



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 01:20 AM UTC

PDB ID : 9BRD / pdb_00009brd
EMDB ID : EMD-44353
Title : Synaptic Vesicle V-ATPase with synaptophysin and SidK, State 3
Authors : Coupland, C.E.; Rubinstein, J.L.
Deposited on : 2024-05-11
Resolution : 3.50 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

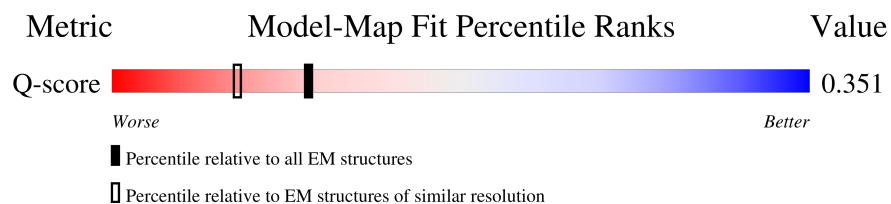
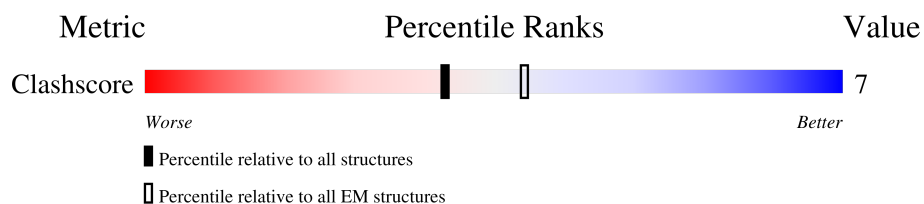
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Q-score	-	25397	13950 (3.00 - 4.00)

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 72445 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 H(+)-transporting two-sector ATPase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	600	Total	C	N	O	S	0	0
			4651	2949	786	889	27		
1	B	600	Total	C	N	O	S	0	0
			4651	2949	786	889	27		
1	C	600	Total	C	N	O	S	0	0
			4651	2949	786	889	27		

- Molecule 2 is a protein called V-type proton ATPase subunit B, brain isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	459	Total	C	N	O	S	0	0
			3595	2282	613	680	20		
2	E	459	Total	C	N	O	S	0	0
			3595	2282	613	680	20		
2	F	459	Total	C	N	O	S	0	0
			3595	2282	613	680	20		

- Molecule 3 is a protein called V-type proton ATPase subunit C 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	G	375	Total	C	N	O	0	0
			2155	1347	400	408		

- Molecule 4 is a protein called ATPase H⁺-transporting V1 subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	214	Total	C	N	O	S	0	0
			1726	1095	311	315	5		

- Molecule 5 is a protein called V-type proton ATPase subunit E 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	225	Total	C	N	O	S	0	0
			1778	1119	315	336	8		
5	J	223	Total	C	N	O	S	0	0
			1779	1120	315	334	10		
5	K	224	Total	C	N	O	S	0	0
			1657	1041	299	309	8		

- Molecule 6 is a protein called V-type proton ATPase subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	109	Total	C	N	O	S	0	0
			864	544	156	162	2		

- Molecule 7 is a protein called V-type proton ATPase subunit G.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	114	Total	C	N	O	S	0	0
			845	506	178	157	4		
7	N	114	Total	C	N	O	S	0	0
			916	548	190	173	5		
7	O	113	Total	C	N	O	S	0	0
			715	427	147	138	3		

- Molecule 8 is a protein called V-type proton ATPase subunit S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	204	Total	C	N	O	S	0	0
			1652	1087	259	297	9		

- Molecule 9 is a protein called Type IV secretion protein Dot.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Q	264	Total	C	N	O	S	0	0
			2130	1352	358	410	10		
9	R	267	Total	C	N	O	S	0	0
			2155	1369	362	413	11		
9	S	263	Total	C	N	O	S	0	0
			2126	1350	357	409	10		

- Molecule 10 is a protein called V-type proton ATPase subunit H.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	T	430	Total	C	N	O	0	0
			2136	1276	430	430		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	428	PHE	ILE	conflict	UNP A0A8I5ZQ24

- Molecule 11 is a protein called Synaptophysin.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	U	214	Total	C	N	O	0	0
			1150	702	221	227		

- Molecule 12 is a protein called V-type proton ATPase 116 kDa subunit a 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	a	770	Total	C	N	O	S	0	0
			6212	4052	1046	1074	40		

- Molecule 13 is a protein called ATPase, H⁺ transporting, V0 subunit B (Predicted), isoform CRA_a.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	b	203	Total	C	N	O	S	0	0
			1503	996	237	259	11		

- Molecule 14 is a protein called V-type proton ATPase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	d	350	Total	C	N	O	S	0	0
			2833	1829	460	530	14		

- Molecule 15 is a protein called V-type proton ATPase subunit e 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	e	80	Total	C	N	O	S	0	0
			644	443	100	98	3		

- Molecule 16 is a protein called Rnasek protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	f	86	Total	C	N	O	S	0	0
			666	440	103	116	7		

- Molecule 17 is a protein called V-type proton ATPase 16 kDa proteolipid subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	g	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		
17	h	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		
17	i	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		
17	j	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		
17	k	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		
17	l	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		
17	m	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		
17	n	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		
17	o	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		

- Molecule 18 is a protein called Renin receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	p	52	Total	C	N	O	S	0	0
			432	290	63	76	3		

- Molecule 19 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



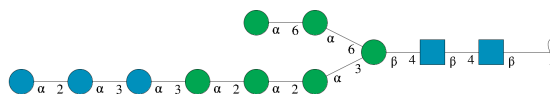
Mol	Chain	Residues	Atoms				AltConf	Trace
19	V	2	Total	C	N	O	0	0
			28	16	2	10		
19	W	2	Total	C	N	O	0	0
			28	16	2	10		

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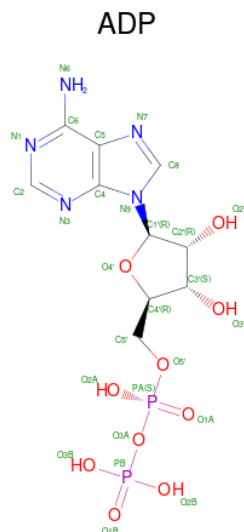
Mol	Chain	Residues	Atoms				AltConf	Trace
19	X	2	Total	C	N	O	0	0
			28	16	2	10		
19	Y	2	Total	C	N	O	0	0
			28	16	2	10		
19	Z	2	Total	C	N	O	0	0
			28	16	2	10		
19	c	2	Total	C	N	O	0	0
			28	16	2	10		
19	q	2	Total	C	N	O	0	0
			28	16	2	10		
19	r	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 20 is an oligosaccharide called alpha-D-glucopyranose-(1-2)-alpha-D-glucopyranos e-(1-3)-alpha-D-glucopyranose-(1-3)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose -(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranos e-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-ace tamido-2-deoxy-beta-D-glucopyranose.



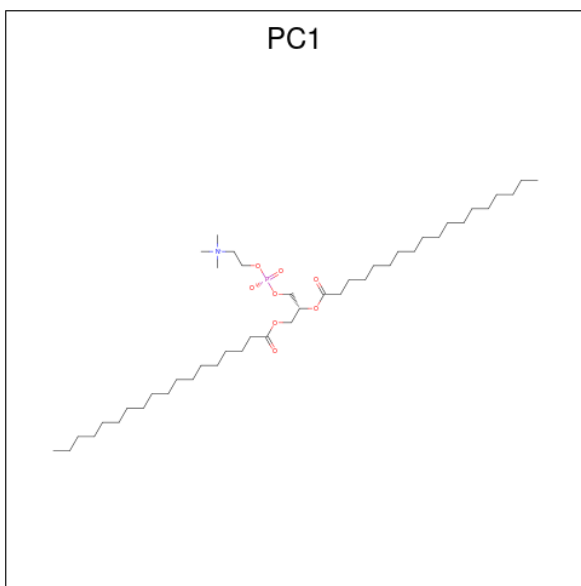
Mol	Chain	Residues	Atoms				AltConf	Trace
20	s	11	Total	C	N	O	0	0
			127	70	2	55		

- Molecule 21 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					AltConf
21	A	1	Total 27	C 10	N 5	O 10	P 2	0

- Molecule 22 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



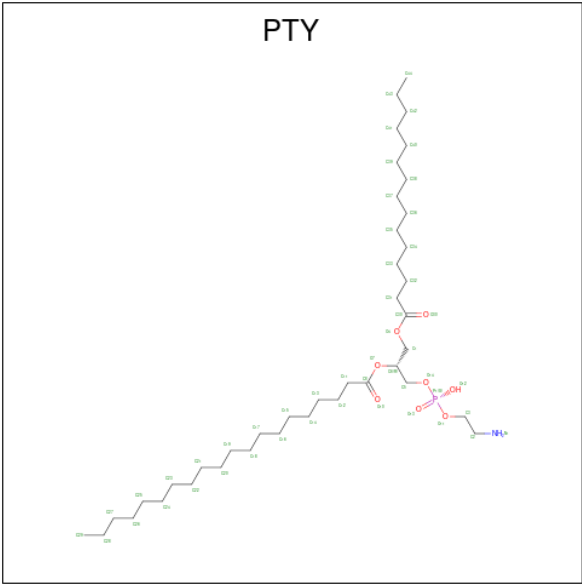
Mol	Chain	Residues	Atoms					AltConf
22	P	1	Total 54	C 44	N 1	O 8	P 1	0
22	P	1	Total 54	C 44	N 1	O 8	P 1	0

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Mol	Chain	Residues	Atoms					AltConf
22	a	1	Total	C	N	O	P	0
			54	44	1	8	1	
22	b	1	Total	C	N	O	P	0
			54	44	1	8	1	
22	l	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 23 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: C₄₀H₈₀NO₈P).



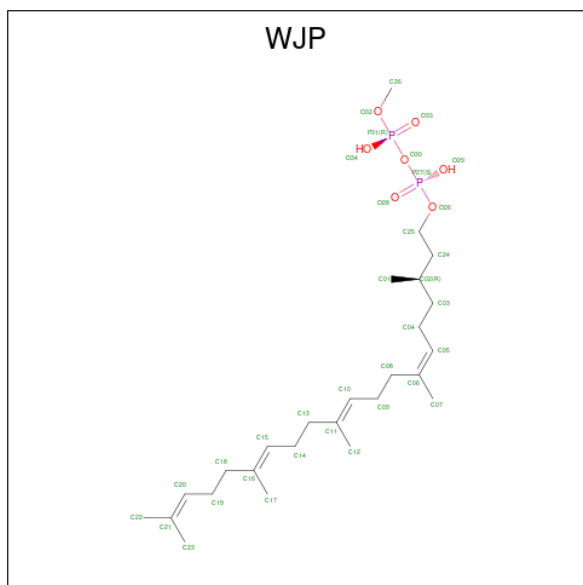
Mol	Chain	Residues	Atoms					AltConf
23	a	1	Total	C	N	O	P	0
			50	40	1	8	1	
23	a	1	Total	C	N	O	P	0
			50	40	1	8	1	
23	a	1	Total	C	N	O	P	0
			50	40	1	8	1	
23	b	1	Total	C	N	O	P	0
			50	40	1	8	1	
23	b	1	Total	C	N	O	P	0
			50	40	1	8	1	
23	p	1	Total	C	N	O	P	0
			50	40	1	8	1	
23	p	1	Total	C	N	O	P	0
			50	40	1	8	1	
23	p	1	Total	C	N	O	P	0
			50	40	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
23	p	1	Total	C	N	O	P	0
			50	40	1	8	1	

- Molecule 24 is methyl (3R,6Z,10E,14E)-3,7,11,15,19-pentamethylicos-6,10,14,18-tetraen-1-yl dihydrogen diphosphate (CCD ID: WJP) (formula: $C_{26}H_{48}O_7P_2$).



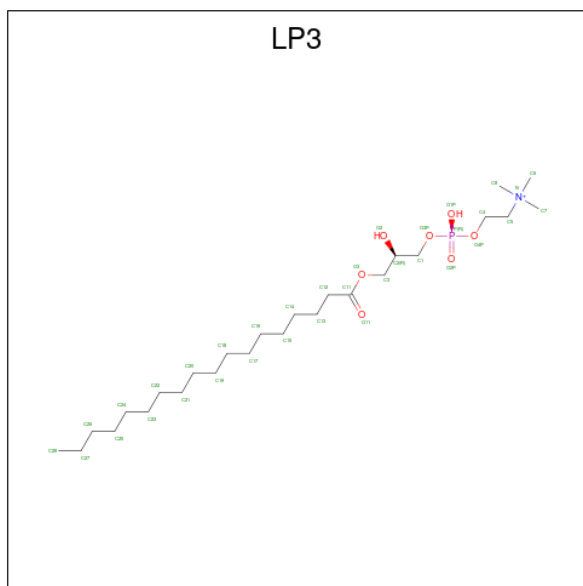
Mol	Chain	Residues	Atoms				AltConf
24	a	1	Total	C	O	P	0
			34	25	7	2	

- Molecule 25 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



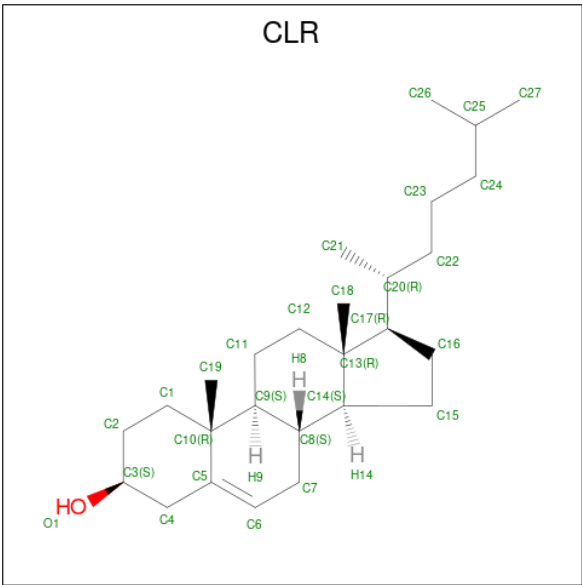
Mol	Chain	Residues	Atoms				AltConf
25	a	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 26 is (7R)-4,7-DIHYDROXY-N,N,N-TRIMETHYL-10-OXO-3,5,9-TRIOXA-4-PHOSPHAHEPTACOSAN-1-AMINIUM 4-OXIDE (CCD ID: LP3) (formula: $C_{26}H_{55}NO_7P$).



Mol	Chain	Residues	Atoms					AltConf
26	a	1	Total	C	N	O	P	0
			35	26	1	7	1	

- Molecule 27 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms			AltConf
27	b	1	Total	C	O	0
			28	27	1	
27	h	1	Total	C	O	0
			28	27	1	
27	h	1	Total	C	O	0
			28	27	1	
27	i	1	Total	C	O	0
			28	27	1	
27	i	1	Total	C	O	0
			28	27	1	
27	i	1	Total	C	O	0
			28	27	1	
27	j	1	Total	C	O	0
			28	27	1	
27	j	1	Total	C	O	0
			28	27	1	
27	j	1	Total	C	O	0
			28	27	1	
27	j	1	Total	C	O	0
			28	27	1	
27	k	1	Total	C	O	0
			28	27	1	
27	k	1	Total	C	O	0
			28	27	1	
27	k	1	Total	C	O	0
			28	27	1	

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Mol	Chain	Residues	Atoms			AltConf
27	l	1	Total	C	O	0
			28	27	1	
27	l	1	Total	C	O	0
			28	27	1	
27	l	1	Total	C	O	0
			28	27	1	
27	l	1	Total	C	O	0
			28	27	1	
27	l	1	Total	C	O	0
			28	27	1	
27	m	1	Total	C	O	0
			28	27	1	
27	m	1	Total	C	O	0
			28	27	1	
27	m	1	Total	C	O	0
			28	27	1	
27	n	1	Total	C	O	0
			28	27	1	
27	n	1	Total	C	O	0
			28	27	1	
27	n	1	Total	C	O	0
			28	27	1	
27	n	1	Total	C	O	0
			28	27	1	
27	n	1	Total	C	O	0
			28	27	1	
27	o	1	Total	C	O	0
			28	27	1	
27	o	1	Total	C	O	0
			28	27	1	
27	o	1	Total	C	O	0
			28	27	1	

SEQUENCE-PLOTS INFOmissingINFO

3 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	198766	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	37.5	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	1.587	Depositor
Minimum map value	-0.952	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.185	Depositor
Map size (Å)	527.36, 527.36, 527.36	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3733333, 1.3733333, 1.3733333	Depositor

4 Model quality

4.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, ADP, PC1, NAG, MAN, BMA, LP3, PTY, CLR, WJP

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	0.15	0/4746	0.28	0/6425
1	B	0.14	0/4746	0.28	0/6425
1	C	0.14	0/4746	0.28	0/6425
2	D	0.15	0/3666	0.29	0/4967
2	E	0.15	0/3666	0.28	0/4967
2	F	0.16	0/3666	0.28	0/4967
3	G	0.12	0/2177	0.28	0/3017
4	H	0.12	0/1744	0.26	0/2332
5	I	0.12	0/1794	0.25	0/2408
5	J	0.13	0/1796	0.28	0/2408
5	K	0.13	0/1671	0.27	0/2255
6	L	0.11	0/877	0.29	0/1183
7	M	0.13	0/850	0.28	0/1140
7	N	0.11	0/921	0.23	0/1226
7	O	0.12	0/718	0.26	0/981
8	P	0.19	0/1707	0.36	0/2324
9	Q	0.11	0/2164	0.25	0/2915
9	R	0.12	0/2189	0.26	0/2947
9	S	0.12	0/2160	0.25	0/2910
10	T	0.08	0/2134	0.20	0/2976
11	U	0.10	0/1158	0.26	0/1601
12	a	0.18	0/6367	0.35	1/8613 (0.0%)
13	b	0.19	0/1537	0.30	0/2088
14	d	0.14	0/2899	0.27	0/3927
15	e	0.16	0/669	0.28	0/920
16	f	0.12	0/682	0.23	0/926
17	g	0.19	0/1083	0.30	0/1466
17	h	0.18	0/1083	0.29	0/1466
17	i	0.18	0/1083	0.30	0/1466
17	j	0.18	0/1083	0.31	0/1466
17	k	0.18	0/1083	0.27	0/1466
17	l	0.18	0/1083	0.28	0/1466

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	m	0.17	0/1083	0.28	0/1466
17	n	0.19	0/1083	0.29	0/1466
17	o	0.19	0/1083	0.31	0/1466
18	p	0.18	0/445	0.29	0/609
All	All	0.15	0/71642	0.28	1/97076 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
12	a	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	a	829	GLU	N-CA-C	-5.12	106.28	112.88

