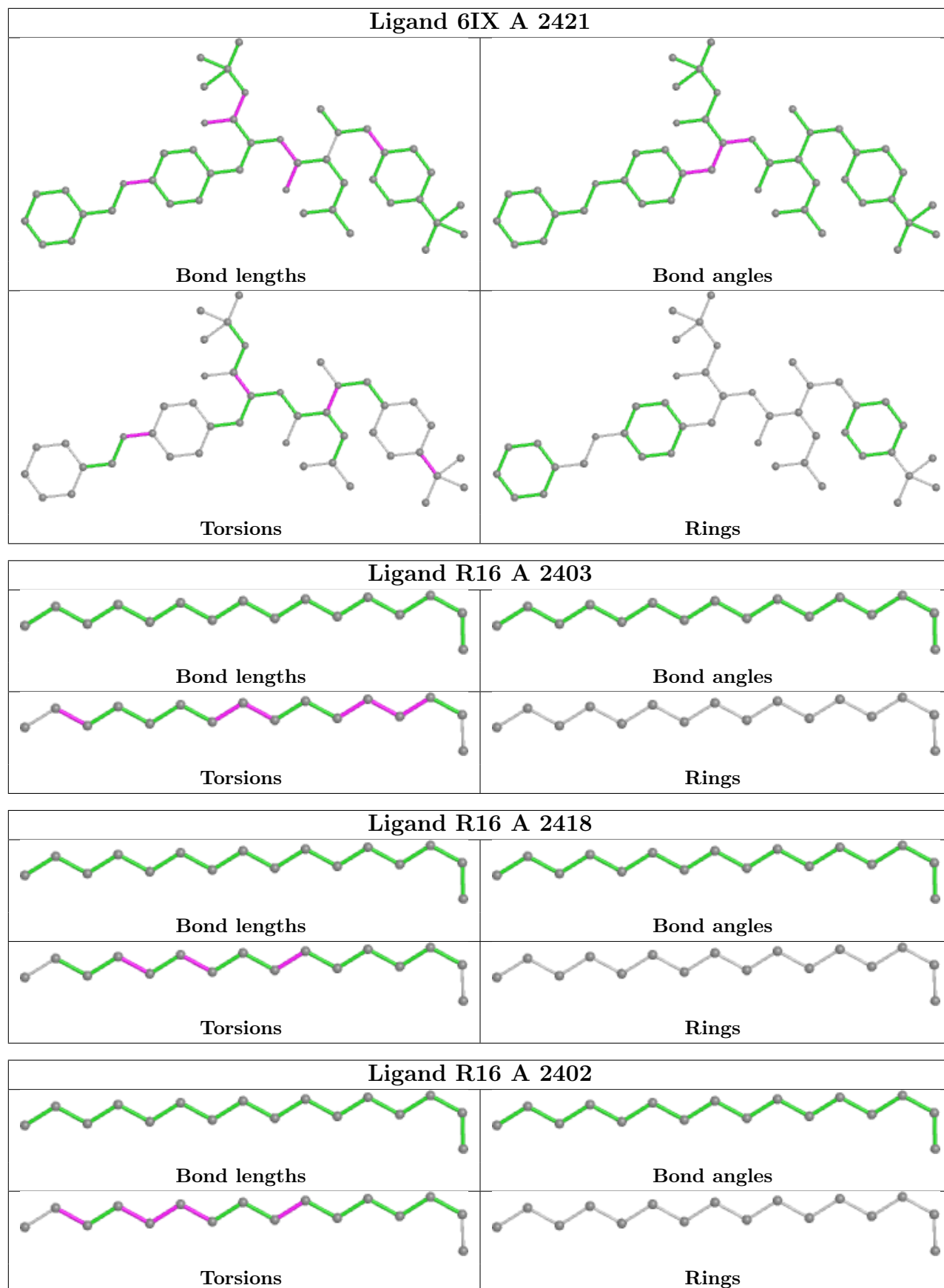
14 monomers are involved in 27 short contacts:

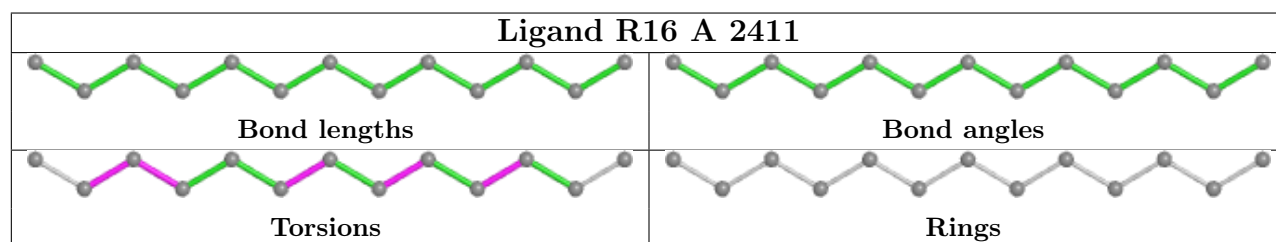
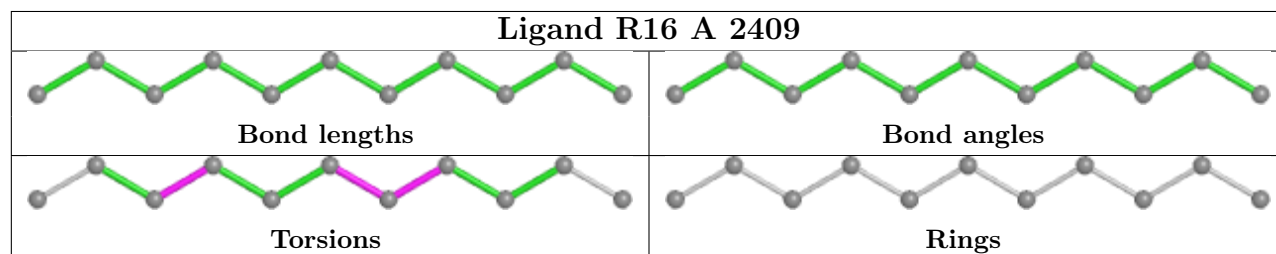
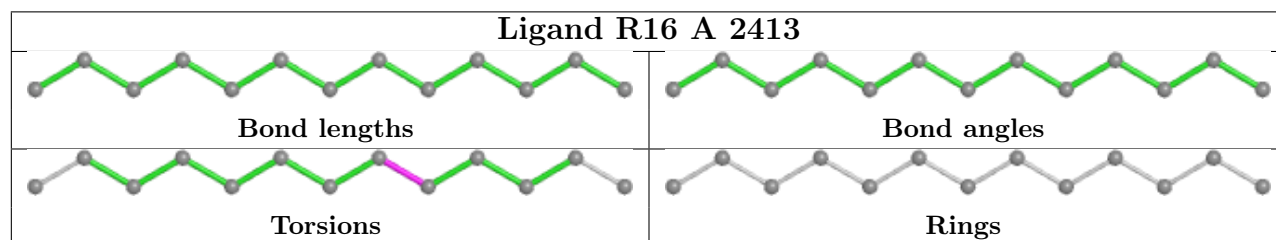
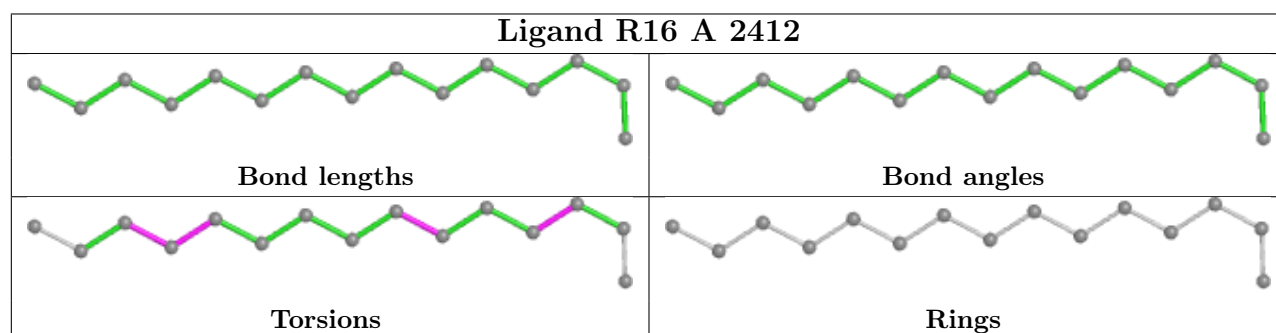
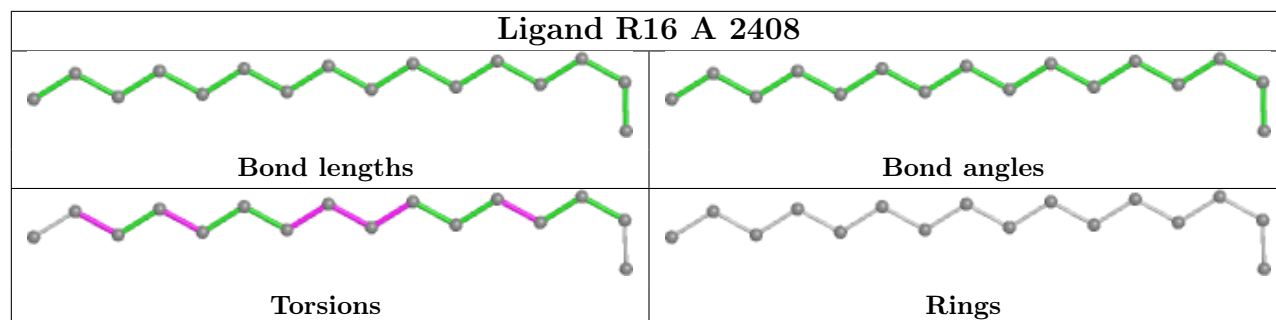
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2401	R16	3	0
11	B	1209	NAG	1	0
7	A	2404	Y01	2	0
7	A	2419	Y01	3	0
6	A	2415	R16	2	0
9	A	2421	6IX	1	0
6	A	2403	R16	1	0
6	A	2408	R16	2	0
11	B	1205	NAG	1	0
6	A	2411	R16	1	0
8	A	2420	PT5	7	0
11	B	1206	NAG	1	0
6	A	2407	R16	1	0
7	A	2410	Y01	3	0