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	a	298	ARG	Sidechain

4.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4651	0	4644	78	0
1	B	4651	0	4644	63	0
1	C	4651	0	4644	60	0
2	D	3595	0	3602	59	0
2	E	3595	0	3602	45	0
2	F	3595	0	3602	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	2155	0	1372	22	0
4	H	1726	0	1835	21	0
5	I	1778	0	1811	18	0
5	J	1779	0	1823	30	0
5	K	1657	0	1605	21	0
6	L	864	0	874	18	0
7	M	845	0	780	13	0
7	N	916	0	917	12	0
7	O	715	0	562	5	0
8	P	1652	0	1579	32	0
9	Q	2130	0	2168	27	0
9	R	2155	0	2201	29	0
9	S	2126	0	2165	14	0
10	T	2136	0	948	0	0
11	U	1150	0	644	7	0
12	a	6212	0	6186	136	0
13	b	1503	0	1551	30	0
14	d	2833	0	2770	37	0
15	e	644	0	659	19	0
16	f	666	0	663	5	0
17	g	1068	0	1136	37	0
17	h	1068	0	1136	13	0
17	i	1068	0	1136	24	0
17	j	1068	0	1136	21	0
17	k	1068	0	1136	11	0
17	l	1068	0	1136	13	0
17	m	1068	0	1136	11	0
17	n	1068	0	1136	21	0
17	o	1068	0	1136	23	0
18	p	432	0	428	16	0
19	V	28	0	25	2	0
19	W	28	0	25	1	0
19	X	28	0	25	2	0
19	Y	28	0	25	1	0
19	Z	28	0	25	0	0
19	c	28	0	25	1	0
19	q	28	0	25	3	0
19	r	28	0	25	1	0
20	s	127	0	106	3	0
21	A	27	0	12	2	0
22	P	108	0	176	4	0
22	a	54	0	88	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	b	54	0	88	0	0
22	l	54	0	88	0	0
23	a	150	0	237	2	0
23	b	100	0	158	1	0
23	p	200	0	316	6	0
24	a	34	0	0	1	0
25	a	14	0	13	3	0
26	a	35	0	54	0	0
27	b	28	0	46	1	0
27	h	56	0	92	3	0
27	i	112	0	184	8	0
27	j	112	0	184	7	0
27	k	84	0	138	2	0
27	l	140	0	230	1	0
27	m	84	0	138	1	0
27	n	140	0	230	7	0
27	o	84	0	138	8	0
All	All	72445	0	71419	947	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (947) 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)
5:I:75:LEU:HD11	7:M:73:VAL:HG11	1.47	0.97
17:g:72:VAL:HG21	17:g:99:VAL:HG21	1.47	0.95
2:D:55:GLY:O	2:D:102:THR:OG1	1.90	0.89
12:a:477:SER:OG	12:a:520:ASP:OD1	1.94	0.86
5:J:54:MET:HE1	7:N:47:TYR:CE2	2.12	0.85
17:j:71:VAL:HG11	27:j:203:CLR:H182	1.57	0.84
1:C:161:LEU:HD11	1:C:296:MET:HE2	1.60	0.84
12:a:748:ALA:HB2	17:g:143:LEU:HD11	1.59	0.82
2:D:106:ASP:OD1	2:D:107:ALA:N	2.13	0.82
19:Y:1:NAG:O3	19:Y:2:NAG:O5	1.97	0.81
14:d:40:GLU:OE1	14:d:40:GLU:N	2.13	0.81
5:K:57:TYR:OH	7:O:48:ARG:O	1.98	0.80
5:K:175:GLU:OE1	5:K:175:GLU:N	2.13	0.80
3:G:106:GLN:OE1	3:G:107:TRP:N	2.14	0.80
9:Q:146:THR:OG1	9:Q:149:ASN:OD1	1.99	0.79
12:a:356:GLN:N	12:a:356:GLN:OE1	2.17	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:125:GLU:OE2	2:F:291:LYS:NZ	2.16	0.78
6:L:37:LEU:HD22	6:L:51:THR:HG21	1.64	0.78
9:R:42:LEU:HD23	9:R:45:ILE:HD12	1.64	0.77
13:b:77:ILE:HG21	17:g:117:GLY:HA2	1.67	0.77
12:a:363:THR:OG1	12:a:384:GLY:O	2.03	0.75
15:e:14:THR:HG1	15:e:49:TYR:HH	1.29	0.75
27:o:202:CLR:H272	27:o:202:CLR:H213	1.69	0.75
1:B:296:MET:HE1	1:B:308:ARG:HD3	1.68	0.74
13:b:55:GLY:O	13:b:59:SER:OG	2.05	0.74
14:d:104:TYR:OH	14:d:323:GLU:OE2	2.05	0.74
2:E:82:ARG:NH1	2:E:101:GLY:O	2.20	0.73
12:a:57:ARG:NH2	12:a:94:MET:SD	2.61	0.73
1:A:151:ASP:OD2	1:A:397:ASN:ND2	2.22	0.72
12:a:175:ILE:HD13	12:a:242:ALA:HB2	1.70	0.72
1:C:459:ARG:NH1	1:C:462:ASP:OD2	2.23	0.72
9:R:195:GLU:N	9:R:195:GLU:OE1	2.22	0.72
12:a:316:GLN:OE1	12:a:317:LYS:N	2.23	0.71
9:R:213:PHE:O	9:R:222:GLN:NE2	2.23	0.71
1:C:159:ASN:ND2	1:C:307:LYS:O	2.23	0.71
17:i:71:VAL:HG21	27:i:203:CLR:H231	1.72	0.70
7:N:52:GLU:O	7:N:56:GLN:NE2	2.24	0.70
5:J:102:LEU:O	5:J:106:VAL:HG13	1.91	0.70
1:A:395:LEU:HD22	9:Q:21:GLN:NE2	2.07	0.70
12:a:176:ASN:OD1	12:a:217:LYS:NZ	2.24	0.70
12:a:757:TRP:CE3	12:a:761:ILE:HD11	2.27	0.70
3:G:51:LEU:HD21	3:G:307:VAL:CG1	2.22	0.70
2:D:106:ASP:OD1	2:D:108:LYS:N	2.24	0.69
1:C:263:LEU:O	1:C:267:SER:OG	2.09	0.69
17:l:11:SER:O	17:l:89:SER:OG	2.04	0.69
1:A:156:VAL:HG21	1:A:205:MET:HE3	1.75	0.69
17:l:50:GLU:OE1	17:l:50:GLU:N	2.25	0.69
1:C:274:TYR:OH	1:C:349:ASP:OD1	2.11	0.68
3:G:317:GLN:OE1	3:G:317:GLN:N	2.25	0.68
23:p:401:PTY:O12	23:p:401:PTY:N1	2.26	0.68
1:A:232:ARG:NH2	1:A:529:ASP:OD1	2.26	0.68
1:B:55:ILE:CD1	1:B:365:LEU:HD21	2.23	0.68
12:a:7:SER:O	12:a:387:ARG:NH1	2.25	0.68
6:L:15:ASP:OD2	6:L:94:LYS:NZ	2.27	0.68
2:D:276:ARG:NH2	2:D:330:ASP:OD1	2.24	0.67
17:g:99:VAL:HG23	17:g:149:ALA:HB2	1.76	0.67
2:E:447:ASP:OD1	2:E:448:ASP:N	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:MET:HE1	1:C:271:VAL:HG13	1.76	0.67
1:A:507:ILE:HD11	1:A:555:VAL:HG21	1.77	0.67
14:d:260:ASP:OD1	14:d:261:TYR:N	2.27	0.67
15:e:14:THR:OG1	15:e:49:TYR:OH	2.03	0.67
1:A:263:LEU:HD22	1:A:347:MET:HE1	1.76	0.66
12:a:132:LEU:HD11	12:a:257:MET:HG2	1.77	0.66
12:a:755:VAL:HG11	17:g:71:VAL:HG22	1.77	0.66
12:a:30:GLU:OE1	12:a:303:ILE:HG13	1.95	0.66
1:B:419:ASP:OD2	1:B:421:VAL:HG12	1.96	0.66
12:a:311:ASN:OD1	12:a:312:ILE:N	2.28	0.66
17:h:48:ARG:NH1	17:h:122:ALA:O	2.29	0.66
5:J:170:GLU:N	5:J:170:GLU:OE1	2.29	0.66
2:E:47:TYR:HB3	2:E:49:THR:HG22	1.78	0.65
2:F:380:ASP:OD2	2:F:393:ASN:ND2	2.28	0.65
6:L:37:LEU:CD2	6:L:51:THR:HG21	2.24	0.65
14:d:217:ASP:OD2	14:d:274:TYR:OH	2.14	0.65
1:B:558:THR:HG21	1:B:565:ILE:HD12	1.78	0.65
5:K:102:LEU:O	5:K:106:VAL:HG13	1.96	0.65
5:I:113:GLN:NE2	5:I:117:ASP:OD1	2.29	0.65
6:L:68:GLN:NE2	6:L:99:ASP:OD1	2.29	0.65
1:C:360:GLU:OE2	2:F:329:THR:OG1	2.09	0.65
2:F:55:GLY:O	2:F:102:THR:OG1	2.07	0.64
2:E:100:GLU:OE1	2:E:100:GLU:N	2.31	0.64
5:J:100:GLN:O	5:J:100:GLN:NE2	2.31	0.64
9:R:42:LEU:HD23	9:R:45:ILE:CD1	2.27	0.64
5:J:54:MET:HE1	7:N:47:TYR:CZ	2.33	0.64
9:Q:256:THR:OG1	9:Q:258:THR:OG1	2.12	0.64
14:d:208:MET:HE1	14:d:316:TYR:CD1	2.33	0.64
2:D:374:GLU:OE2	2:D:401:LEU:HD21	1.98	0.64
13:b:196:LEU:CD1	17:o:74:VAL:HG22	2.28	0.64
1:B:234:LEU:HD21	1:B:448:VAL:HG21	1.78	0.63
17:h:16:VAL:HG11	17:i:90:PHE:O	1.98	0.63
5:J:54:MET:HE2	5:J:54:MET:N	2.14	0.63
12:a:187:LEU:HD11	12:a:222:ILE:HD11	1.79	0.63
2:E:465:GLN:NE2	2:E:469:GLU:O	2.32	0.62
2:F:276:ARG:NH2	2:F:330:ASP:OD1	2.29	0.62
1:A:275:VAL:HG21	1:A:346:MET:HE3	1.81	0.62
5:I:101:ARG:HB2	7:M:100:LEU:HD11	1.81	0.62
5:K:136:CYS:CB	5:K:144:VAL:HG21	2.29	0.62
2:D:283:GLU:HA	2:D:348:ILE:HD11	1.79	0.62
2:F:354:LEU:HD11	2:F:369:THR:HG21	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ILE:HD12	1:A:365:LEU:HD11	1.82	0.62
2:E:462:PHE:O	2:E:471:ARG:NH2	2.32	0.62
2:D:485:ARG:NH1	2:D:504:TYR:O	2.33	0.61
18:p:342:MET:HE3	18:p:342:MET:HA	1.81	0.61
9:S:248:ALA:O	9:S:251:SER:OG	2.10	0.61
9:Q:23:VAL:HG22	9:Q:65:ILE:HG22	1.81	0.61
12:a:36:GLN:NE2	12:a:824:LEU:O	2.34	0.61
17:o:143:LEU:HD11	27:o:202:CLR:H232	1.82	0.61
12:a:535:SER:OG	20:s:1:NAG:H82	2.00	0.61
12:a:594:LYS:NZ	20:s:1:NAG:O5	2.29	0.61
17:n:11:SER:O	17:n:89:SER:OG	2.14	0.61
2:D:272:ILE:CD1	2:D:310:VAL:HG21	2.31	0.61
12:a:743:TRP:CH2	13:b:109:ILE:HD11	2.36	0.61
4:H:94:ILE:HD11	4:H:146:VAL:CG2	2.31	0.60
9:Q:98:ILE:HG22	9:Q:98:ILE:O	2.01	0.60
15:e:70:ASN:OD1	15:e:71:GLU:N	2.33	0.60
18:p:310:VAL:HG11	23:p:401:PTY:H151	1.82	0.60
17:g:16:VAL:HG11	17:h:90:PHE:O	2.01	0.60
2:D:82:ARG:NH1	2:D:101:GLY:O	2.34	0.60
1:A:574:MET:HE2	1:A:611:ALA:HB3	1.83	0.60
1:A:574:MET:HE1	1:A:612:PHE:CG	2.37	0.60
2:E:188:LYS:NZ	2:E:374:GLU:OE2	2.29	0.60
9:R:90:GLU:OE2	9:R:93:ARG:NH1	2.35	0.60
9:S:159:LEU:HD21	9:S:179:PHE:CE1	2.36	0.60
27:n:204:CLR:H182	27:n:205:CLR:H191	1.84	0.60
5:J:208:MET:HE2	5:J:208:MET:HA	1.83	0.59
1:A:486:GLU:OE2	1:A:516:LYS:NZ	2.32	0.59
1:B:111:SER:O	1:B:114:GLN:NE2	2.35	0.59
17:o:120:GLY:O	17:o:124:GLN:N	2.34	0.59
6:L:47:GLU:O	6:L:51:THR:HG22	2.03	0.59
5:I:101:ARG:CB	7:M:100:LEU:HD11	2.33	0.59
17:n:74:VAL:HG11	27:n:201:CLR:H72	1.85	0.59
2:E:283:GLU:HA	2:E:348:ILE:HD11	1.84	0.59
2:E:253:SER:O	2:E:257:VAL:HG23	2.03	0.59
1:A:264:SER:HA	1:A:272:ILE:HD13	1.85	0.59
1:C:95:MET:HE1	1:C:271:VAL:CG1	2.32	0.59
5:J:11:GLN:O	5:J:15:MET:SD	2.61	0.59
1:A:444:HIS:ND1	1:A:444:HIS:O	2.36	0.59
2:F:268:THR:HG21	2:F:309:GLU:OE1	2.02	0.59
12:a:757:TRP:CD2	12:a:761:ILE:HD11	2.38	0.58
27:j:203:CLR:H151	27:j:204:CLR:H181	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:75:LEU:HD11	7:M:73:VAL:CG1	2.28	0.58
13:b:24:ILE:HG23	13:b:28:ILE:HD12	1.85	0.58
12:a:802:HIS:CE1	17:g:140:VAL:HG11	2.38	0.58
3:G:181:TYR:O	3:G:231:LYS:N	2.34	0.58
17:j:71:VAL:HG13	27:j:202:CLR:H161	1.84	0.58
2:D:189:ILE:O	2:D:189:ILE:HG23	2.03	0.58
3:G:219:ASP:N	3:G:222:SER:O	2.37	0.58
2:D:183:ILE:HG12	2:D:189:ILE:HD13	1.85	0.58
3:G:65:VAL:HG21	3:G:297:ILE:HD12	1.85	0.58
12:a:211:THR:HG22	12:a:213:ASP:OD1	2.03	0.58
12:a:713:ASP:OD1	12:a:713:ASP:N	2.33	0.58
2:E:400:ARG:O	2:E:403:LYS:NZ	2.37	0.58
3:G:51:LEU:HD21	3:G:307:VAL:HG13	1.86	0.58
1:C:234:LEU:HD21	1:C:448:VAL:HG21	1.84	0.58
5:J:116:LEU:HD21	5:J:144:VAL:HG23	1.85	0.58
5:K:185:ASN:OD1	5:K:188:ARG:N	2.36	0.58
12:a:444:PHE:O	12:a:447:ARG:NH1	2.35	0.57
1:B:95:MET:HE3	1:B:337:PHE:CZ	2.39	0.57
17:k:47:MET:SD	17:k:47:MET:N	2.77	0.57
14:d:233:SER:OG	14:d:236:ASP:OD2	2.21	0.57
1:C:604:LEU:O	1:C:608:MET:HG3	2.05	0.57
1:A:172:SER:OG	1:A:201:GLU:OE2	2.20	0.57
1:B:558:THR:HG21	1:B:565:ILE:CD1	2.34	0.57
2:D:206:ILE:O	2:D:210:ALA:HB2	2.04	0.57
12:a:592:PHE:O	12:a:596:THR:HG23	2.05	0.57
2:D:192:PHE:CE1	2:D:354:LEU:HD21	2.40	0.57
7:N:11:LEU:HD12	12:a:168:LEU:HD11	1.86	0.57
17:j:47:MET:SD	18:p:342:MET:HE1	2.45	0.57
19:q:1:NAG:O3	19:q:2:NAG:O5	2.19	0.57
2:D:172:THR:HG21	2:D:183:ILE:HD12	1.87	0.57
12:a:295:ILE:HD11	12:a:831:ILE:HA	1.87	0.57
17:n:143:LEU:HD11	27:n:204:CLR:H231	1.87	0.57
1:A:115:SER:OG	5:I:226:ASP:OD2	2.15	0.56
7:N:42:MET:N	7:N:42:MET:HE2	2.20	0.56
12:a:557:LEU:HD22	12:a:573:PHE:CE2	2.40	0.56
1:B:495:LEU:HD13	4:H:29:GLY:HA2	1.86	0.56
1:C:95:MET:HE2	1:C:337:PHE:CE1	2.39	0.56
2:D:97:GLN:OE1	2:D:310:VAL:HG11	2.05	0.56
2:E:64:LYS:NZ	5:J:129:GLU:OE2	2.27	0.56
1:C:242:GLN:OE1	1:C:268:ASN:ND2	2.39	0.56
1:C:369:PRO:O	4:H:196:ARG:NH1	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:269:ILE:HD12	2:D:310:VAL:HG22	1.86	0.56
17:j:23:MET:HE3	17:j:23:MET:O	2.05	0.56
4:H:94:ILE:HD11	4:H:146:VAL:HG21	1.87	0.56
17:l:87:TYR:OH	17:l:155:LYS:NZ	2.39	0.56
1:A:167:MET:HE1	1:A:339:ASP:HB2	1.87	0.56
1:A:157:ASN:OD1	1:A:163:LYS:NZ	2.36	0.56
1:B:98:ILE:HD13	2:E:161:GLN:OE1	2.06	0.56
1:A:436:ASP:O	1:A:447:SER:OG	2.23	0.56
5:K:208:MET:HE2	5:K:208:MET:HA	1.88	0.56
2:D:235:GLY:N	2:D:262:ASN:O	2.36	0.56
2:D:411:THR:OG1	2:D:412:ARG:N	2.31	0.56
9:S:222:GLN:O	9:S:226:VAL:HG23	2.06	0.56
17:i:23:MET:HE3	17:i:23:MET:O	2.05	0.56
1:A:372:SER:O	1:A:372:SER:OG	2.16	0.56
2:E:201:GLU:OE1	2:E:201:GLU:N	2.39	0.56
17:h:79:SER:O	17:h:79:SER:OG	2.21	0.56
9:S:201:LYS:HG3	9:S:260:LEU:HD21	1.89	0.55
13:b:196:LEU:HD13	17:o:74:VAL:HG22	1.88	0.55
1:C:161:LEU:HD11	1:C:296:MET:CE	2.34	0.55
1:B:55:ILE:HD12	1:B:365:LEU:HD21	1.87	0.55
2:F:126:ASP:OD2	5:K:212:ARG:NH2	2.36	0.55
12:a:208:ASP:OD1	12:a:213:ASP:N	2.38	0.55
17:j:71:VAL:HG11	27:j:203:CLR:C18	2.32	0.55
17:i:35:ALA:HB3	18:p:331:MET:HE1	1.89	0.55
1:B:573:HIS:ND1	1:B:615:LEU:HD13	2.21	0.55
6:L:13:ASP:O	6:L:17:VAL:HG23	2.07	0.55
12:a:135:THR:OG1	12:a:221:ILE:HD11	2.06	0.55
8:P:270:VAL:CG1	8:P:279:LEU:HD11	2.37	0.55
14:d:338:GLN:OE1	14:d:338:GLN:N	2.39	0.55
15:e:2:THR:HG23	15:e:2:THR:O	2.06	0.55
1:C:288:LEU:HD23	1:C:311:LEU:HD23	1.89	0.55
2:E:55:GLY:O	2:E:102:THR:OG1	2.14	0.55
2:E:189:ILE:HG23	2:E:189:ILE:O	2.06	0.55
3:G:40:ILE:CD1	3:G:299:ALA:HB1	2.37	0.55
6:L:17:VAL:O	6:L:21:LEU:HD22	2.07	0.55
12:a:26:VAL:HG11	12:a:307:LEU:HD21	1.89	0.55
12:a:138:PHE:HD2	12:a:221:ILE:HD12	1.71	0.55
12:a:249:GLU:N	12:a:249:GLU:OE1	2.40	0.55
12:a:609:LEU:CD2	12:a:629:LEU:HD11	2.36	0.55
12:a:801:LEU:HB3	17:g:136:ILE:HD13	1.89	0.55
1:B:366:ALA:HA	2:E:317:VAL:HG21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:253:SER:O	2:D:257:VAL:HG23	2.06	0.54
1:B:540:MET:O	1:B:544:MET:HG2	2.07	0.54
17:j:112:ILE:HD13	18:p:331:MET:HE2	1.89	0.54
12:a:298:ARG:HD2	12:a:830:HIS:HB3	1.88	0.54
17:k:16:VAL:HG11	17:l:90:PHE:O	2.07	0.54
17:n:71:VAL:HG22	27:n:202:CLR:H17	1.89	0.54
1:A:55:ILE:CD1	1:A:365:LEU:HD11	2.38	0.54
14:d:32:ASP:O	14:d:36:LEU:HD23	2.06	0.54
12:a:751:GLN:HG3	17:g:150:LEU:HD13	1.89	0.54
1:C:90:LEU:CD2	1:C:333:LEU:HD23	2.37	0.54
2:F:300:MET:HE2	2:F:335:TYR:CE1	2.43	0.54
7:N:8:ILE:HD12	12:a:223:PHE:CE1	2.43	0.54
1:A:95:MET:HE2	1:A:95:MET:HA	1.90	0.54
1:C:156:VAL:HG21	1:C:205:MET:HE3	1.90	0.54
2:E:60:LEU:HD21	2:E:112:CYS:SG	2.48	0.54
12:a:476:GLY:O	15:e:4:HIS:NE2	2.39	0.54
2:F:123:VAL:HG21	2:F:151:LEU:HD12	1.89	0.54
2:F:203:ALA:HB2	2:F:353:ILE:CD1	2.38	0.54
9:R:94:LEU:HD22	9:R:126:TYR:OH	2.08	0.54
9:R:45:ILE:HG12	9:R:112:TYR:CD2	2.43	0.54
12:a:743:TRP:HH2	13:b:109:ILE:HD11	1.73	0.54
9:Q:148:LYS:NZ	9:Q:188:MET:O	2.41	0.53
17:m:81:THR:HG23	17:m:84:ILE:HG23	1.90	0.53
5:J:38:PHE:CD2	7:N:36:ALA:HB2	2.44	0.53
5:J:55:GLU:OE1	5:J:56:TYR:N	2.41	0.53
8:P:410:ASP:OD1	8:P:410:ASP:N	2.41	0.53
9:S:170:GLU:OE1	9:S:170:GLU:N	2.41	0.53
2:F:126:ASP:OD2	5:K:87:ARG:NH1	2.38	0.53
3:G:289:GLU:OE1	3:G:290:ALA:N	2.42	0.53
5:K:136:CYS:HB2	5:K:144:VAL:HG21	1.90	0.53
9:Q:209:GLU:N	9:Q:209:GLU:OE1	2.42	0.53
9:R:42:LEU:HB3	9:R:45:ILE:HD12	1.91	0.53
12:a:175:ILE:CD1	12:a:242:ALA:HB2	2.36	0.53
1:C:486:GLU:OE1	1:C:516:LYS:NZ	2.41	0.53
2:E:82:ARG:NH2	2:E:103:SER:O	2.42	0.53
4:H:97:LYS:HB3	4:H:108:VAL:HG23	1.90	0.53
13:b:62:VAL:HG13	17:g:141:LEU:HB3	1.89	0.53
17:i:97:LEU:HD21	18:p:317:LEU:HD21	1.91	0.53
12:a:187:LEU:HD11	12:a:222:ILE:CD1	2.39	0.53
17:g:72:VAL:CG2	17:g:99:VAL:HG21	2.32	0.53
5:J:119:LEU:O	5:J:194:ASN:ND2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:i:47:MET:HE2	17:i:47:MET:HA	1.90	0.53
1:B:562:ASP:OD1	1:B:563:ASN:N	2.42	0.53
2:F:123:VAL:HG21	2:F:151:LEU:CD1	2.39	0.53
8:P:270:VAL:HG11	8:P:279:LEU:HD11	1.91	0.53
12:a:748:ALA:CB	17:g:143:LEU:HD11	2.36	0.53
2:D:60:LEU:HD21	2:D:112:CYS:SG	2.49	0.52
17:n:24:VAL:HG13	17:o:101:LEU:HB3	1.91	0.52
1:A:25:SER:O	1:A:364:ARG:NH1	2.42	0.52
2:F:411:THR:HG21	2:F:415:HIS:ND1	2.24	0.52
12:a:49:ARG:O	12:a:52:VAL:HG13	2.10	0.52
17:i:154:THR:HG21	27:i:203:CLR:H192	1.90	0.52
2:E:49:THR:HG21	2:E:61:ASP:O	2.08	0.52
17:i:35:ALA:O	17:i:39:THR:HG23	2.09	0.52
12:a:27:SER:HA	12:a:303:ILE:HD11	1.90	0.52
14:d:247:LEU:HD23	14:d:271:TYR:CE1	2.44	0.52
5:J:11:GLN:O	5:J:15:MET:CE	2.58	0.52
14:d:284:ASN:ND2	14:d:287:ASP:OD2	2.43	0.52
1:C:280:ARG:NE	2:F:373:THR:O	2.41	0.52
9:Q:168:ILE:HD12	9:Q:169:THR:N	2.25	0.52
12:a:22:ALA:HB1	12:a:319:LEU:HD12	1.90	0.52
12:a:801:LEU:CD1	17:g:136:ILE:HG21	2.39	0.52
14:d:137:GLN:NE2	14:d:157:ASP:O	2.42	0.52
17:i:71:VAL:HG11	27:i:203:CLR:H183	1.92	0.52
17:o:11:SER:O	17:o:89:SER:OG	2.27	0.52
7:N:15:GLU:OE2	12:a:166:LEU:N	2.43	0.52
9:S:33:MET:HE1	9:S:45:ILE:HG22	1.92	0.52
14:d:75:LYS:O	14:d:79:VAL:HG23	2.09	0.52
1:C:407:VAL:O	1:C:407:VAL:HG12	2.10	0.52
12:a:27:SER:OG	12:a:28:GLU:OE2	2.28	0.52
12:a:35:VAL:HG22	12:a:325:CYS:SG	2.49	0.52
8:P:344:ASN:O	8:P:344:ASN:ND2	2.43	0.51
12:a:336:ALA:HA	12:a:339:ARG:HE	1.74	0.51
1:A:574:MET:HE2	1:A:611:ALA:CB	2.40	0.51
5:J:36:GLU:O	5:J:40:ILE:HG22	2.10	0.51
6:L:74:VAL:HG12	6:L:74:VAL:O	2.11	0.51
12:a:377:ILE:HG23	12:a:804:LEU:CD2	2.40	0.51
13:b:59:SER:HB2	17:g:101:LEU:HD23	1.92	0.51
17:g:99:VAL:HG23	17:g:149:ALA:CB	2.40	0.51
2:D:229:ILE:HB	2:D:257:VAL:HG22	1.93	0.51
14:d:279:GLU:OE2	14:d:280:GLY:N	2.44	0.51
27:k:201:CLR:H272	27:k:201:CLR:H221	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:72:MET:SD	7:N:69:LEU:HD23	2.51	0.51
12:a:111:ILE:HD11	12:a:278:HIS:ND1	2.25	0.51
14:d:11:VAL:O	17:g:36:LYS:NZ	2.40	0.51
1:A:558:THR:HG21	1:A:565:ILE:CD1	2.41	0.51
1:B:80:LEU:HD23	1:B:81:ARG:H	1.75	0.51
1:B:376:ALA:HB1	2:F:309:GLU:HA	1.93	0.51
17:k:17:MET:O	17:k:21:SER:OG	2.26	0.51
1:A:261:GLN:NE2	1:A:286:GLU:OE2	2.38	0.51
5:I:123:GLY:HA3	5:I:183:ILE:HD13	1.92	0.51
8:P:399:ASN:OD1	19:q:1:NAG:O5	2.16	0.51
8:P:429:MET:HE1	17:g:17:MET:SD	2.51	0.51
12:a:331:ASP:OD1	12:a:331:ASP:N	2.43	0.51
17:n:35:ALA:O	17:n:39:THR:HG23	2.10	0.51
1:A:511:VAL:HG11	1:A:548:TYR:HB2	1.92	0.51
2:E:60:LEU:HD21	2:E:112:CYS:HB2	1.93	0.51
12:a:325:CYS:SG	12:a:333:ILE:HD13	2.51	0.51
17:g:140:VAL:HA	17:g:143:LEU:HB3	1.93	0.51
17:i:53:MET:HE2	17:i:53:MET:HA	1.93	0.51
17:m:11:SER:O	17:m:89:SER:OG	2.20	0.51
1:B:55:ILE:HD11	1:B:365:LEU:HD21	1.93	0.51
2:D:100:GLU:N	2:D:100:GLU:OE1	2.44	0.51
2:F:484:LEU:HD13	2:F:495:ILE:HD11	1.93	0.51
3:G:61:LEU:HB3	3:G:297:ILE:HD13	1.93	0.51
8:P:314:THR:HG23	8:P:314:THR:O	2.09	0.51
12:a:527:THR:N	15:e:67:GLN:O	2.42	0.51
1:A:167:MET:HE1	1:A:339:ASP:CB	2.41	0.51
1:B:438:LYS:O	1:B:442:ARG:HG2	2.11	0.51
1:C:95:MET:HE2	1:C:337:PHE:CZ	2.46	0.51
2:E:175:SER:OG	2:E:471:ARG:NH2	2.39	0.51
12:a:543:ILE:HG12	12:a:588:VAL:HG13	1.93	0.51
12:a:755:VAL:HG11	17:g:71:VAL:CG2	2.41	0.51
12:a:793:ILE:HD12	22:a:901:PC1:H2G1	1.92	0.51
1:B:391:ARG:NH1	1:B:401:GLU:OE1	2.44	0.50
7:M:45:GLU:OE2	7:M:46:GLN:N	2.44	0.50
9:Q:83:ARG:NH2	9:Q:116:LYS:O	2.44	0.50
12:a:170:PHE:CE2	12:a:221:ILE:HG23	2.46	0.50
13:b:59:SER:O	13:b:63:VAL:HG23	2.12	0.50
1:C:190:VAL:HG13	1:C:190:VAL:O	2.10	0.50
8:P:412:ALA:O	22:P:501:PC1:H152	2.11	0.50
2:D:106:ASP:OD1	2:D:106:ASP:C	2.55	0.50
12:a:406:MET:HE2	12:a:742:LEU:HD23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:d:204:THR:HA	14:d:311:HIS:HB2	1.93	0.50
17:j:72:VAL:HG11	17:j:99:VAL:HG11	1.92	0.50
1:B:491:GLU:O	1:B:495:LEU:HG	2.11	0.50
9:R:29:ILE:HG21	9:R:52:VAL:HG21	1.94	0.50
12:a:794:MET:HE3	17:g:60:VAL:HG11	1.93	0.50
1:A:397:ASN:HB2	1:A:398:PRO:HD3	1.94	0.50
12:a:620:SER:O	12:a:620:SER:OG	2.17	0.50
12:a:126:THR:HA	12:a:265:ILE:HD11	1.93	0.50
15:e:75:TYR:CD2	16:f:41:ILE:HD12	2.47	0.50
17:o:44:MET:HE2	17:o:118:VAL:HG13	1.94	0.50
2:E:60:LEU:HD21	2:E:112:CYS:CB	2.42	0.49
13:b:89:LYS:NZ	13:b:166:ASP:OD2	2.41	0.49
1:C:558:THR:HG21	1:C:565:ILE:CD1	2.42	0.49
2:D:272:ILE:HD11	2:D:310:VAL:HG21	1.93	0.49
5:J:121:LEU:HD22	5:J:154:MET:HE3	1.94	0.49
12:a:48:GLN:OE1	12:a:48:GLN:HA	2.11	0.49
13:b:36:ASP:HB3	13:b:39:TRP:HB3	1.94	0.49
17:n:24:VAL:O	17:n:28:MET:HG3	2.12	0.49
1:C:102:ILE:O	1:C:102:ILE:CG2	2.59	0.49
2:F:121:THR:HG21	2:F:277:LEU:HG	1.94	0.49
8:P:251:PRO:HD2	19:X:2:NAG:H83	1.95	0.49
2:E:226:ASN:OD1	2:E:226:ASN:N	2.45	0.49
27:h:201:CLR:H213	17:i:147:ILE:HD13	1.94	0.49
1:A:116:ILE:HG21	2:D:341:VAL:HG11	1.94	0.49
1:C:284:MET:SD	1:C:313:ALA:HB1	2.52	0.49
3:G:104:ARG:NH1	3:G:104:ARG:HA	2.27	0.49
8:P:328:VAL:HG12	8:P:328:VAL:O	2.13	0.49
9:R:94:LEU:HD13	9:R:168:ILE:HD12	1.93	0.49
12:a:22:ALA:CB	12:a:319:LEU:HD12	2.41	0.49
12:a:823:PHE:CD1	12:a:823:PHE:C	2.90	0.49
2:D:306:ALA:O	2:D:310:VAL:HG23	2.12	0.49
2:E:168:GLU:OE1	2:E:185:ARG:NH2	2.44	0.49
13:b:18:CYS:SG	27:b:304:CLR:H272	2.53	0.49
17:g:143:LEU:HD12	17:g:143:LEU:O	2.13	0.49
17:n:17:MET:HE1	17:o:97:LEU:HD12	1.94	0.49
3:G:48:LEU:HD21	5:J:18:PHE:CD2	2.48	0.49
14:d:79:VAL:HG21	14:d:131:PRO:HB2	1.94	0.49
3:G:57:GLU:OE2	3:G:57:GLU:HA	2.13	0.49
5:K:134:VAL:HG22	5:K:183:ILE:HD12	1.95	0.49
1:A:346:MET:HE1	1:A:385:PHE:CZ	2.48	0.49
1:C:529:ASP:OD2	1:C:529:ASP:C	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:180:MET:HA	2:D:402:MET:HE1	1.95	0.49
2:D:327:MET:HE3	2:D:331:LEU:HD11	1.95	0.49
6:L:13:ASP:OD1	6:L:14:GLU:N	2.46	0.49
1:C:241:VAL:O	1:C:244:GLY:N	2.44	0.49
2:F:68:TYR:OH	2:F:314:ARG:NH2	2.43	0.49
14:d:90:TYR:O	14:d:94:ALA:N	2.40	0.49
1:A:356:GLU:O	1:A:360:GLU:HG3	2.12	0.48
1:A:558:THR:HG21	1:A:565:ILE:HD11	1.95	0.48
8:P:446:MET:HE2	17:g:39:THR:HG23	1.95	0.48
1:A:298:VAL:O	1:A:298:VAL:HG13	2.13	0.48
1:A:425:THR:O	1:A:429:VAL:HG22	2.14	0.48
7:M:75:GLN:OE1	7:M:79:ARG:NE	2.46	0.48
17:n:67:ILE:O	17:n:71:VAL:HG23	2.12	0.48
1:A:334:SER:HA	1:A:344:VAL:HG11	1.95	0.48
3:G:42:ASP:OD1	3:G:42:ASP:C	2.57	0.48
7:M:93:GLU:OE2	7:M:93:GLU:HA	2.14	0.48
8:P:266:GLN:HB3	8:P:392:ASN:HB2	1.96	0.48
9:Q:139:TYR:OH	9:Q:149:ASN:ND2	2.46	0.48
1:A:394:CYS:SG	1:A:402:GLY:N	2.87	0.48
8:P:405:PHE:O	18:p:294:ASN:ND2	2.41	0.48
13:b:133:ALA:HA	13:b:201:VAL:CG2	2.43	0.48
17:n:16:VAL:HG11	17:o:90:PHE:O	2.13	0.48
1:A:226:PRO:HG3	1:A:461:LEU:HD22	1.95	0.48
14:d:106:ILE:O	14:d:109:VAL:HG12	2.13	0.48
1:A:442:ARG:NH1	2:D:431:ASP:OD2	2.46	0.48
2:D:180:MET:O	2:D:181:ASN:ND2	2.47	0.48
6:L:39:VAL:HG22	6:L:48:ILE:HD12	1.96	0.48
9:S:94:LEU:HD22	9:S:168:ILE:HD11	1.96	0.48
1:A:574:MET:HE1	1:A:612:PHE:CD2	2.48	0.48
1:C:425:THR:O	1:C:429:VAL:HG22	2.14	0.48
4:H:83:VAL:O	4:H:119:TYR:OH	2.27	0.48
8:P:278:ASP:C	8:P:278:ASP:OD1	2.56	0.48
8:P:352:VAL:HG22	8:P:378:LEU:HD23	1.95	0.48
14:d:337:ALA:O	14:d:339:ARG:NE	2.46	0.48
27:n:201:CLR:H151	27:n:202:CLR:H152	1.95	0.48
1:C:486:GLU:OE2	1:C:487:GLU:N	2.46	0.48
2:D:149:ASP:OD2	5:I:222:ARG:NH2	2.45	0.48
2:D:450:LEU:HD22	2:D:486:ILE:HG22	1.95	0.48
4:H:122:THR:HG23	4:H:131:LEU:HD23	1.94	0.48
12:a:138:PHE:CD2	12:a:221:ILE:HD12	2.49	0.48
17:l:84:ILE:HG23	17:l:84:ILE:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:a:801:LEU:HD13	17:g:136:ILE:HG21	1.95	0.48
1:C:297:GLU:HG2	1:C:302:VAL:HG22	1.96	0.48
2:E:203:ALA:HB2	2:E:353:ILE:HD11	1.95	0.48
9:Q:86:LEU:HD21	9:Q:122:TRP:CD1	2.49	0.48
11:U:72:HIS:O	12:a:482:ARG:NH2	2.46	0.48
9:R:112:TYR:CD1	9:R:112:TYR:C	2.92	0.47
12:a:222:ILE:HG21	12:a:233:VAL:HG11	1.95	0.47
17:g:44:MET:HE3	17:g:118:VAL:CG1	2.44	0.47
17:j:49:PRO:O	17:j:52:ILE:HG22	2.13	0.47
2:E:183:ILE:HG12	2:E:189:ILE:HG21	1.96	0.47
11:U:49:VAL:O	11:U:58:ALA:N	2.47	0.47
12:a:26:VAL:HG11	12:a:307:LEU:CD2	2.43	0.47
15:e:28:VAL:HG21	15:e:38:ILE:HG13	1.95	0.47
1:A:149:GLY:O	9:Q:21:GLN:NE2	2.42	0.47
1:B:133:TRP:HB2	1:B:205:MET:HE1	1.96	0.47
2:F:100:GLU:OE1	2:F:100:GLU:N	2.42	0.47
2:F:236:VAL:HG22	2:F:240:THR:HB	1.96	0.47
4:H:198:GLU:OE2	4:H:198:GLU:N	2.47	0.47
9:S:220:GLU:OE1	9:S:220:GLU:N	2.42	0.47
17:g:44:MET:HE3	17:g:118:VAL:HG13	1.97	0.47
1:C:264:SER:O	1:C:308:ARG:NH2	2.41	0.47
12:a:557:LEU:HD22	12:a:573:PHE:CZ	2.48	0.47
17:n:72:VAL:HG21	17:n:99:VAL:HG21	1.96	0.47
2:F:82:ARG:NH1	2:F:101:GLY:O	2.48	0.47
17:k:44:MET:HG3	17:k:122:ALA:HB2	1.96	0.47
4:H:72:ALA:HB1	4:H:131:LEU:HD12	1.97	0.47
9:R:42:LEU:CD2	9:R:45:ILE:HD12	2.41	0.47
12:a:377:ILE:HD12	12:a:804:LEU:HD21	1.96	0.47