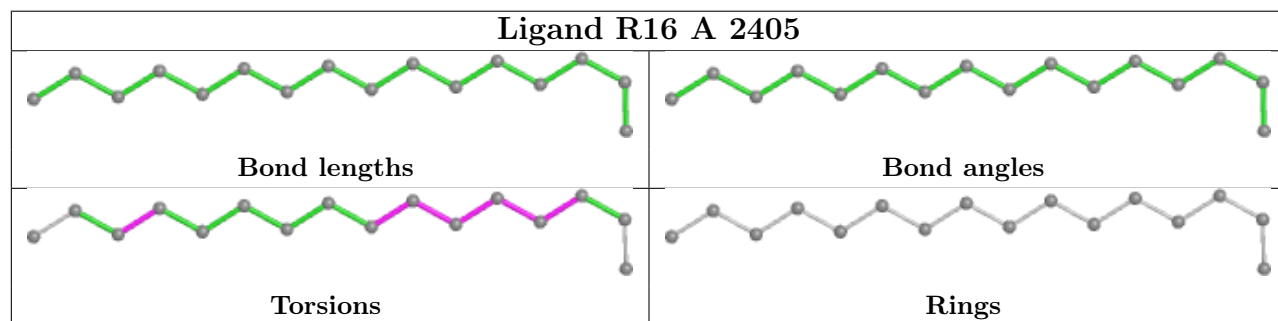
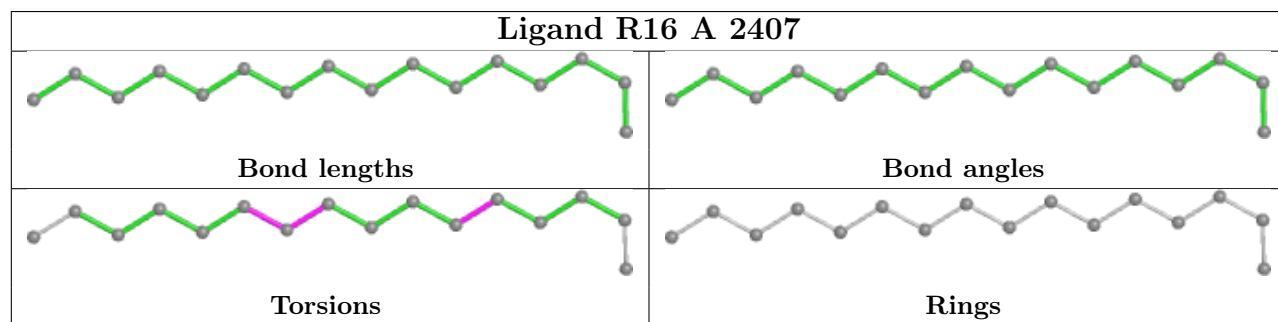
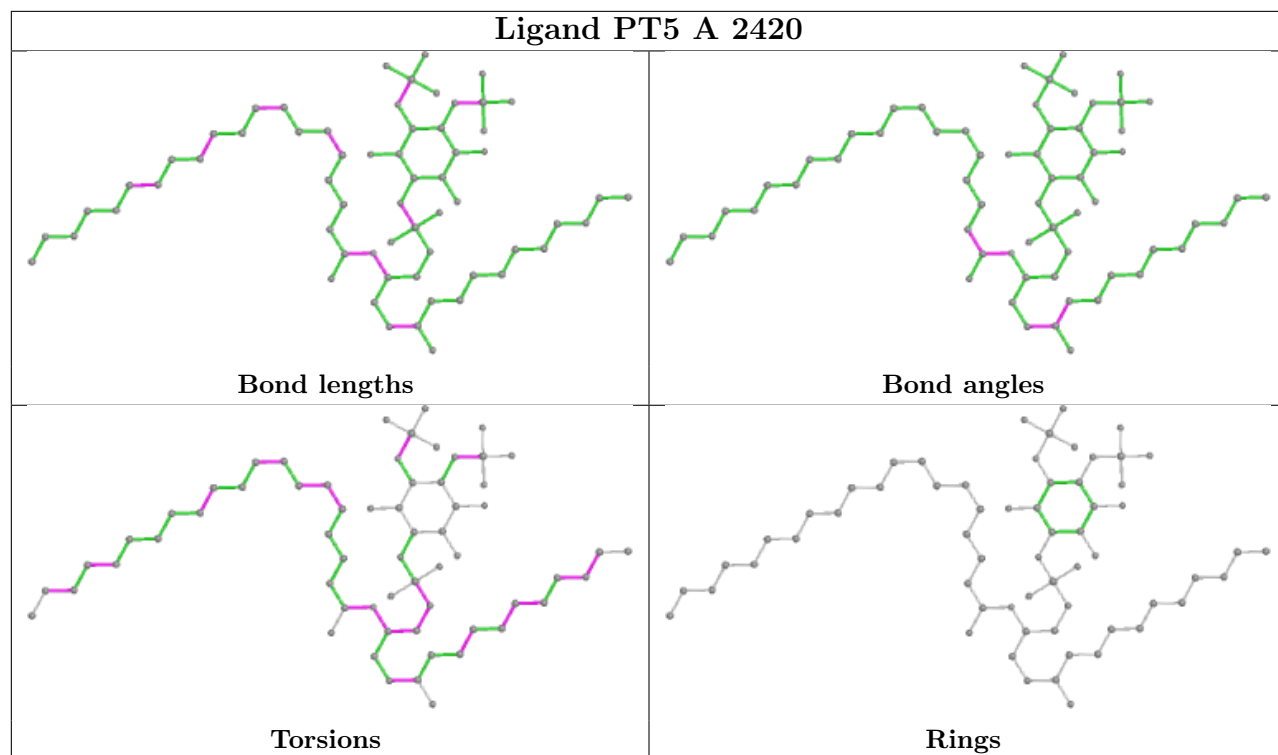
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