1:A:412:PRO:O	2:D:371:TYR:OH	2.25	0.47
1:B:88:VAL:HG13	1:B:211:VAL:HG12	1.97	0.47
2:D:201:GLU:OE1	2:D:201:GLU:N	2.45	0.47
2:F:158:ILE:HD11	2:F:287:TYR:CE2	2.50	0.47
2:F:193:SER:O	2:F:356:MET:N	2.46	0.47
4:H:111:HIS:C	4:H:111:HIS:CD2	2.92	0.47
4:H:130:GLN:HA	4:H:130:GLN:OE1	2.14	0.47
5:I:38:PHE:CD2	7:M:36:ALA:HB2	2.48	0.47
6:L:31:ASN:OD1	6:L:31:ASN:C	2.57	0.47
7:O:74:GLU:C	7:O:74:GLU:OE1	2.58	0.47
12:a:399:PHE:HB3	12:a:400:PRO:HD3	1.96	0.47
12:a:489:ASN:HB2	25:a:906:NAG:H2	1.97	0.47
13:b:175:LYS:HB3	17:o:52:ILE:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:e:30:LYS:CD	15:e:30:LYS:N	2.78	0.47
17:j:52:ILE:HD12	17:k:127:LEU:HA	1.97	0.47
1:C:34:MET:HE1	1:C:43:VAL:HG11	1.96	0.47
2:F:236:VAL:HG13	2:F:236:VAL:O	2.14	0.47
9:Q:181:LEU:HD23	9:Q:203:TYR:HB2	1.95	0.47
2:D:459:GLU:O	2:D:464:THR:OG1	2.24	0.47
2:E:166:PRO:HG2	2:E:401:LEU:HD13	1.96	0.47
4:H:62:MET:HE2	4:H:141:ALA:HB1	1.96	0.47
2:E:279:LEU:CD1	2:E:334:ILE:HG23	2.45	0.47
17:j:44:MET:HG3	17:j:122:ALA:HB2	1.97	0.47
17:j:128:PHE:O	17:j:132:ILE:HG12	2.14	0.47
17:k:85:THR:HG23	17:k:88:ARG:H	1.79	0.47
1:C:558:THR:HG21	1:C:565:ILE:HD12	1.97	0.46
2:D:327:MET:HE2	2:D:368:LEU:HD22	1.96	0.46
2:D:354:LEU:CD2	2:D:369:THR:HG21	2.45	0.46
5:I:192:VAL:HG13	5:I:192:VAL:O	2.15	0.46
14:d:21:ARG:NH2	14:d:308:ASN:O	2.47	0.46
15:e:79:LEU:HD11	16:f:36:HIS:O	2.15	0.46
1:A:197:GLU:HA	1:A:197:GLU:OE1	2.15	0.46
9:S:151:PHE:O	9:S:155:MET:HG3	2.15	0.46
1:A:462:ASP:OD1	1:A:463:GLU:N	2.48	0.46
13:b:41:LEU:O	13:b:135:TYR:OH	2.30	0.46
17:j:11:SER:O	17:j:89:SER:OG	2.28	0.46
17:m:22:ALA:O	17:m:26:SER:OG	2.14	0.46
17:o:45:SER:HB2	17:o:52:ILE:HD11	1.98	0.46
2:D:74:LEU:HD23	2:D:112:CYS:SG	2.55	0.46
5:J:136:CYS:CB	5:J:144:VAL:HG21	2.45	0.46
8:P:256:ASP:OD1	8:P:256:ASP:C	2.58	0.46
15:e:36:VAL:O	15:e:40:MET:HG3	2.14	0.46
2:E:174:ILE:HG23	2:E:390:PRO:HG3	1.98	0.46
2:E:459:GLU:O	2:E:464:THR:OG1	2.31	0.46
1:B:40:TYR:N	1:B:54:ILE:O	2.40	0.46
1:B:43:VAL:HG21	1:B:64:ILE:HD13	1.97	0.46
1:B:251:ALA:HB2	1:B:435:LEU:HD22	1.97	0.46
1:C:536:LYS:O	1:C:540:MET:HG3	2.15	0.46
12:a:135:THR:HA	12:a:221:ILE:HD11	1.97	0.46
12:a:240:PHE:O	12:a:241:ARG:HG2	2.15	0.46
2:E:60:LEU:HD22	2:E:114:PHE:CE1	2.51	0.46
8:P:352:VAL:HG22	8:P:378:LEU:CD2	2.45	0.46
9:R:42:LEU:HD21	9:R:108:ILE:HG21	1.96	0.46
13:b:114:MET:HE3	13:b:201:VAL:HG12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:m:16:VAL:CG1	17:n:91:LEU:HD23	2.46	0.46
1:A:38:ALA:HA	2:E:106:ASP:HB3	1.98	0.46
1:A:77:ASP:OD1	7:M:113:ASN:ND2	2.43	0.46
1:B:161:LEU:HD21	1:B:296:MET:HE3	1.96	0.46
2:F:300:MET:HE1	2:F:334:ILE:HG21	1.98	0.46
5:I:55:GLU:OE1	5:I:56:TYR:N	2.48	0.46
9:Q:217:LEU:HD12	9:Q:217:LEU:H	1.81	0.46
13:b:91:LEU:HD23	13:b:95:ILE:HG12	1.98	0.46
17:i:71:VAL:CG1	27:i:203:CLR:H183	2.46	0.46
17:n:129:VAL:O	17:n:133:LEU:HD23	2.16	0.46
17:h:114:GLY:O	17:h:118:VAL:HG22	2.15	0.46
1:B:503:GLU:O	1:B:507:ILE:HG12	2.16	0.46
1:B:588:ASP:OD2	1:B:591:LYS:NZ	2.38	0.46
9:R:39:GLU:N	9:R:39:GLU:OE1	2.48	0.46
9:R:246:LEU:CD1	9:R:266:ILE:HG21	2.46	0.46
17:j:52:ILE:HG23	17:j:53:MET:N	2.31	0.46
1:C:615:LEU:O	1:C:615:LEU:HD23	2.16	0.45
1:B:220:LYS:HG2	1:B:392:VAL:HG12	1.98	0.45
1:C:331:ILE:HD13	1:C:406:ILE:HD11	1.97	0.45
6:L:39:VAL:HG21	6:L:70:ILE:HD13	1.98	0.45
11:U:72:HIS:O	12:a:482:ARG:NH1	2.47	0.45
14:d:208:MET:HE1	14:d:316:TYR:CE1	2.51	0.45
16:f:35:VAL:HG12	16:f:35:VAL:O	2.16	0.45
1:B:349:ASP:O	1:B:409:ALA:HB3	2.15	0.45
1:B:581:LEU:HD23	1:B:584:MET:SD	2.56	0.45
12:a:51:PHE:HB2	12:a:308:ASN:OD1	2.16	0.45
12:a:396:VAL:HG11	15:e:40:MET:SD	2.57	0.45
15:e:25:PRO:O	15:e:28:VAL:HG22	2.17	0.45
17:l:22:ALA:HB2	17:l:96:GLY:HA2	1.97	0.45
17:n:81:THR:HG22	17:n:82:ASP:N	2.32	0.45
1:A:159:ASN:ND2	1:A:307:LYS:O	2.45	0.45
1:B:34:MET:HE2	1:B:64:ILE:HD11	1.99	0.45
1:B:66:VAL:HG12	1:B:68:GLU:H	1.80	0.45
1:C:334:SER:OG	1:C:404:VAL:HG13	2.16	0.45
2:D:380:ASP:N	2:D:391:PRO:O	2.37	0.45
8:P:313:ALA:HB3	19:V:1:NAG:H82	1.98	0.45
14:d:224:THR:HG23	14:d:241:PHE:CZ	2.51	0.45
15:e:70:ASN:O	15:e:73:ILE:HG22	2.17	0.45
17:h:88:ARG:O	17:h:92:GLN:HG3	2.16	0.45
17:m:150:LEU:HD22	27:m:202:CLR:H12	1.98	0.45
1:A:234:LEU:HD21	1:A:448:VAL:HG21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Q:111:GLN:NE2	9:Q:169:THR:OG1	2.38	0.45
12:a:505:PRO:HG2	12:a:600:ALA:HB2	1.98	0.45
17:l:16:VAL:CG1	17:l:80:LEU:HD21	2.46	0.45
1:C:486:GLU:OE2	1:C:486:GLU:C	2.60	0.45
8:P:376:SER:O	8:P:376:SER:OG	2.26	0.45
12:a:567:LEU:HD11	12:a:658:ILE:HG21	1.98	0.45
1:B:495:LEU:HD13	4:H:29:GLY:CA	2.47	0.45
2:F:504:TYR:N	2:F:505:PRO:HD2	2.32	0.45
13:b:140:ALA:O	13:b:144:VAL:HG12	2.17	0.45
1:B:479:ALA:HB2	1:B:541:LEU:HD11	1.98	0.45
5:K:103:SER:O	5:K:106:VAL:HG22	2.17	0.45
5:K:169:LEU:HD23	5:K:172:TYR:OH	2.17	0.45
22:P:502:PC1:H2B2	23:b:302:PTY:H293	1.99	0.45
12:a:118:LEU:HB3	12:a:272:LEU:HD21	1.99	0.45
12:a:489:ASN:HB2	25:a:906:NAG:O5	2.16	0.45
27:j:203:CLR:H211	27:j:203:CLR:H241	1.99	0.45
17:m:70:LEU:HD21	27:n:205:CLR:H151	1.99	0.45
17:o:75:LEU:HD22	17:o:150:LEU:HD23	1.98	0.45
1:B:29:VAL:HG12	1:B:30:THR:N	2.32	0.45
3:G:52:VAL:HG22	3:G:308:LEU:HD11	1.98	0.45
5:J:23:ALA:HB2	7:N:18:ALA:HB1	1.99	0.45
9:Q:226:VAL:HG23	9:Q:255:LEU:HD12	1.99	0.45
9:R:124:SER:O	9:R:128:VAL:HG23	2.17	0.45
14:d:42:LEU:H	14:d:42:LEU:HD12	1.81	0.45
1:A:466:ASP:OD1	1:A:466:ASP:C	2.60	0.45
5:K:121:LEU:HD22	5:K:154:MET:CE	2.47	0.45
15:e:6:PHE:CG	15:e:6:PHE:O	2.69	0.45
17:m:53:MET:HE3	17:m:53:MET:HA	1.98	0.45
1:C:471:GLU:OE1	1:C:471:GLU:N	2.30	0.44
4:H:133:LYS:O	4:H:137:ASN:OD1	2.35	0.44
15:e:63:LEU:HD12	20:s:1:NAG:H2	1.99	0.44
2:D:276:ARG:NH1	2:D:334:ILE:HD11	2.33	0.44
2:F:436:LYS:HB2	2:F:444:LEU:HD11	1.99	0.44
9:Q:234:MET:HG2	9:Q:235:PRO:HD3	1.99	0.44
1:A:590:VAL:HG23	1:A:591:LYS:N	2.33	0.44
4:H:48:LEU:HD11	6:L:109:ALA:HB1	1.99	0.44
12:a:132:LEU:HD12	12:a:258:ALA:HA	1.98	0.44
17:l:128:PHE:O	17:l:132:ILE:HG12	2.18	0.44
17:o:8:PRO:HG2	17:o:86:LEU:HD13	1.98	0.44
12:a:175:ILE:HG22	12:a:176:ASN:N	2.32	0.44
12:a:367:THR:CG2	12:a:372:HIS:HA	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:a:401:PHE:O	12:a:405:VAL:HG23	2.17	0.44
17:h:56:ILE:O	17:h:56:ILE:CG2	2.66	0.44
27:h:201:CLR:H183	27:h:202:CLR:H212	1.99	0.44
1:B:152:ILE:HD11	1:B:400:ARG:NE	2.33	0.44
2:E:395:LEU:HB2	2:E:396:PRO:HD3	2.00	0.44
7:N:47:TYR:C	7:N:47:TYR:CD2	2.95	0.44
9:R:112:TYR:CD1	9:R:112:TYR:O	2.71	0.44
9:R:148:LYS:NZ	9:R:185:LEU:O	2.42	0.44
12:a:17:LEU:HD23	12:a:17:LEU:N	2.32	0.44
17:l:71:VAL:HG22	27:l:203:CLR:H222	1.98	0.44
1:A:37:ALA:O	1:A:57:LEU:HD22	2.18	0.44
1:A:100:ASP:OD1	1:A:104:ARG:N	2.39	0.44
1:B:217:VAL:HG11	1:B:392:VAL:HG21	2.00	0.44
1:C:156:VAL:HG21	1:C:205:MET:CE	2.47	0.44
2:E:365:ILE:HB	2:E:366:PRO:CD	2.48	0.44
2:E:402:MET:HG3	2:E:406:ILE:HD13	1.99	0.44
9:Q:195:GLU:OE1	9:Q:195:GLU:N	2.47	0.44
9:S:201:LYS:CG	9:S:260:LEU:HD21	2.46	0.44
14:d:279:GLU:CD	14:d:279:GLU:C	2.85	0.44
16:f:15:GLY:O	16:f:19:SER:OG	2.29	0.44
17:i:114:GLY:O	17:i:118:VAL:HG23	2.17	0.44
27:n:201:CLR:H183	27:o:202:CLR:H182	2.00	0.44
17:o:75:LEU:HD11	27:o:203:CLR:H193	1.99	0.44
1:B:275:VAL:HG13	1:B:275:VAL:O	2.18	0.44
9:Q:194:ASP:OD2	9:Q:194:ASP:C	2.59	0.44
9:R:97:SER:O	9:R:160:GLN:NE2	2.50	0.44
12:a:178:GLU:HA	12:a:178:GLU:OE1	2.18	0.44
12:a:407:PHE:CD1	12:a:407:PHE:O	2.70	0.44
17:i:56:ILE:HG22	17:i:56:ILE:O	2.17	0.44
17:i:130:GLY:O	17:i:134:ILE:HG13	2.17	0.44
1:A:258:VAL:HG11	21:A:701:ADP:C5	2.53	0.44
1:B:298:VAL:O	1:B:298:VAL:HG13	2.16	0.44
1:C:574:MET:HE1	1:C:612:PHE:CE2	2.53	0.44
2:E:208:ARG:NH2	2:E:467:PRO:O	2.46	0.44
2:F:428:ILE:O	2:F:432:VAL:HG23	2.17	0.44
5:K:155:TYR:CD1	5:K:163:VAL:HG11	2.53	0.44
7:M:38:GLU:C	7:M:38:GLU:CD	2.85	0.44
12:a:801:LEU:CB	17:g:136:ILE:HD13	2.47	0.44
17:g:34:THR:HG23	17:g:59:VAL:HG13	2.00	0.44
17:i:55:SER:O	17:i:58:PRO:HD2	2.18	0.44
17:m:81:THR:CG2	17:m:84:ILE:HG23	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:ILE:HG21	2:D:341:VAL:CG1	2.47	0.44
1:C:504:THR:O	1:C:507:ILE:HG22	2.18	0.44
17:h:35:ALA:O	17:h:39:THR:HG23	2.18	0.44
17:o:81:THR:HG22	17:o:82:ASP:N	2.33	0.44
2:D:121:THR:OG1	2:D:277:LEU:HD23	2.18	0.43
2:D:134:GLY:N	2:D:261:LEU:O	2.50	0.43
2:E:229:ILE:HB	2:E:257:VAL:HG22	2.00	0.43
3:G:45:VAL:HG21	3:G:312:LEU:HD11	1.99	0.43
5:K:97:GLU:HG3	7:O:96:LEU:HD11	1.99	0.43
11:U:30:PHE:O	11:U:31:ALA:HB3	2.19	0.43
12:a:367:THR:HG21	12:a:372:HIS:ND1	2.33	0.43
13:b:64:GLY:HA3	13:b:149:LEU:HA	1.99	0.43
14:d:105:MET:HE3	14:d:160:LEU:HD13	1.99	0.43
17:g:72:VAL:HG21	17:g:99:VAL:CG2	2.35	0.43
5:J:67:GLN:OE1	5:J:67:GLN:HA	2.18	0.43
17:g:49:PRO:HB2	17:h:126:ARG:HE	1.83	0.43
1:B:53:GLU:OE1	1:B:67:TYR:OH	2.33	0.43
1:B:88:VAL:HG13	1:B:211:VAL:CG1	2.48	0.43
1:B:395:LEU:HD22	9:R:21:GLN:CD	2.43	0.43
1:C:217:VAL:HG11	1:C:392:VAL:HG21	1.99	0.43
5:J:103:SER:O	5:J:106:VAL:HG22	2.19	0.43
12:a:556:SER:O	12:a:560:HIS:ND1	2.51	0.43
17:i:35:ALA:CB	18:p:331:MET:HE1	2.48	0.43
1:C:469:PHE:O	1:C:470:THR:C	2.61	0.43
2:F:61:ASP:OD2	2:F:93:LYS:NZ	2.50	0.43
3:G:40:ILE:HD11	3:G:299:ALA:HB1	2.01	0.43
5:I:94:LEU:HD13	5:I:215:LEU:HD11	2.01	0.43
5:J:168:ASP:OD2	5:J:188:ARG:NH1	2.51	0.43
7:O:74:GLU:OE1	7:O:75:GLN:N	2.51	0.43
12:a:430:ILE:HD13	12:a:440:PHE:HZ	1.84	0.43
17:j:65:ILE:CD1	17:j:110:ILE:HD12	2.48	0.43
1:A:239:PRO:O	1:A:455:SER:OG	2.31	0.43
1:B:274:TYR:OH	1:B:349:ASP:OD1	2.25	0.43
1:C:368:MET:HE1	4:H:196:ARG:HG2	2.00	0.43
2:E:341:VAL:HG23	2:E:344:ARG:HB2	1.99	0.43
2:F:283:GLU:HA	2:F:348:ILE:HD11	1.98	0.43
2:F:351:ILE:O	2:F:351:ILE:HG22	2.19	0.43
5:J:37:GLU:HA	5:J:40:ILE:HG22	2.00	0.43
8:P:310:LEU:HD23	8:P:311:PHE:CG	2.53	0.43
9:R:42:LEU:N	9:R:42:LEU:HD12	2.32	0.43
9:R:172:ASN:OD1	9:R:174:GLY:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:a:12:LEU:HD23	12:a:324:TRP:CD2	2.53	0.43
12:a:224:PHE:CD1	12:a:224:PHE:N	2.86	0.43
12:a:311:ASN:ND2	12:a:315:THR:OG1	2.52	0.43
17:h:24:VAL:O	17:h:28:MET:HG3	2.18	0.43
17:n:45:SER:OG	17:n:52:ILE:HD11	2.19	0.43
27:o:201:CLR:H263	27:o:203:CLR:H272	1.99	0.43
1:B:144:GLY:N	1:B:176:VAL:O	2.39	0.43
1:C:268:ASN:OD1	1:C:268:ASN:N	2.46	0.43
2:D:135:SER:O	2:D:135:SER:OG	2.36	0.43
2:E:450:LEU:HD22	2:E:486:ILE:HG22	1.99	0.43
2:F:245:LYS:NZ	2:F:249:GLU:OE2	2.30	0.43
22:P:502:PC1:O13	22:P:502:PC1:H143	2.18	0.43
9:S:51:ASP:OD1	9:S:51:ASP:N	2.51	0.43
14:d:115:GLY:HA3	14:d:125:LEU:HD11	2.00	0.43
1:A:88:VAL:HG13	1:A:211:VAL:CG1	2.48	0.43
1:B:34:MET:HE1	1:B:43:VAL:HG11	2.01	0.43
1:B:328:TYR:HA	1:B:331:ILE:HG22	2.00	0.43
8:P:403:GLU:HG2	19:X:2:NAG:H82	1.99	0.43
12:a:180:ILE:N	12:a:181:PRO:HD2	2.34	0.43
1:A:56:ARG:HB2	1:A:63:THR:CG2	2.48	0.43
5:J:102:LEU:HD12	5:J:200:LEU:HD22	2.01	0.43
5:K:174:PRO:HD2	5:K:177:ILE:HD12	2.01	0.43
14:d:272:PRO:HD2	17:n:123:GLN:HG3	2.01	0.43
17:o:154:THR:HG21	27:o:201:CLR:H42	2.00	0.43
1:A:147:ILE:HG23	1:A:168:LEU:HD11	2.01	0.43
1:B:80:LEU:HD23	1:B:81:ARG:N	2.34	0.43
1:C:232:ARG:CD	1:C:540:MET:HE2	2.49	0.43
2:D:180:MET:HE1	2:D:394:VAL:HG21	2.00	0.43
3:G:307:VAL:HA	3:G:316:PHE:CZ	2.54	0.43
9:Q:98:ILE:O	9:Q:98:ILE:CG2	2.67	0.43
12:a:57:ARG:HB2	12:a:94:MET:HE1	2.01	0.43
17:i:56:ILE:O	17:i:56:ILE:CG2	2.66	0.43
2:F:354:LEU:CD2	2:F:365:ILE:HG22	2.49	0.43
8:P:381:ASN:OD1	19:c:1:NAG:H82	2.19	0.43
13:b:172:LEU:HD13	17:o:45:SER:HB2	2.01	0.43
17:g:84:ILE:O	17:g:84:ILE:HG23	2.18	0.43
17:j:31:ALA:HB1	17:k:109:ALA:HB2	2.01	0.43
23:p:403:PTY:HN11	23:p:403:PTY:P1	2.41	0.43
1:A:280:ARG:NH1	2:D:372:ILE:O	2.45	0.42
5:I:121:LEU:HD22	5:I:154:MET:HE2	2.00	0.42
8:P:369:SER:OG	8:P:389:THR:OG1	2.29	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:408:ALA:CB	18:p:296:ALA:HB2	2.49	0.42
9:Q:159:LEU:HD21	9:Q:179:PHE:CE1	2.54	0.42
9:R:51:ASP:OD1	9:R:51:ASP:N	2.51	0.42
12:a:377:ILE:HG23	12:a:804:LEU:HD21	2.00	0.42
14:d:41:THR:HG22	14:d:42:LEU:N	2.33	0.42
1:C:397:ASN:HB2	1:C:398:PRO:HD3	2.00	0.42
2:E:43:PRO:HB2	5:J:192:VAL:CG2	2.49	0.42
2:F:300:MET:HE2	2:F:335:TYR:HE1	1.82	0.42
9:R:192:LYS:O	9:R:196:GLN:HG3	2.19	0.42
12:a:131:ILE:HD11	12:a:173:GLY:HA2	2.02	0.42
12:a:368:ASN:OD1	12:a:369:LYS:N	2.50	0.42
12:a:757:TRP:CZ3	12:a:761:ILE:HD11	2.54	0.42
17:i:28:MET:SD	17:j:105:ALA:HB2	2.59	0.42
1:C:550:MET:HE3	1:C:612:PHE:CD2	2.54	0.42
2:F:40:LEU:O	5:K:202:LEU:HD21	2.18	0.42
2:F:121:THR:HG23	2:F:153:ILE:CG2	2.49	0.42
12:a:419:PHE:O	12:a:423:MET:HG3	2.19	0.42
13:b:81:VAL:HG13	17:g:123:GLN:HB3	1.99	0.42
17:g:11:SER:O	17:g:89:SER:OG	2.25	0.42
27:i:203:CLR:H221	27:i:203:CLR:H262	2.01	0.42
17:l:77:ALA:O	17:m:155:LYS:CE	2.67	0.42
1:A:106:LEU:HD13	2:D:160:PRO:HD2	2.02	0.42
1:A:338:ARG:HD3	1:A:404:VAL:HG23	2.01	0.42
1:C:615:LEU:HD23	1:C:615:LEU:C	2.45	0.42
9:R:115:MET:HE2	9:R:126:TYR:CE1	2.54	0.42
12:a:610:LEU:O	12:a:614:ILE:HG12	2.19	0.42
13:b:42:THR:CG2	13:b:123:PRO:HB3	2.49	0.42
17:l:55:SER:O	17:l:58:PRO:HD2	2.19	0.42
1:A:275:VAL:O	1:A:276:GLY:C	2.62	0.42
1:B:148:THR:HG21	9:R:20:SER:O	2.19	0.42
1:B:419:ASP:OD2	1:B:419:ASP:C	2.62	0.42
2:F:374:GLU:OE1	2:F:401:LEU:HD11	2.19	0.42
4:H:144:LEU:O	4:H:144:LEU:HD23	2.19	0.42
11:U:30:PHE:C	11:U:32:ILE:H	2.27	0.42
12:a:484:MET:SD	12:a:507:ILE:HD11	2.60	0.42
12:a:628:MET:HA	12:a:628:MET:HE2	2.01	0.42
17:h:87:TYR:CZ	17:h:91:LEU:HD11	2.55	0.42
27:j:203:CLR:C18	27:j:203:CLR:H213	2.50	0.42
17:m:87:TYR:OH	17:m:155:LYS:HD3	2.20	0.42
17:n:16:VAL:CG1	17:o:94:GLY:HA3	2.50	0.42
18:p:332:ASP:OD1	18:p:334:GLY:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:ILE:O	1:C:102:ILE:HG22	2.18	0.42
5:I:183:ILE:HD12	5:I:183:ILE:N	2.35	0.42
5:K:129:GLU:H	5:K:132:MET:CE	2.33	0.42
8:P:399:ASN:OD1	19:q:1:NAG:H2	2.19	0.42
12:a:471:SER:OG	12:a:524:ASN:HB2	2.19	0.42
23:a:903:PTY:HN11	23:a:903:PTY:P1	2.42	0.42
17:g:90:PHE:HD1	17:g:93:LEU:HD23	1.83	0.42
27:h:201:CLR:H272	27:i:204:CLR:H263	2.00	0.42
27:j:201:CLR:H272	27:j:202:CLR:H273	2.02	0.42
18:p:336:ASP:HA	18:p:339:ILE:HD12	2.02	0.42
1:A:216:PRO:HB2	1:A:395:LEU:HD11	2.02	0.42
2:D:203:ALA:CB	2:D:353:ILE:HD11	2.50	0.42
2:F:49:THR:OG1	2:F:61:ASP:O	2.34	0.42
6:L:55:PHE:HB3	6:L:61:ILE:HD13	2.02	0.42
9:Q:133:LEU:HD13	9:Q:159:LEU:HD23	2.02	0.42
12:a:547:ILE:HD13	15:e:50:LEU:HD11	2.00	0.42
13:b:70:TYR:CD1	13:b:70:TYR:C	2.98	0.42
14:d:119:GLN:O	14:d:119:GLN:HG2	2.20	0.42
1:C:475:LEU:HD21	1:C:542:SER:CB	2.49	0.42
2:D:317:VAL:HG13	2:D:317:VAL:O	2.19	0.42
2:D:365:ILE:HB	2:D:366:PRO:CD	2.50	0.42
5:I:38:PHE:HD2	7:M:36:ALA:HB2	1.83	0.42
5:I:197:GLU:OE1	5:I:197:GLU:N	2.52	0.42
9:S:111:GLN:NE2	9:S:167:GLY:HA3	2.34	0.42
12:a:35:VAL:HG11	12:a:37:PHE:HE1	1.85	0.42
12:a:131:ILE:HG12	12:a:219:VAL:HG23	2.02	0.42
12:a:549:MET:HE3	12:a:580:MET:CE	2.50	0.42
12:a:609:LEU:N	24:a:905:WJP:O28	2.52	0.42
19:V:1:NAG:O7	19:V:1:NAG:C1	2.68	0.42
1:B:574:MET:HE2	1:B:611:ALA:HB1	2.01	0.42
2:D:56:PRO:HA	2:D:102:THR:HG23	2.02	0.42
5:K:72:MET:O	5:K:76:MET:HG2	2.20	0.42
6:L:24:GLY:C	6:L:25:ILE:HD12	2.44	0.42
6:L:45:ILE:HD12	6:L:45:ILE:H	1.85	0.42
8:P:319:PHE:HB3	8:P:336:MET:HE2	2.02	0.42
12:a:369:LYS:NZ	12:a:448:TYR:OH	2.25	0.42
12:a:392:ALA:O	12:a:396:VAL:HG23	2.20	0.42
12:a:518:GLY:O	15:e:59:GLN:NE2	2.46	0.42
17:k:71:VAL:HG22	27:k:201:CLR:H161	2.01	0.42
1:C:229:THR:HG22	1:C:263:LEU:HD23	2.02	0.42
1:C:377:TYR:O	1:C:381:ARG:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:445:THR:OG1	2:E:447:ASP:OD1	2.37	0.42
5:I:141:PHE:CE1	5:I:169:LEU:HD21	2.55	0.42
8:P:432:ILE:HG23	17:g:101:LEU:HD13	2.01	0.42
12:a:186:MET:HA	12:a:186:MET:HE2	2.02	0.42
12:a:368:ASN:OD1	23:a:904:PTY:N1	2.53	0.42
17:g:99:VAL:HG22	17:g:146:LEU:HA	2.01	0.42
17:o:127:LEU:HG	17:o:127:LEU:O	2.19	0.42
1:A:191:VAL:HG21	1:A:205:MET:CG	2.50	0.41
2:F:354:LEU:HD21	2:F:365:ILE:HG22	2.01	0.41
2:F:365:ILE:HB	2:F:366:PRO:CD	2.50	0.41
6:L:39:VAL:HG22	6:L:48:ILE:CD1	2.50	0.41
9:Q:98:ILE:HG22	9:Q:101:PHE:O	2.20	0.41
12:a:177:ARG:NH1	12:a:201:GLU:OE2	2.52	0.41
1:C:503:GLU:OE1	1:C:567:TRP:N	2.41	0.41
2:D:82:ARG:NH1	2:D:103:SER:O	2.51	0.41
12:a:69:GLU:O	12:a:73:ARG:HG2	2.19	0.41
12:a:579:PHE:CZ	12:a:583:LEU:HD12	2.55	0.41
17:o:150:LEU:HD13	27:o:201:CLR:H152	2.02	0.41
18:p:338:ILE:O	18:p:338:ILE:HG22	2.19	0.41
1:A:116:ILE:HD13	2:D:341:VAL:HG11	2.02	0.41
1:A:229:THR:HG22	1:A:263:LEU:HG	2.01	0.41
21:A:701:ADP:O3B	2:D:400:ARG:NH2	2.54	0.41
1:C:102:ILE:O	1:C:103:GLN:HB3	2.20	0.41
2:D:435:MET:O	2:D:439:VAL:HG22	2.20	0.41
7:M:41:GLN:HA	7:M:44:VAL:HG22	2.03	0.41
12:a:187:LEU:HD21	12:a:233:VAL:HG22	2.01	0.41
19:r:1:NAG:O3	19:r:2:NAG:O5	2.30	0.41
1:A:92:PRO:HG3	1:A:205:MET:HE2	2.01	0.41
1:C:254:CYS:SG	1:C:255:GLY:N	2.93	0.41
2:E:173:GLY:O	2:E:465:GLN:NE2	2.50	0.41
5:K:92:THR:O	5:K:96:ASN:ND2	2.53	0.41
9:S:163:ILE:O	9:S:167:GLY:N	2.54	0.41
12:a:629:LEU:N	12:a:633:GLN:OE1	2.50	0.41
13:b:7:LEU:HD12	23:p:403:PTY:H141	2.03	0.41
13:b:176:ILE:O	13:b:176:ILE:HG22	2.21	0.41
14:d:222:ILE:HG22	14:d:226:ASN:OD1	2.20	0.41
17:g:137:PHE:HA	17:g:140:VAL:HG22	2.03	0.41
17:l:16:VAL:HG13	17:l:80:LEU:HD21	2.02	0.41
1:A:44:ARG:HG2	1:A:44:ARG:HH11	1.86	0.41
1:A:268:ASN:OD1	1:A:268:ASN:N	2.48	0.41
1:A:270:ASP:OD1	1:A:270:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:148:GLU:OE2	5:J:219:ASN:ND2	2.48	0.41
3:G:51:LEU:HD21	3:G:307:VAL:HG11	2.02	0.41
8:P:414:PHE:CZ	22:P:501:PC1:H142	2.56	0.41
9:Q:32:CYS:O	9:Q:36:ILE:HG22	2.21	0.41
12:a:32:LEU:O	12:a:32:LEU:HD12	2.20	0.41
17:j:114:GLY:O	17:j:118:VAL:HG22	2.20	0.41
4:H:50:LYS:HB3	4:H:151:LEU:HD13	2.03	0.41
5:J:50:ARG:HG2	5:J:54:MET:HE3	2.02	0.41
12:a:619:PHE:CE2	12:a:641:ILE:HG21	2.54	0.41
14:d:109:VAL:HG11	14:d:160:LEU:HD23	2.03	0.41
14:d:126:VAL:N	14:d:127:PRO:HD2	2.35	0.41
15:e:28:VAL:HG21	15:e:38:ILE:CG1	2.50	0.41
17:g:55:SER:O	17:g:58:PRO:HD2	2.20	0.41
17:l:49:PRO:O	17:l:52:ILE:HD12	2.21	0.41
1:A:98:ILE:HG12	1:A:106:LEU:HD12	2.01	0.41
1:A:395:LEU:HD22	9:Q:21:GLN:CD	2.44	0.41
1:A:562:ASP:OD1	1:A:563:ASN:N	2.54	0.41
1:C:338:ARG:HD3	1:C:404:VAL:HG23	2.03	0.41
2:F:76:LEU:HD21	2:F:82:ARG:CZ	2.51	0.41
3:G:305:GLU:HG3	3:G:370:VAL:HG22	2.02	0.41
4:H:144:LEU:HD23	4:H:144:LEU:C	2.46	0.41
5:J:50:ARG:O	5:J:54:MET:HG2	2.20	0.41
9:Q:126:TYR:HB3	9:Q:168:ILE:HD13	2.01	0.41
12:a:357:THR:HG22	12:a:358:ASN:H	1.85	0.41
12:a:648:VAL:HB	12:a:649:PRO:HD3	2.02	0.41
17:n:84:ILE:O	17:n:84:ILE:HG23	2.20	0.41
1:A:99:PHE:HB3	1:A:103:GLN:HA	2.03	0.41
1:A:479:ALA:HB2	1:A:541:LEU:HD11	2.03	0.41
1:A:503:GLU:O	1:A:507:ILE:HG13	2.21	0.41
1:B:397:ASN:HB3	9:R:28:TYR:CB	2.50	0.41
1:B:523:ASN:OD1	1:B:526:THR:HG23	2.21	0.41
2:D:233:ALA:HB1	2:D:236:VAL:HG21	2.02	0.41
2:F:173:GLY:O	2:F:465:GLN:NE2	2.45	0.41
2:F:234:MET:HE1	2:F:300:MET:SD	2.60	0.41
2:F:488:PRO:HD2	2:F:491:MET:SD	2.61	0.41
4:H:90:ALA:HB2	6:L:27:GLU:HB3	2.02	0.41
4:H:117:ASP:OD1	4:H:118:SER:N	2.53	0.41
8:P:290:ASN:OD1	19:W:1:NAG:O5	2.32	0.41
9:Q:29:ILE:HG21	9:Q:52:VAL:HG21	2.02	0.41
11:U:119:THR:O	11:U:123:LEU:N	2.54	0.41
12:a:357:THR:HG22	12:a:358:ASN:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:b:38:ALA:HB1	17:o:10:TYR:CE1	2.56	0.41
14:d:253:ALA:O	14:d:257:ARG:HG3	2.21	0.41
18:p:338:ILE:O	18:p:342:MET:HG2	2.21	0.41
1:B:147:ILE:HG13	1:B:168:LEU:HD22	2.02	0.41
1:B:573:HIS:CD2	1:B:573:HIS:C	2.99	0.41
1:C:102:ILE:O	1:C:103:GLN:CB	2.69	0.41
2:D:180:MET:CE	2:D:394:VAL:HG21	2.51	0.41
2:F:168:GLU:O	2:F:185:ARG:N	2.45	0.41
2:F:189:ILE:HD11	2:F:377:ILE:HD11	2.03	0.41
2:F:272:ILE:HD11	2:F:307:LEU:N	2.36	0.41
12:a:329:ASP:OD1	12:a:329:ASP:N	2.54	0.41
13:b:58:ILE:HD13	13:b:105:ILE:HG22	2.02	0.41
13:b:150:PHE:CZ	17:o:28:MET:HE2	2.56	0.41
14:d:276:LEU:HD22	17:n:47:MET:HE1	2.03	0.41
14:d:328:ASN:ND2	14:d:348:ILE:O	2.49	0.41
17:j:56:ILE:O	17:j:56:ILE:CG2	2.68	0.41
1:B:248:ILE:O	1:B:409:ALA:HA	2.21	0.40
1:B:276:GLY:HA2	1:B:349:ASP:HB2	2.03	0.40
1:C:24:VAL:HG13	1:C:29:VAL:HG22	2.02	0.40
2:D:207:CYS:SG	2:D:296:ILE:CD1	3.09	0.40
8:P:410:ASP:OD2	18:p:299:TYR:CD2	2.74	0.40
9:R:119:VAL:HG13	9:R:120:ASN:N	2.36	0.40
12:a:489:ASN:CB	25:a:906:NAG:O5	2.69	0.40
27:o:202:CLR:H162	27:o:202:CLR:H221	1.89	0.40
18:p:302:GLU:O	18:p:306:VAL:HG12	2.21	0.40
1:B:103:GLN:HG3	1:B:103:GLN:O	2.21	0.40
1:B:389:ALA:HB2	1:B:406:ILE:HD12	2.02	0.40
2:E:298:THR:O	2:E:353:ILE:HB	2.21	0.40
3:G:53:GLY:O	3:G:57:GLU:HG2	2.21	0.40
8:P:336:MET:SD	8:P:352:VAL:HG11	2.61	0.40
9:R:254:VAL:HG22	9:R:255:LEU:N	2.36	0.40
12:a:298:ARG:CD	12:a:830:HIS:HB3	2.50	0.40
13:b:56:LEU:HD13	13:b:142:LEU:HD12	2.03	0.40
17:h:110:ILE:HG23	17:h:135:LEU:HD22	2.02	0.40
17:k:101:LEU:HD13	23:p:401:PTY:H291	2.04	0.40
1:A:275:VAL:O	1:A:312:VAL:O	2.40	0.40
1:B:273:ILE:O	1:B:346:MET:HA	2.22	0.40
1:B:570:ILE:O	1:B:574:MET:HG2	2.21	0.40
2:E:188:LYS:HG2	2:E:338:ALA:HB3	2.03	0.40
2:F:162:CYS:O	2:F:342:GLU:N	2.53	0.40
3:G:48:LEU:HD11	5:J:18:PHE:CD1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:a:358:ASN:N	12:a:358:ASN:OD1	2.55	0.40
17:i:14:PHE:HB2	17:i:89:SER:OG	2.21	0.40
17:m:16:VAL:HG11	17:n:91:LEU:HD23	2.04	0.40
1:A:346:MET:HE1	1:A:385:PHE:HZ	1.85	0.40
2:D:358:ASN:ND2	2:D:358:ASN:O	2.54	0.40
5:K:101:ARG:HB3	7:O:100:LEU:HD11	2.03	0.40
7:N:42:MET:HE2	7:N:42:MET:CA	2.50	0.40
8:P:274:ASP:OD1	8:P:274:ASP:N	2.54	0.40
12:a:324:TRP:CZ2	12:a:361:PRO:HA	2.56	0.40
14:d:110:ILE:O	14:d:114:THR:OG1	2.34	0.40
17:i:75:LEU:HD21	27:i:203:CLR:H193	2.03	0.40
17:j:17:MET:HE1	17:k:97:LEU:HD12	2.04	0.40
17:o:41:ILE:HA	17:o:44:MET:HE3	2.03	0.40
18:p:314:MET:HE2	23:p:401:PTY:H191	2.03	0.40
1:A:212:ARG:NH2	1:A:324:GLU:OE2	2.47	0.40
1:B:164:HIS:CE1	1:B:340:MET:HE1	2.56	0.40
5:I:214:ALA:O	7:M:91:ASN:ND2	2.54	0.40
9:S:140:LEU:HD21	9:S:152:LEU:HB3	2.04	0.40
11:U:75:TYR:HB3	11:U:90:PHE:CD1	2.57	0.40
12:a:32:LEU:HD12	12:a:32:LEU:C	2.47	0.40
14:d:306:PHE:CE2	14:d:314:VAL:HG13	2.57	0.40
16:f:13:ALA:HA	16:f:16:ILE:HG22	2.03	0.40
17:h:137:PHE:O	17:h:140:VAL:HG22	2.22	0.40
17:i:71:VAL:HG21	27:i:203:CLR:C23	2.46	0.40
17:i:77:ALA:O	17:j:155:LYS:HE3	2.22	0.40
17:i:92:GLN:HA	17:i:92:GLN:OE1	2.22	0.40
17:j:67:ILE:O	17:j:71:VAL:HG23	2.21	0.40
17:k:87:TYR:CE2	17:k:91:LEU:HD21	2.57	0.40
17:n:36:LYS:O	17:n:115:ASP:OD1	2.39	0.40