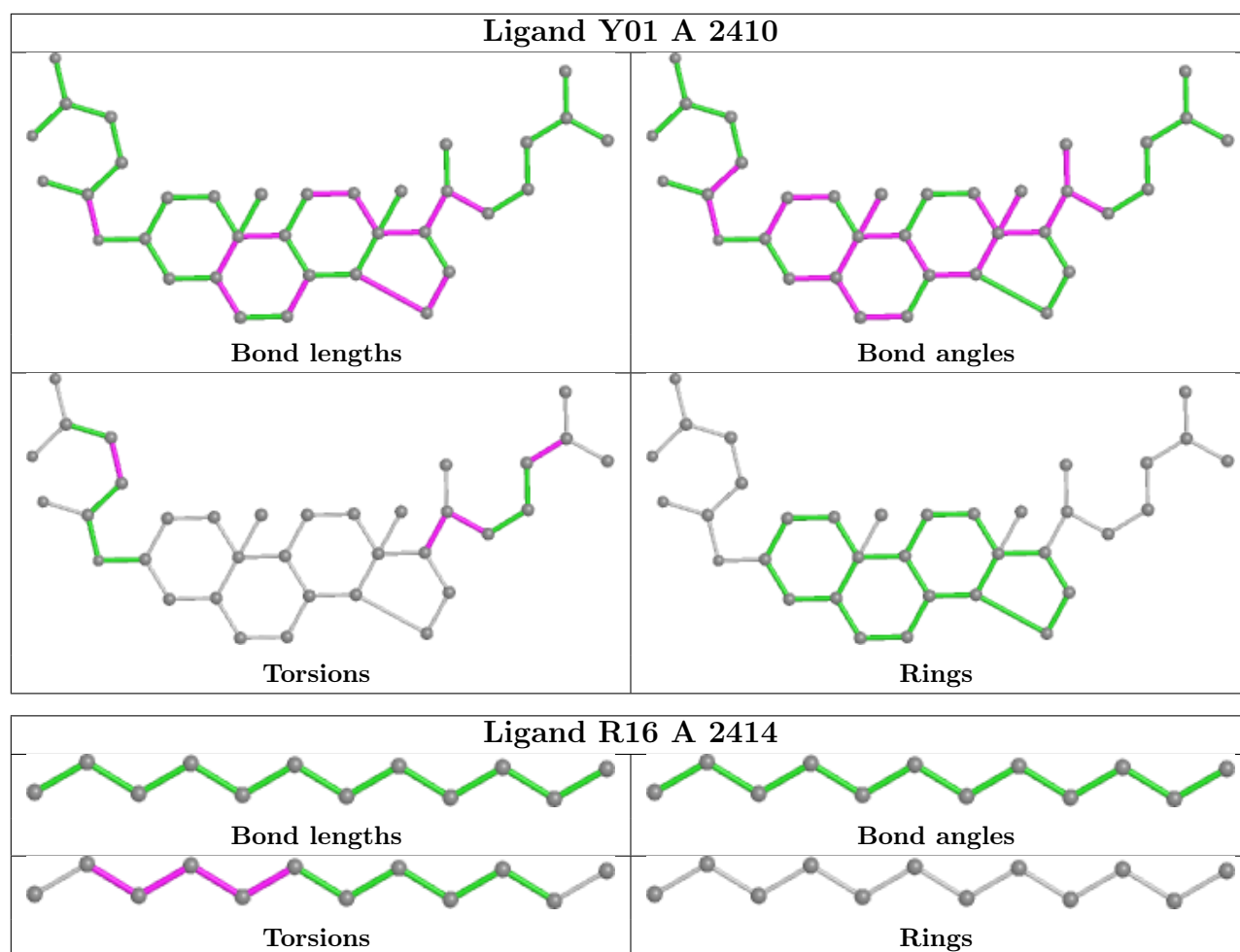












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

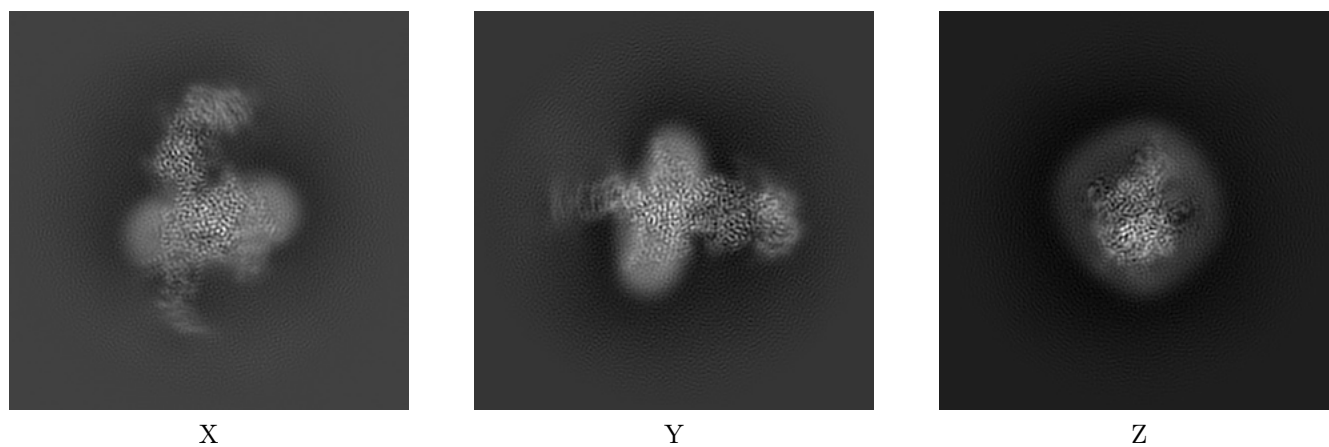
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31960. 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](#)