There are no symmetry-related clashes.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

4.3.2 Protein sidechains [i](#)

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

4.3.3 RNA ⓘ

There are no RNA molecules in this entry.

4.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

4.5 Carbohydrates ⓘ

27 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	$\# Z > 2$
19	NAG	V	1	19	14,14,15	0.74	0	17,19,21	1.13	1 (5%)
19	NAG	V	2	19	14,14,15	0.71	0	17,19,21	0.86	0
19	NAG	W	1	19,8	14,14,15	0.70	0	17,19,21	1.21	1 (5%)
19	NAG	W	2	19	14,14,15	0.80	0	17,19,21	0.99	1 (5%)
19	NAG	X	1	19,8	14,14,15	0.59	0	17,19,21	1.16	2 (11%)
19	NAG	X	2	19	14,14,15	0.81	0	17,19,21	0.77	0
19	NAG	Y	1	19,8	14,14,15	0.83	0	17,19,21	1.58	4 (23%)
19	NAG	Y	2	19	14,14,15	0.70	0	17,19,21	1.06	1 (5%)
19	NAG	Z	1	19,8	14,14,15	0.74	0	17,19,21	1.37	2 (11%)
19	NAG	Z	2	19	14,14,15	0.71	0	17,19,21	1.36	2 (11%)
19	NAG	c	1	19	14,14,15	0.71	0	17,19,21	1.40	1 (5%)
19	NAG	c	2	19	14,14,15	0.67	0	17,19,21	1.13	1 (5%)
19	NAG	q	1	19,8	14,14,15	0.77	0	17,19,21	0.80	0
19	NAG	q	2	19	14,14,15	0.72	0	17,19,21	1.16	1 (5%)
19	NAG	r	1	19	14,14,15	0.74	0	17,19,21	0.71	0
19	NAG	r	2	19	14,14,15	0.70	0	17,19,21	0.82	0
20	NAG	s	1	20	14,14,15	0.77	0	17,19,21	0.81	0
20	MAN	s	10	20	11,11,12	0.69	0	15,15,17	1.19	1 (6%)
20	MAN	s	11	20	11,11,12	0.74	0	15,15,17	0.93	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	NAG	s	2	20	14,14,15	0.74	0	17,19,21	0.82	1 (5%)
20	BMA	s	3	20	11,11,12	0.78	0	15,15,17	2.16	3 (20%)
20	MAN	s	4	20	11,11,12	0.68	0	15,15,17	1.35	1 (6%)
20	MAN	s	5	20	11,11,12	0.72	0	15,15,17	1.25	1 (6%)
20	MAN	s	6	20	11,11,12	0.84	1 (9%)	15,15,17	0.93	0
20	GLC	s	7	20	11,11,12	0.65	0	15,15,17	0.49	0
20	GLC	s	8	20	11,11,12	0.61	0	15,15,17	0.81	0
20	GLC	s	9	20	11,11,12	0.60	0	15,15,17	0.68	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
19	NAG	V	1	19	-	2/6/23/26	0/1/1/1
19	NAG	V	2	19	-	0/6/23/26	0/1/1/1
19	NAG	W	1	19,8	-	0/6/23/26	0/1/1/1
19	NAG	W	2	19	-	0/6/23/26	0/1/1/1
19	NAG	X	1	19,8	-	0/6/23/26	0/1/1/1
19	NAG	X	2	19	-	0/6/23/26	0/1/1/1
19	NAG	Y	1	19,8	-	0/6/23/26	0/1/1/1
19	NAG	Y	2	19	-	1/6/23/26	0/1/1/1
19	NAG	Z	1	19,8	-	2/6/23/26	0/1/1/1
19	NAG	Z	2	19	-	1/6/23/26	0/1/1/1
19	NAG	c	1	19	-	2/6/23/26	0/1/1/1
19	NAG	c	2	19	-	2/6/23/26	0/1/1/1
19	NAG	q	1	19,8	-	1/6/23/26	0/1/1/1
19	NAG	q	2	19	-	2/6/23/26	0/1/1/1
19	NAG	r	1	19	-	2/6/23/26	0/1/1/1
19	NAG	r	2	19	-	0/6/23/26	0/1/1/1
20	NAG	s	1	20	-	0/6/23/26	0/1/1/1
20	MAN	s	10	20	-	0/2/19/22	0/1/1/1
20	MAN	s	11	20	-	0/2/19/22	0/1/1/1
20	NAG	s	2	20	-	2/6/23/26	0/1/1/1
20	BMA	s	3	20	-	1/2/19/22	0/1/1/1
20	MAN	s	4	20	-	2/2/19/22	0/1/1/1
20	MAN	s	5	20	-	2/2/19/22	0/1/1/1
20	MAN	s	6	20	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	GLC	s	7	20	-	1/2/19/22	0/1/1/1
20	GLC	s	8	20	-	0/2/19/22	0/1/1/1
20	GLC	s	9	20	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	s	6	MAN	O5-C1	-2.19	1.40	1.43

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	s	3	BMA	C1-O5-C5	6.32	120.66	112.19
19	c	1	NAG	C2-N2-C7	4.17	128.49	122.90
20	s	4	MAN	C1-O5-C5	4.13	117.72	112.19
19	Y	1	NAG	C1-O5-C5	3.85	117.34	112.19
19	Z	1	NAG	C2-N2-C7	3.77	127.95	122.90
19	Z	2	NAG	C2-N2-C7	3.73	127.90	122.90
19	q	2	NAG	C2-N2-C7	3.55	127.66	122.90
20	s	5	MAN	C1-O5-C5	3.49	116.86	112.19
20	s	10	MAN	C1-O5-C5	3.47	116.84	112.19
19	c	2	NAG	C2-N2-C7	3.39	127.44	122.90
19	V	1	NAG	C2-N2-C7	3.24	127.24	122.90
20	s	3	BMA	C3-C4-C5	3.03	115.73	110.23
19	Y	2	NAG	O5-C1-C2	-2.96	106.71	111.29
19	X	1	NAG	O4-C4-C3	-2.89	103.56	110.38
19	W	1	NAG	O4-C4-C3	-2.78	103.83	110.38
19	W	2	NAG	O5-C1-C2	-2.65	107.19	111.29
19	Z	2	NAG	O5-C1-C2	-2.44	107.52	111.29
19	Y	1	NAG	C3-C4-C5	-2.41	105.87	110.23
19	X	1	NAG	O5-C1-C2	-2.38	107.62	111.29
20	s	3	BMA	O4-C4-C3	-2.35	104.83	110.38
19	Y	1	NAG	O5-C1-C2	2.32	114.88	111.29
19	Z	1	NAG	O4-C4-C3	-2.28	105.00	110.38
20	s	11	MAN	C1-O5-C5	2.15	115.06	112.19
19	Y	1	NAG	O4-C4-C5	2.12	114.56	109.32
20	s	2	NAG	O5-C1-C2	-2.03	108.15	111.29

There are no chirality outliers.

All (23) torsion outliers are listed below:

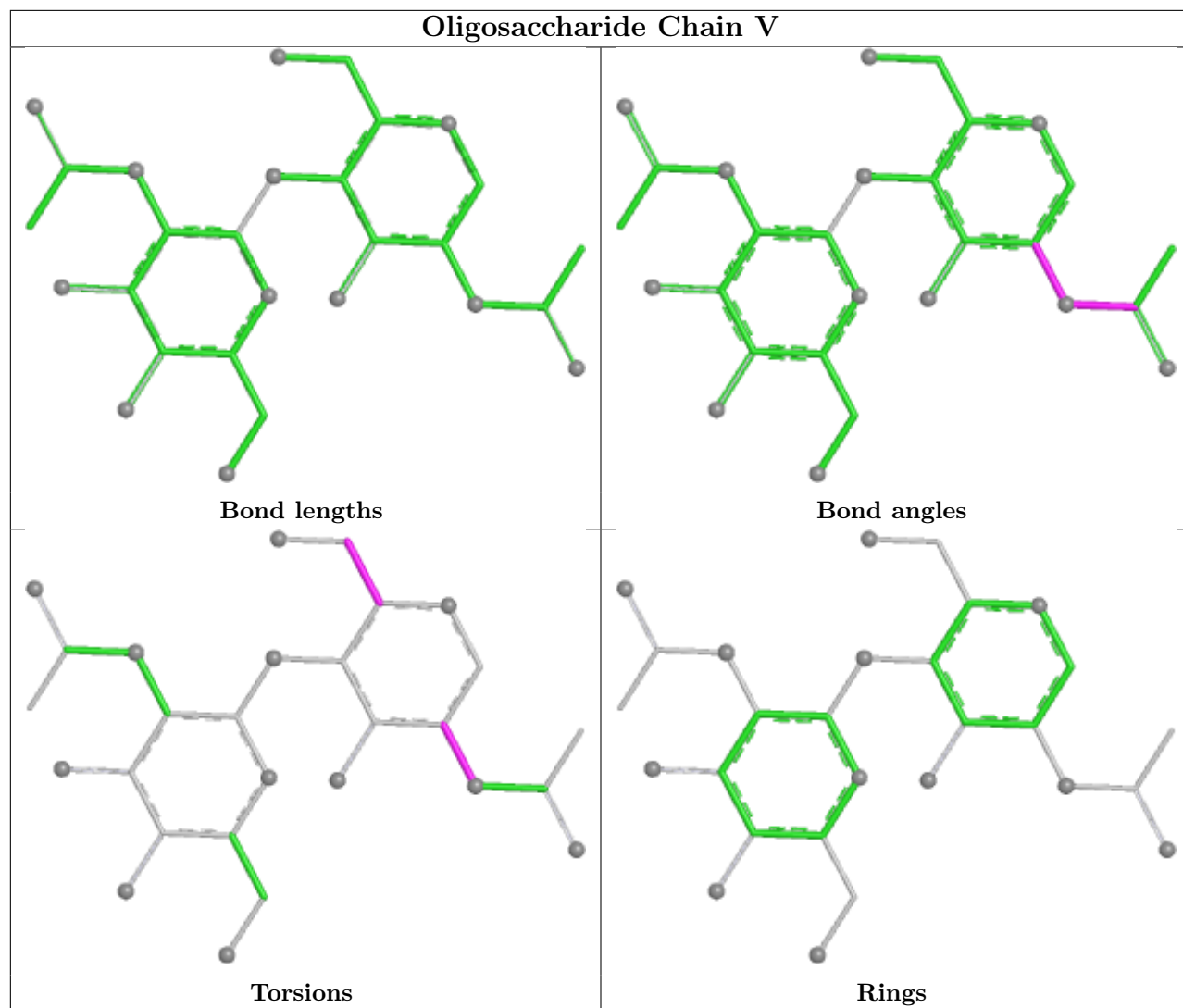
Mol	Chain	Res	Type	Atoms
19	V	1	NAG	C1-C2-N2-C7
19	Y	2	NAG	C1-C2-N2-C7
19	Z	2	NAG	C3-C2-N2-C7
19	q	1	NAG	C1-C2-N2-C7
19	r	1	NAG	C1-C2-N2-C7
20	s	5	MAN	O5-C5-C6-O6
20	s	2	NAG	O5-C5-C6-O6
20	s	4	MAN	O5-C5-C6-O6
20	s	5	MAN	C4-C5-C6-O6
20	s	2	NAG	C4-C5-C6-O6
20	s	4	MAN	C4-C5-C6-O6
19	Z	1	NAG	C8-C7-N2-C2
19	Z	1	NAG	O7-C7-N2-C2
19	c	1	NAG	C8-C7-N2-C2
19	c	1	NAG	O7-C7-N2-C2
19	c	2	NAG	C8-C7-N2-C2
19	c	2	NAG	O7-C7-N2-C2
19	q	2	NAG	C8-C7-N2-C2
19	q	2	NAG	O7-C7-N2-C2
19	V	1	NAG	O5-C5-C6-O6
19	r	1	NAG	C3-C2-N2-C7
20	s	7	GLC	O5-C5-C6-O6
20	s	3	BMA	O5-C5-C6-O6

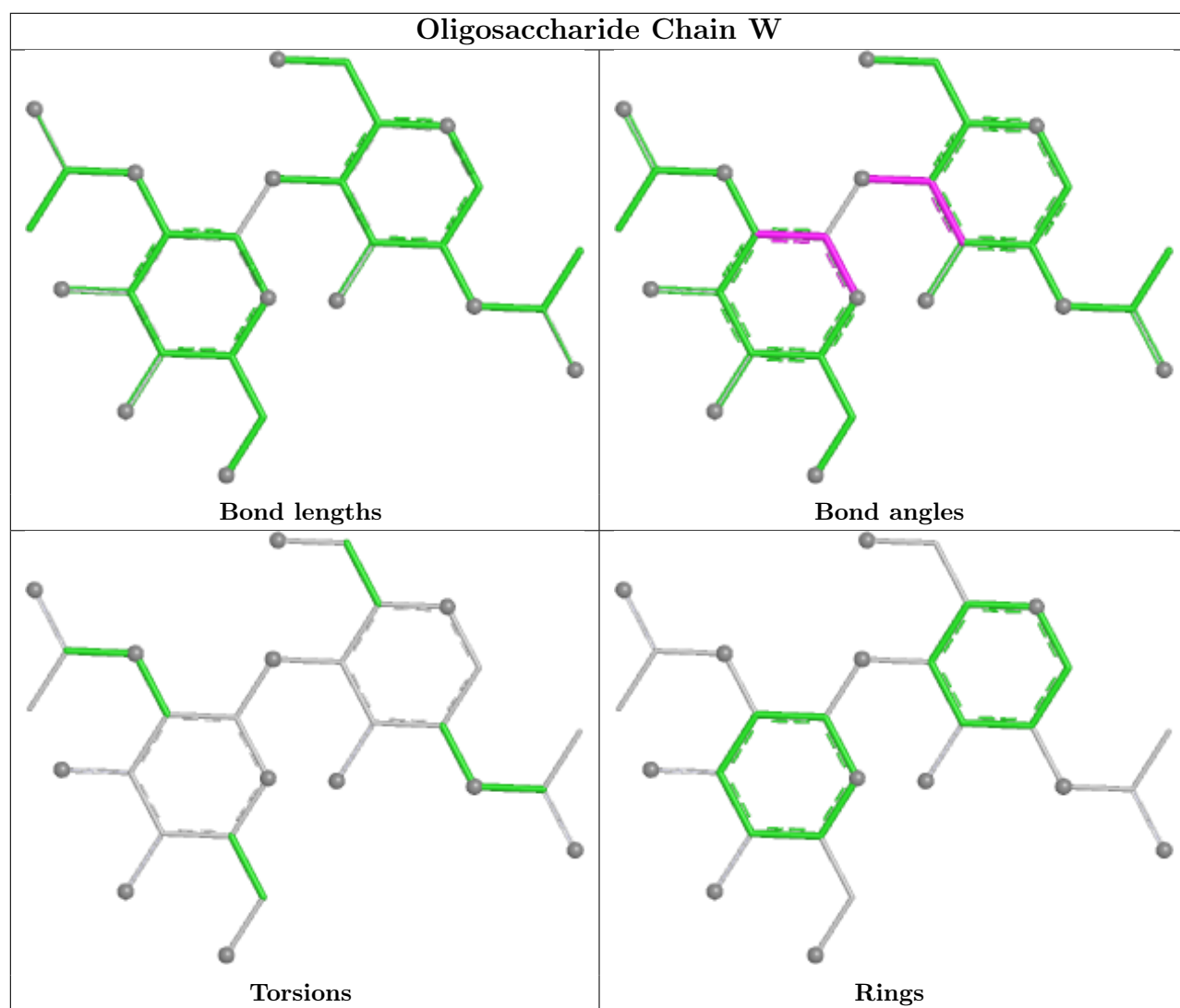
There are no ring outliers.

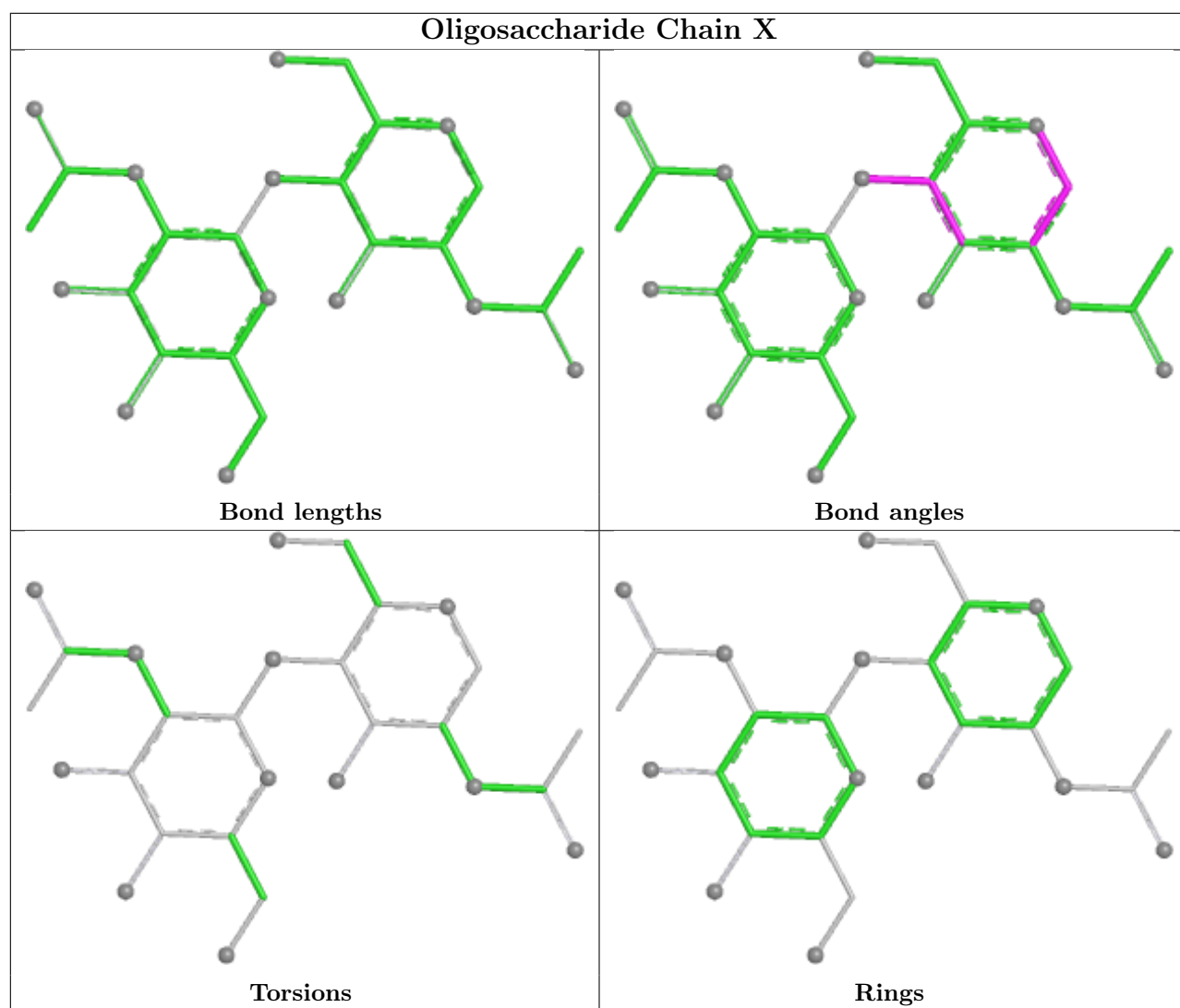
11 monomers are involved in 14 short contacts:

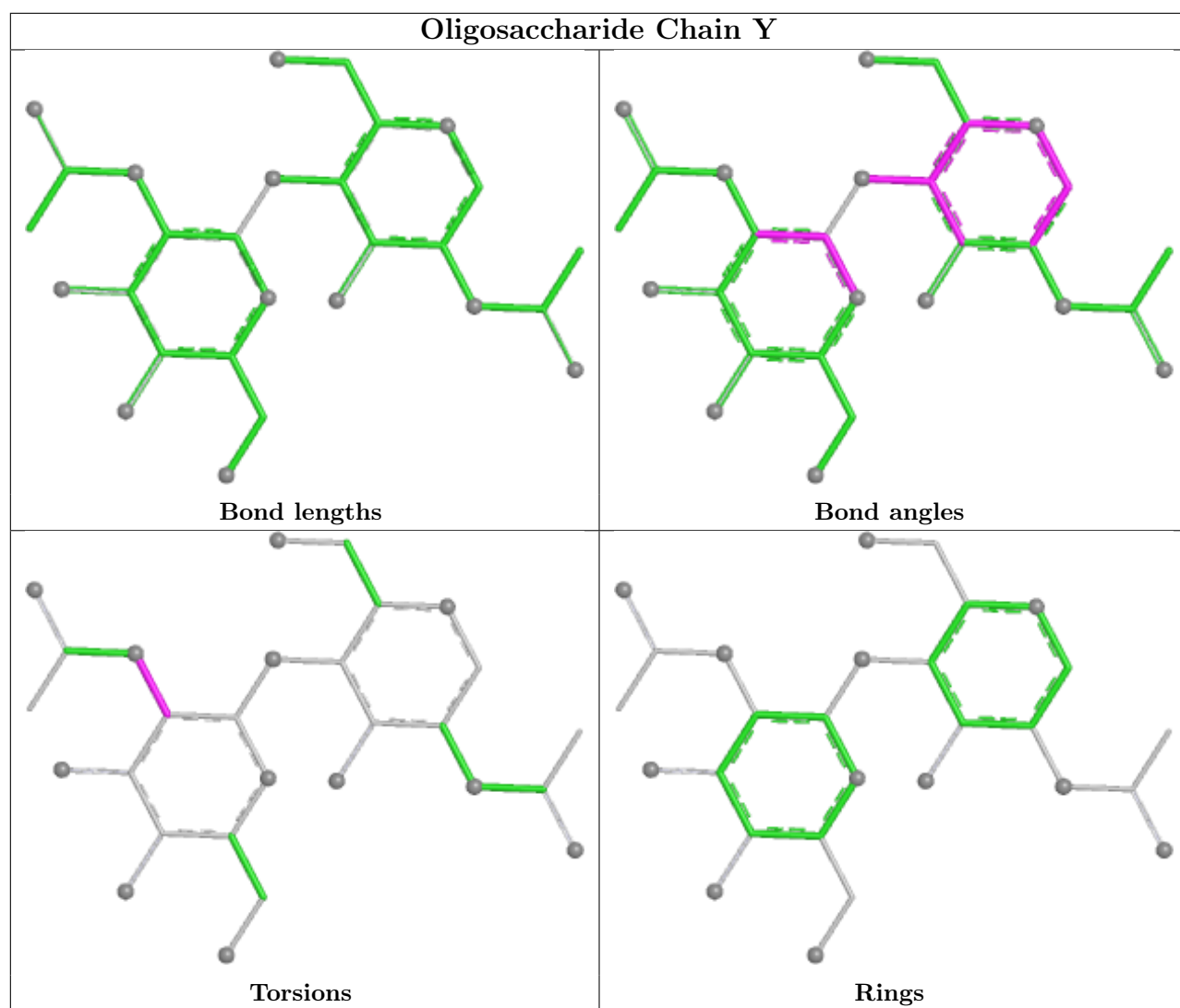
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	r	2	NAG	1	0
19	W	1	NAG	1	0
19	r	1	NAG	1	0
19	X	2	NAG	2	0
19	q	1	NAG	3	0
20	s	1	NAG	3	0
19	c	1	NAG	1	0
19	Y	2	NAG	1	0
19	q	2	NAG	1	0
19	Y	1	NAG	1	0
19	V	1	NAG	2	0

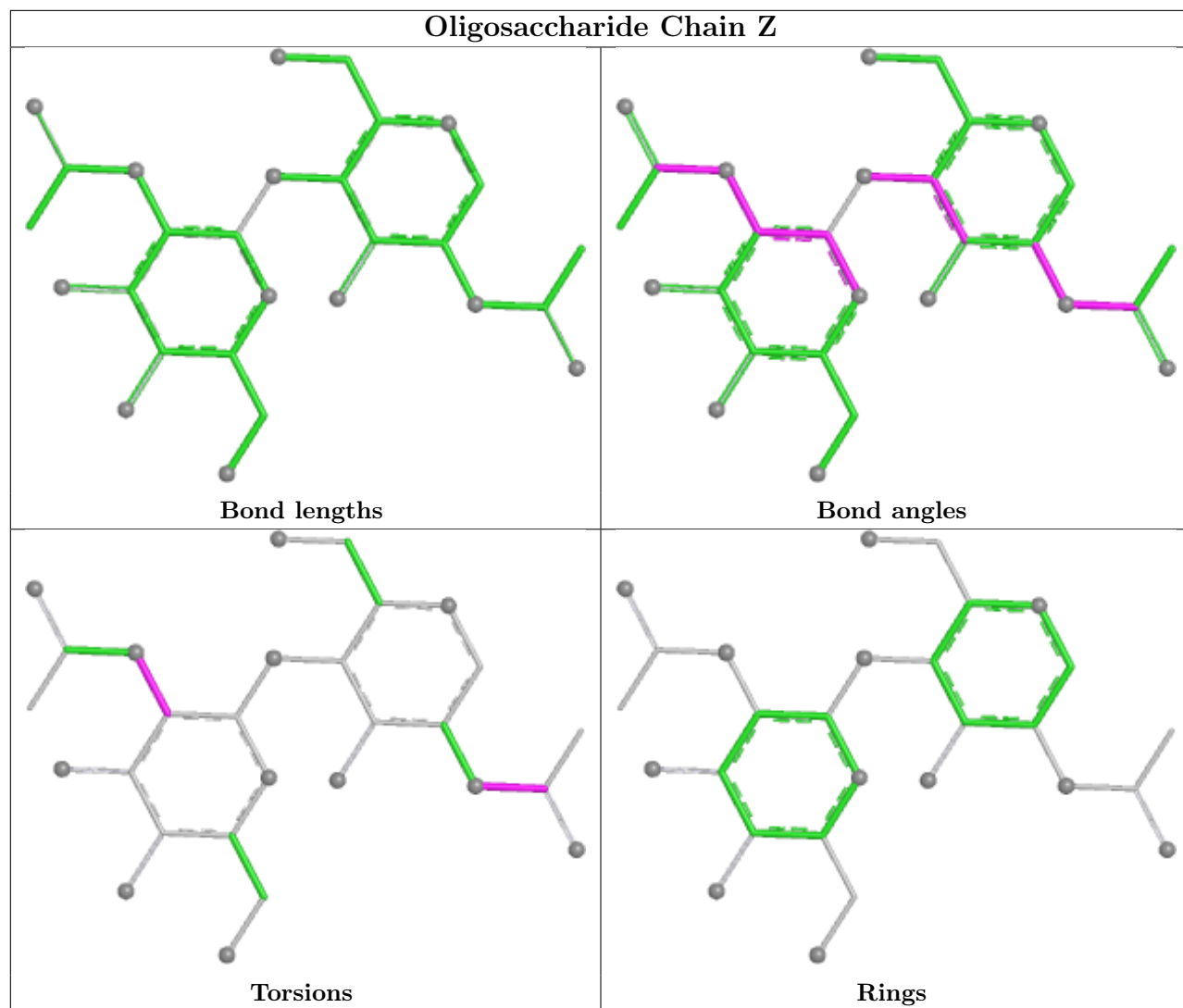
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