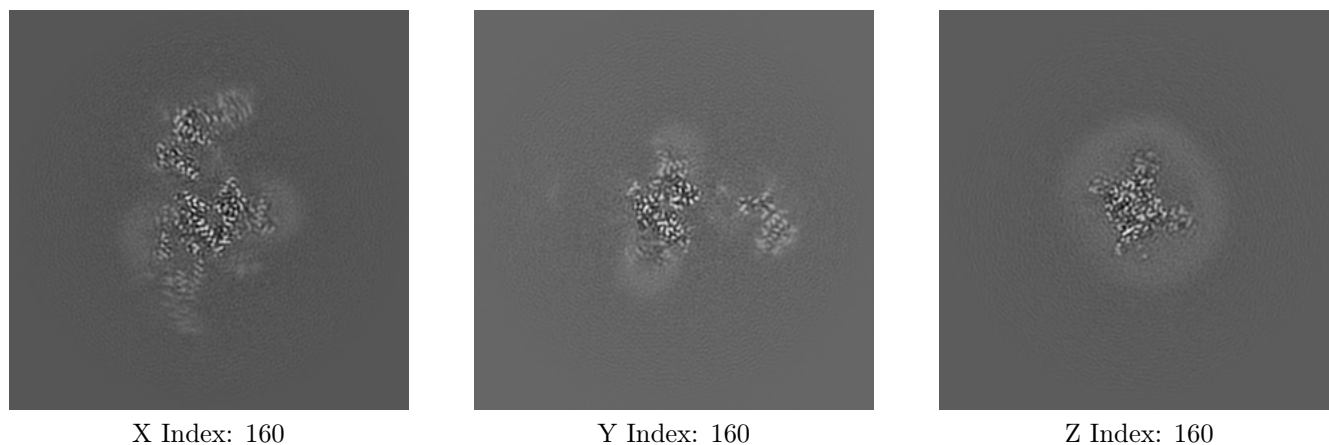
6.1.1 Primary map



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

6.2 Central slices [i](#)

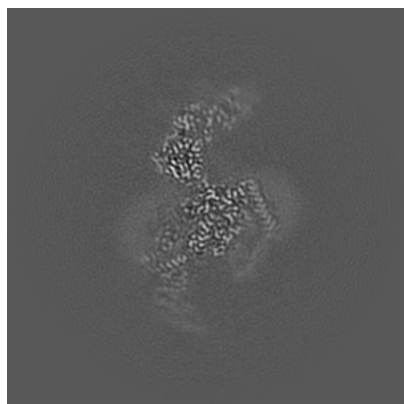
6.2.1 Primary map



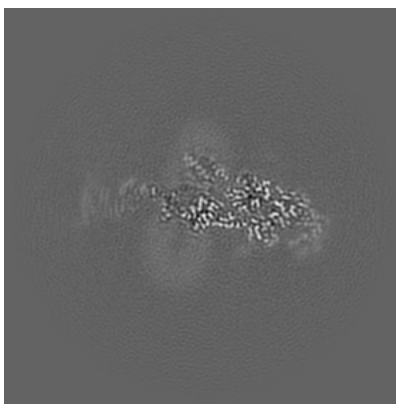
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

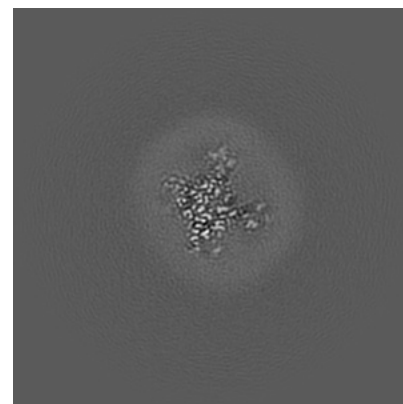
6.3.1 Primary map



X Index: 168



Y Index: 144



Z Index: 157

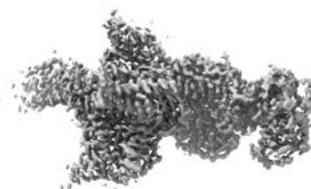
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

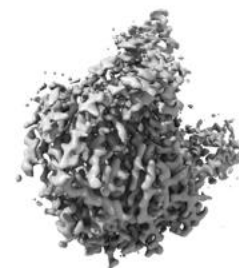
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

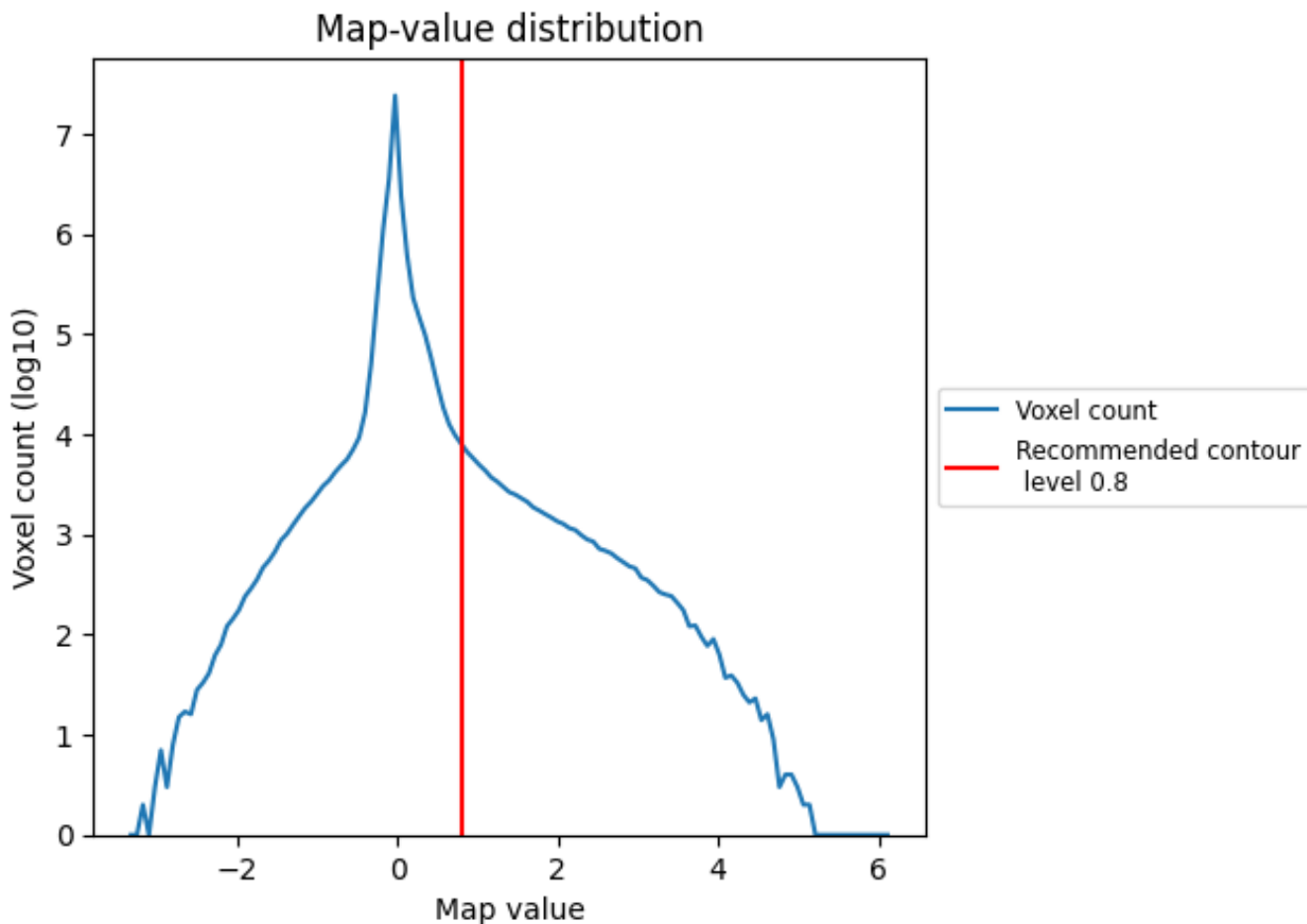
6.5 Mask visualisation

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

7 Map analysis [i](#)

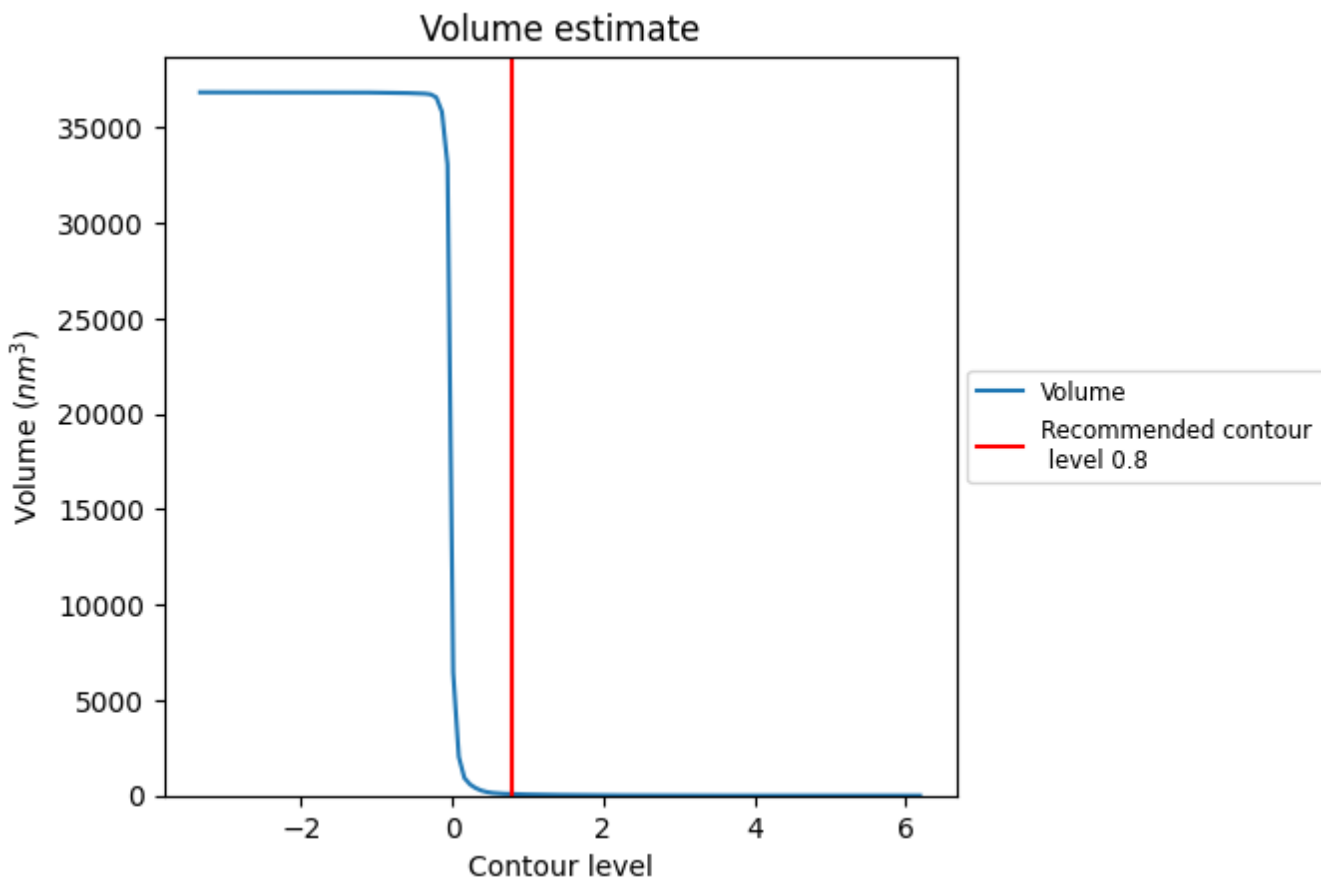
This section contains the results of statistical analysis of the map.

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.

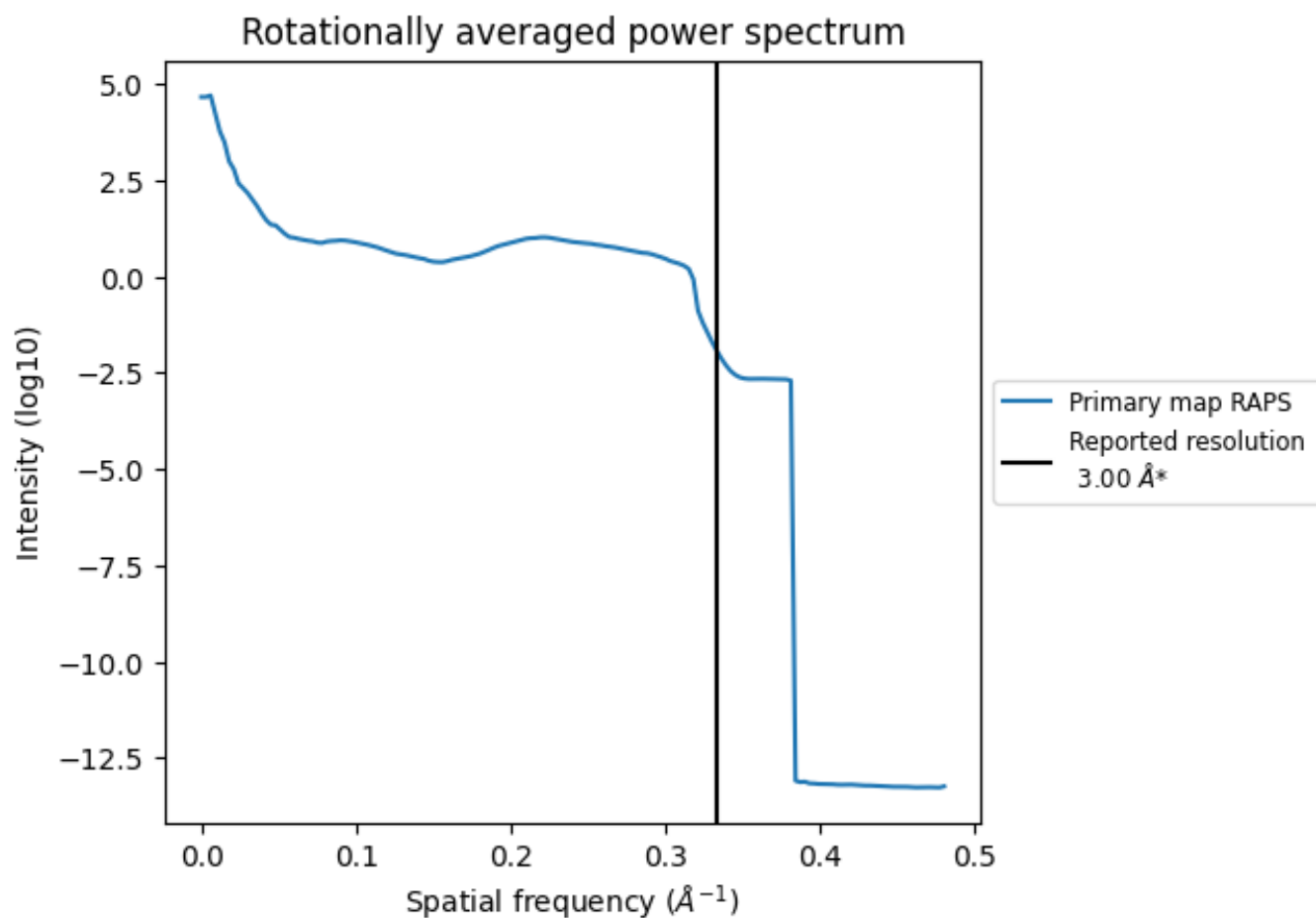
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 78 nm^3 ; this corresponds to an approximate mass of 71 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⁻¹

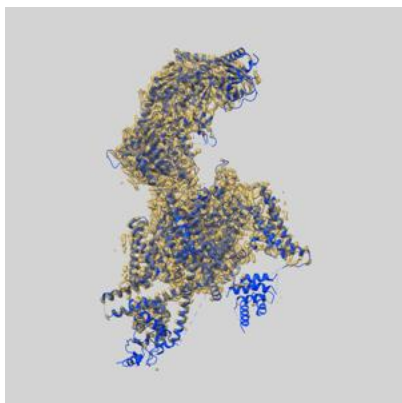
8 Fourier-Shell correlation

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

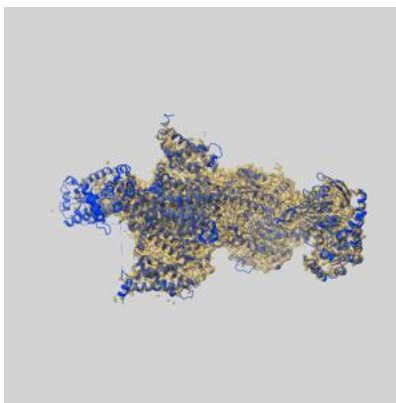
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-31960 and PDB model 7VFV. Per-residue inclusion information can be found in section 3 on page 9.

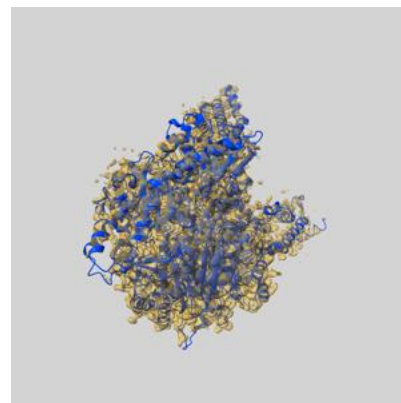
9.1 Map-model overlay [i](#)



X



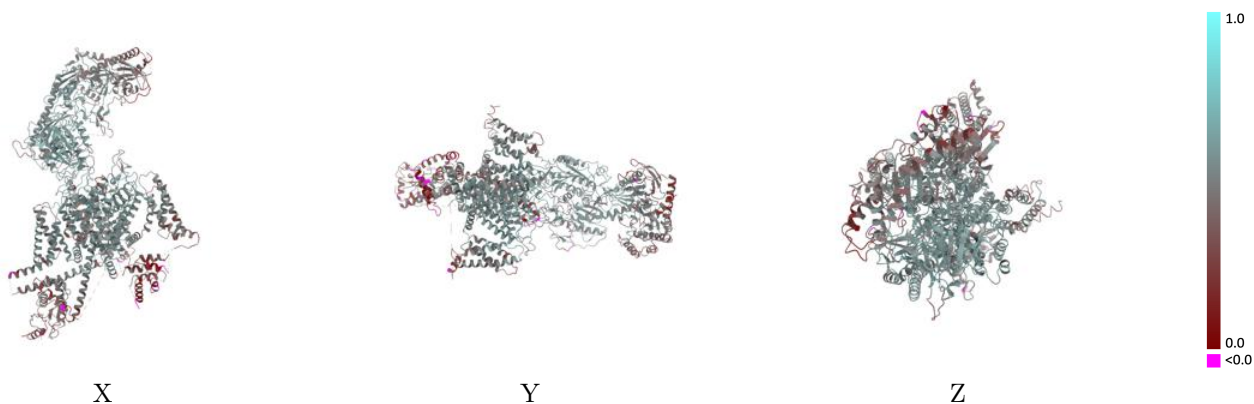
Y



Z

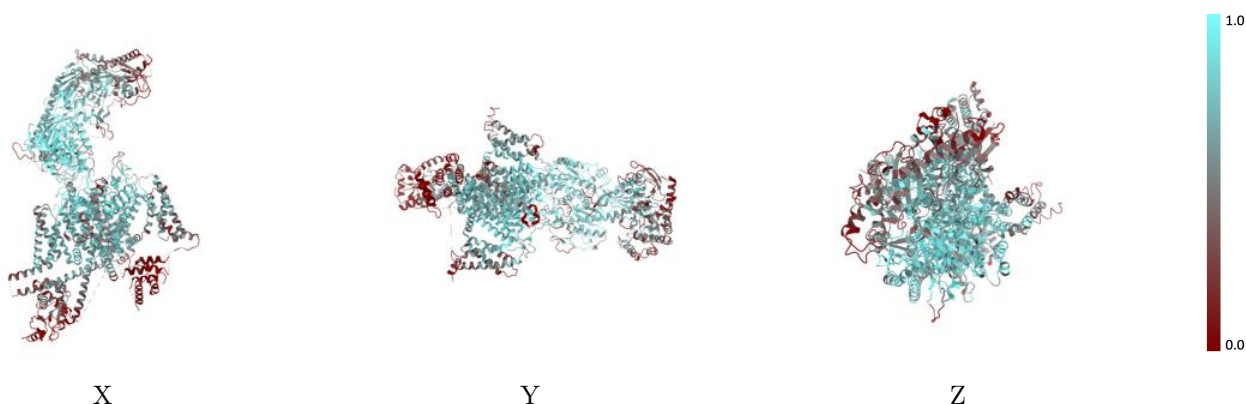
The images above show the 3D surface view of the map at the recommended contour level 0.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



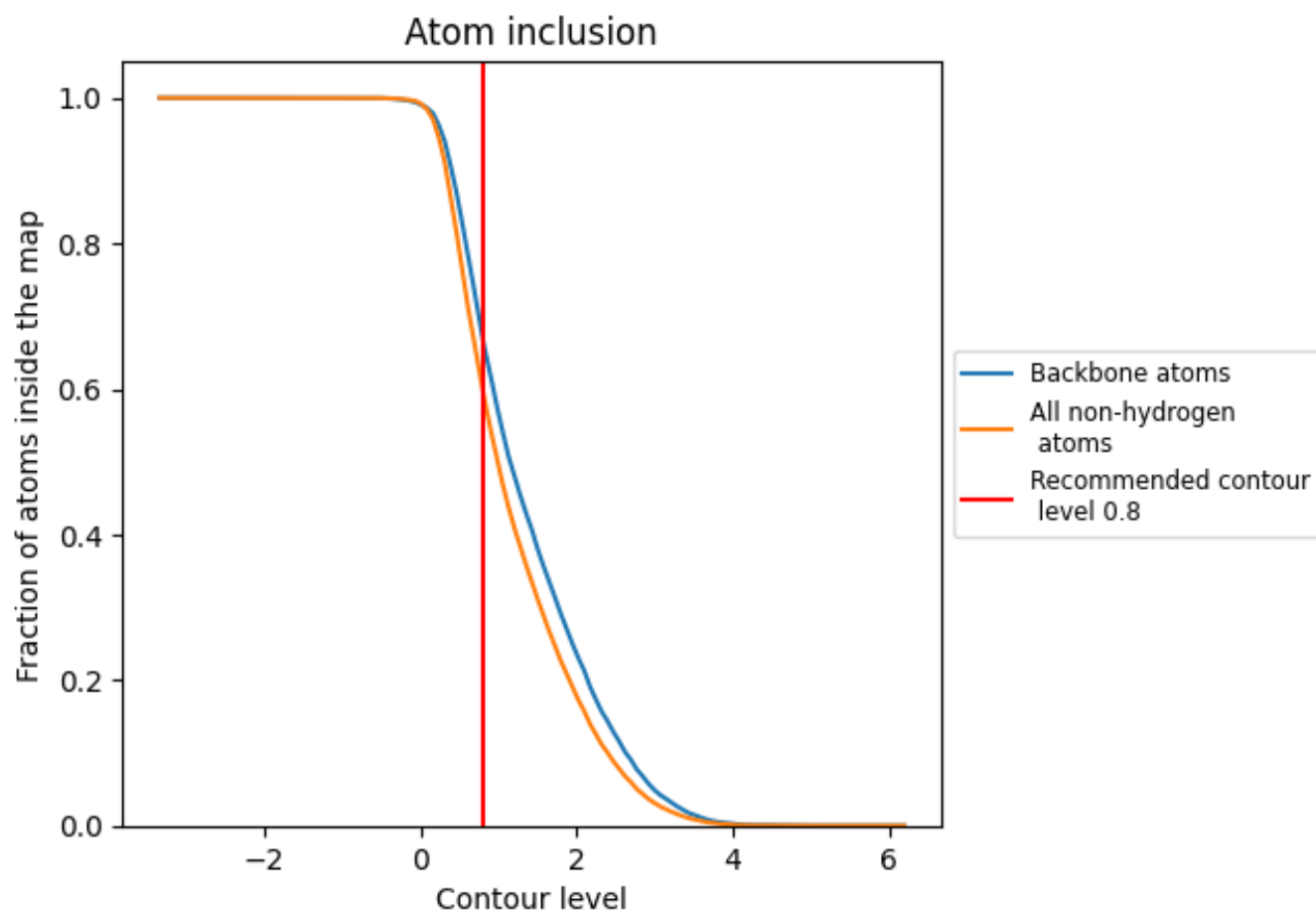
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.8).















9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 60% 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 (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5976	 0.4900
A	 0.6281	 0.5000
B	 0.6216	 0.4960
C	 0.3077	 0.3720
D	 0.2108	 0.3720
E	 0.7949	 0.5400
F	 0.0769	 0.2310