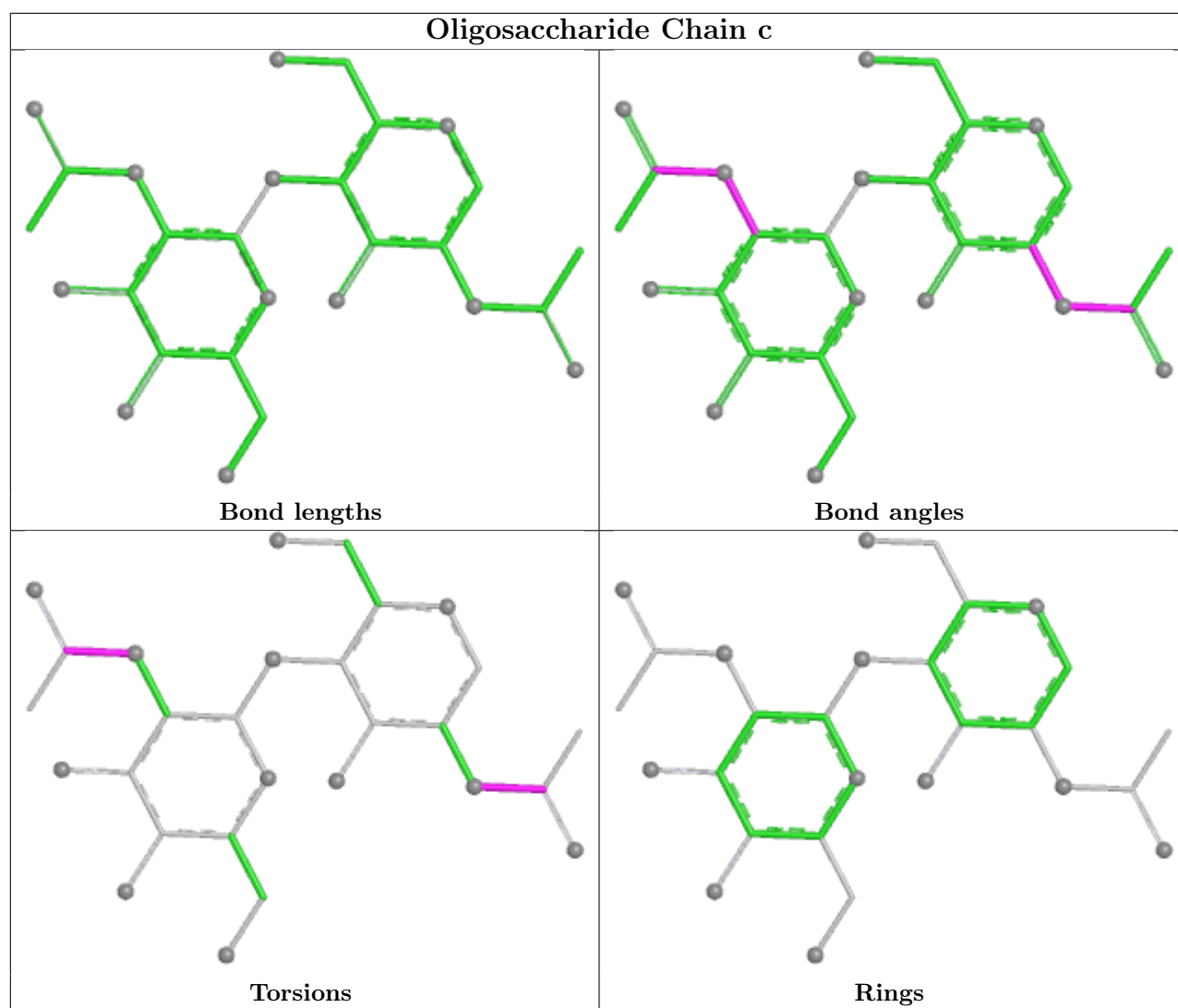


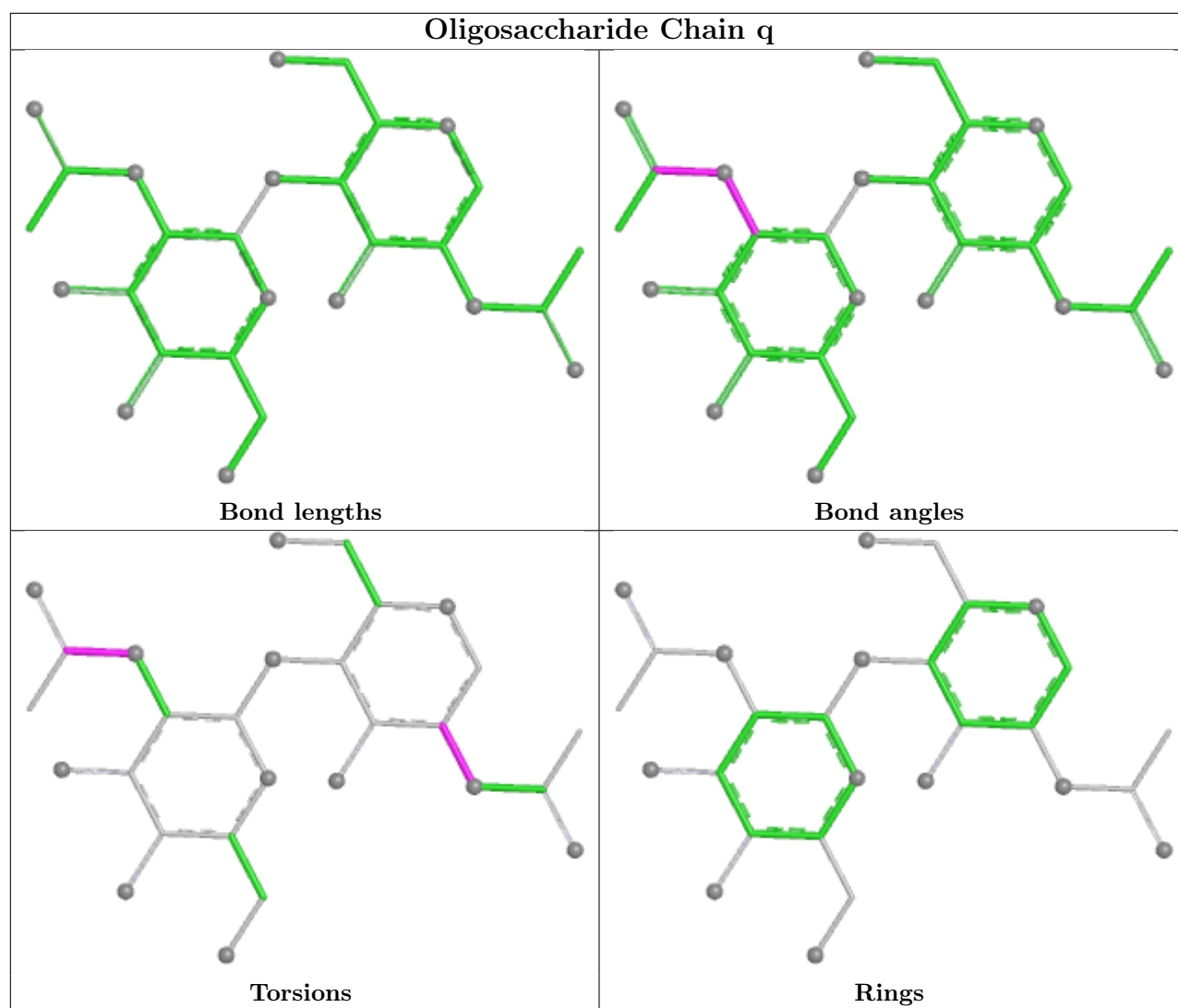


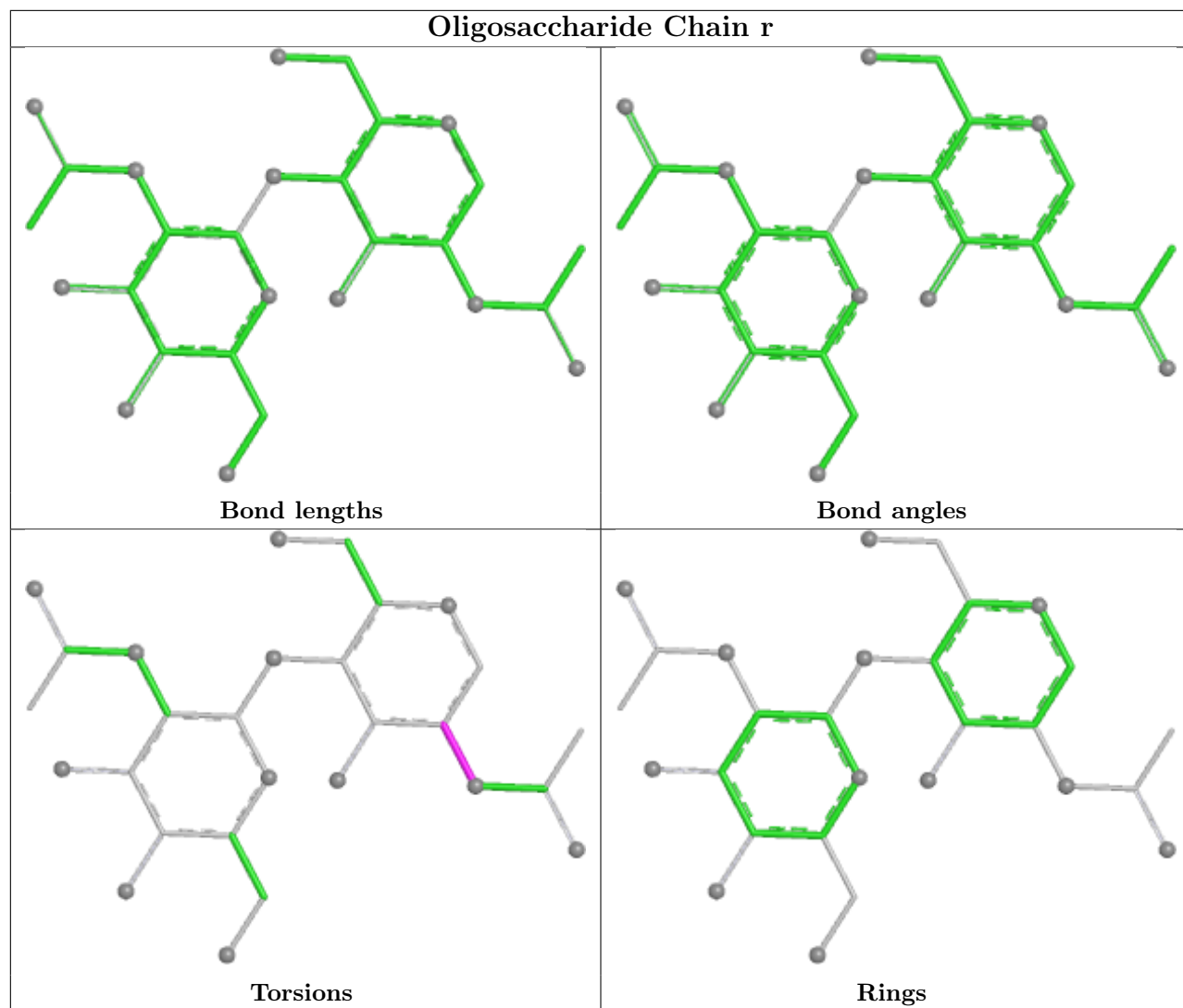


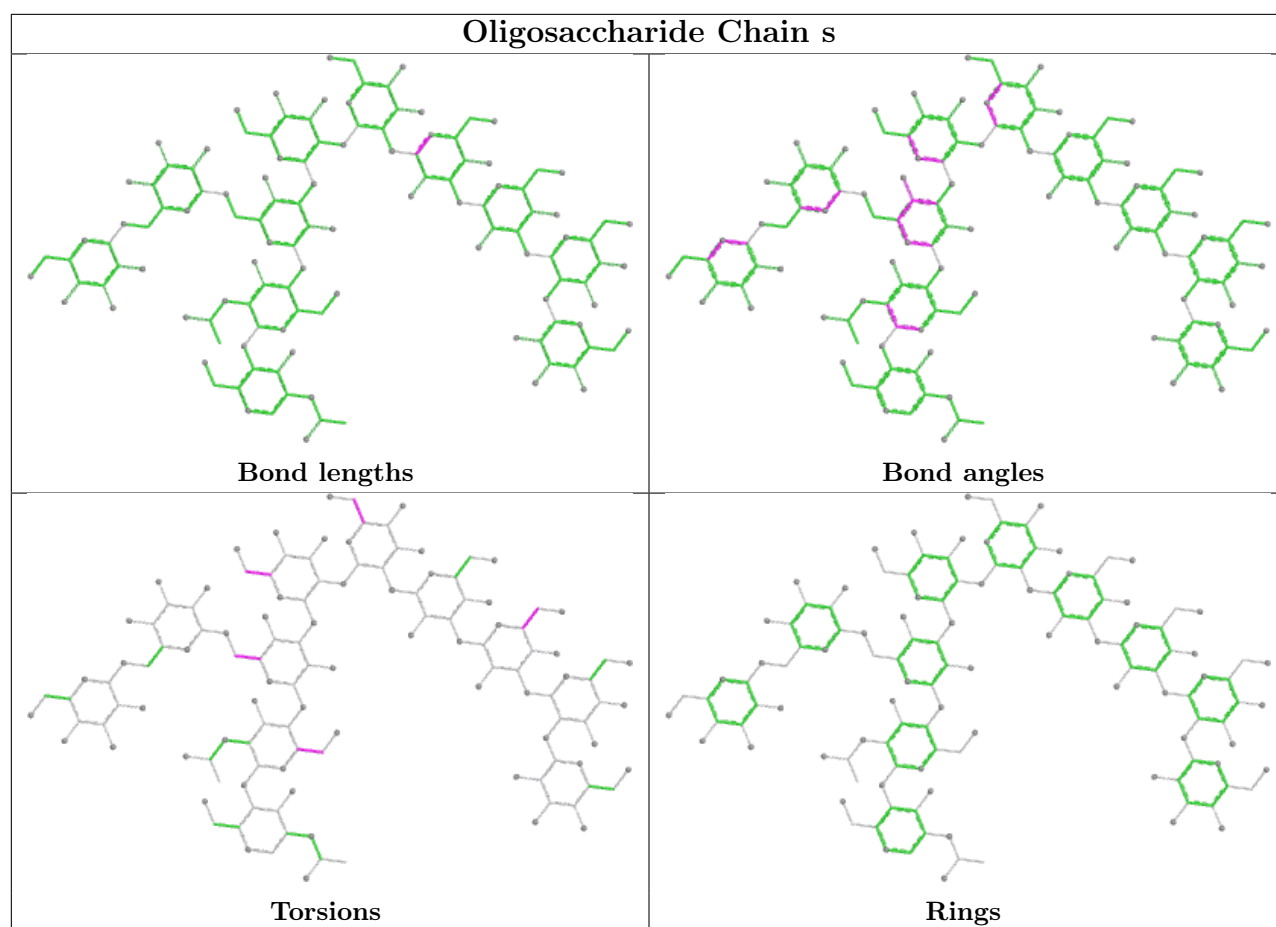












4.6 Ligand geometry [i](#)

48 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	$\# Z > 2$
22	PC1	a	901	-	53,53,53	0.50	0	59,61,61	0.48	1 (1%)
27	CLR	j	203	-	31,31,31	0.44	0	48,48,48	0.75	1 (2%)
27	CLR	h	201	-	31,31,31	0.39	0	48,48,48	0.75	0
27	CLR	i	202	-	31,31,31	0.40	0	48,48,48	0.77	0
27	CLR	m	202	-	31,31,31	0.36	0	48,48,48	0.67	0
25	NAG	a	906	12	14,14,15	0.77	0	17,19,21	1.17	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	ADP	A	701	-	28,29,29	1.39	5 (17%)	43,45,45	1.84	11 (25%)
22	PC1	b	301	-	53,53,53	0.51	0	59,61,61	0.49	1 (1%)
27	CLR	o	201	-	31,31,31	0.40	0	48,48,48	0.88	1 (2%)
23	PTY	p	404	-	49,49,49	0.46	0	52,54,54	0.39	0
27	CLR	i	204	-	31,31,31	0.38	0	48,48,48	0.62	0
27	CLR	k	202	-	31,31,31	0.36	0	48,48,48	0.49	0
27	CLR	l	204	-	31,31,31	0.39	0	48,48,48	0.72	0
27	CLR	j	201	-	31,31,31	0.39	0	48,48,48	0.66	0
27	CLR	k	203	-	31,31,31	0.37	0	48,48,48	0.56	0
27	CLR	j	204	-	31,31,31	0.38	0	48,48,48	0.72	0
27	CLR	n	204	-	31,31,31	0.37	0	48,48,48	0.77	0
22	PC1	l	201	-	53,53,53	0.50	0	59,61,61	0.51	1 (1%)
23	PTY	a	903	-	49,49,49	0.47	0	52,54,54	0.40	0
27	CLR	i	201	-	31,31,31	0.38	0	48,48,48	0.77	1 (2%)
27	CLR	m	203	-	31,31,31	0.41	0	48,48,48	0.79	1 (2%)
27	CLR	o	202	-	31,31,31	0.45	0	48,48,48	1.00	3 (6%)
23	PTY	b	302	-	49,49,49	0.48	0	52,54,54	0.41	0
27	CLR	l	202	-	31,31,31	0.36	0	48,48,48	0.75	0
27	CLR	n	205	-	31,31,31	0.37	0	48,48,48	0.58	0
23	PTY	p	403	-	49,49,49	0.46	0	52,54,54	0.45	0
27	CLR	n	202	-	31,31,31	0.39	0	48,48,48	0.68	0
27	CLR	n	203	-	31,31,31	0.36	0	48,48,48	0.67	0
27	CLR	o	203	-	31,31,31	0.36	0	48,48,48	0.68	0
23	PTY	a	902	-	49,49,49	0.47	0	52,54,54	0.37	0
27	CLR	j	202	-	31,31,31	0.42	0	48,48,48	0.89	3 (6%)
27	CLR	h	202	-	31,31,31	0.38	0	48,48,48	0.98	4 (8%)
23	PTY	p	401	-	49,49,49	0.47	0	52,54,54	0.43	0
22	PC1	P	502	-	53,53,53	0.50	0	59,61,61	0.47	1 (1%)
27	CLR	k	201	-	31,31,31	0.36	0	48,48,48	0.66	0
27	CLR	b	304	-	31,31,31	0.40	0	48,48,48	0.61	0
22	PC1	P	501	-	53,53,53	0.50	0	59,61,61	0.53	1 (1%)
23	PTY	b	303	-	49,49,49	0.48	0	52,54,54	0.39	0
27	CLR	l	203	-	31,31,31	0.36	0	48,48,48	0.62	0
24	WJP	a	905	-	32,33,34	1.81	7 (21%)	39,43,44	6.61	7 (17%)
27	CLR	m	201	-	31,31,31	0.41	0	48,48,48	0.67	0
26	LP3	a	907	-	34,34,34	0.52	0	39,41,41	0.56	0
27	CLR	i	203	-	31,31,31	0.47	0	48,48,48	0.85	1 (2%)
27	CLR	n	201	-	31,31,31	0.36	0	48,48,48	0.83	2 (4%)
23	PTY	p	402	-	49,49,49	0.47	0	52,54,54	0.42	0
27	CLR	l	205	-	31,31,31	0.35	0	48,48,48	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLR	l	206	-	31,31,31	0.39	0	48,48,48	0.55	0
23	PTY	a	904	-	49,49,49	0.47	0	52,54,54	0.37	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
22	PC1	a	901	-	-	21/57/57/57	-
27	CLR	j	203	-	-	6/10/68/68	0/4/4/4
27	CLR	h	201	-	-	3/10/68/68	0/4/4/4
27	CLR	i	202	-	-	4/10/68/68	0/4/4/4
27	CLR	m	202	-	-	1/10/68/68	0/4/4/4
25	NAG	a	906	12	-	2/6/23/26	0/1/1/1
21	ADP	A	701	-	-	3/16/32/32	0/3/3/3
22	PC1	b	301	-	-	23/57/57/57	-
27	CLR	o	201	-	-	6/10/68/68	0/4/4/4
23	PTY	p	404	-	-	23/53/53/53	-
27	CLR	i	204	-	-	6/10/68/68	0/4/4/4
27	CLR	k	202	-	-	2/10/68/68	0/4/4/4
27	CLR	l	204	-	-	2/10/68/68	0/4/4/4
27	CLR	j	201	-	-	4/10/68/68	0/4/4/4
27	CLR	k	203	-	-	2/10/68/68	0/4/4/4
27	CLR	j	204	-	-	4/10/68/68	0/4/4/4
27	CLR	n	204	-	-	3/10/68/68	0/4/4/4
22	PC1	l	201	-	-	21/57/57/57	-
23	PTY	a	903	-	-	19/53/53/53	-
27	CLR	i	201	-	-	3/10/68/68	0/4/4/4
27	CLR	m	203	-	-	5/10/68/68	0/4/4/4
27	CLR	o	202	-	-	6/10/68/68	0/4/4/4
23	PTY	b	302	-	-	22/53/53/53	-
27	CLR	l	202	-	-	4/10/68/68	0/4/4/4
27	CLR	n	205	-	-	4/10/68/68	0/4/4/4
23	PTY	p	403	-	-	24/53/53/53	-
27	CLR	n	202	-	-	1/10/68/68	0/4/4/4
27	CLR	n	203	-	-	2/10/68/68	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLR	o	203	-	-	3/10/68/68	0/4/4/4
23	PTY	a	902	-	-	19/53/53/53	-
27	CLR	j	202	-	-	7/10/68/68	0/4/4/4
27	CLR	h	202	-	-	7/10/68/68	0/4/4/4
23	PTY	p	401	-	-	17/53/53/53	-
22	PC1	P	502	-	-	20/57/57/57	-
27	CLR	k	201	-	-	3/10/68/68	0/4/4/4
27	CLR	b	304	-	-	4/10/68/68	0/4/4/4
22	PC1	P	501	-	-	24/57/57/57	-
23	PTY	b	303	-	-	23/53/53/53	-
27	CLR	l	203	-	-	4/10/68/68	0/4/4/4
24	WJP	a	905	-	-	16/37/37/40	-
27	CLR	m	201	-	-	4/10/68/68	0/4/4/4
26	LP3	a	907	-	-	14/36/36/36	-
27	CLR	i	203	-	-	5/10/68/68	0/4/4/4
27	CLR	n	201	-	-	1/10/68/68	0/4/4/4
23	PTY	p	402	-	-	24/53/53/53	-
27	CLR	l	205	-	-	6/10/68/68	0/4/4/4
27	CLR	l	206	-	-	4/10/68/68	0/4/4/4
23	PTY	a	904	-	-	20/53/53/53	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	905	WJP	P27-O30	4.82	1.64	1.59
21	A	701	ADP	C5-C4	4.43	1.47	1.39
24	a	905	WJP	C18-C16	3.76	1.59	1.51
24	a	905	WJP	C07-C06	3.11	1.58	1.50
24	a	905	WJP	P31-O32	3.07	1.66	1.54
24	a	905	WJP	C17-C16	2.75	1.57	1.50
24	a	905	WJP	C13-C11	2.65	1.56	1.51
21	A	701	ADP	C5-C6	2.54	1.48	1.41
21	A	701	ADP	C5-N7	-2.53	1.34	1.39
21	A	701	ADP	C8-N7	2.29	1.36	1.31
24	a	905	WJP	C14-C15	2.07	1.56	1.50
21	A	701	ADP	C4-N9	-2.05	1.33	1.37

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	905	WJP	C08-C06-C05	20.90	168.09	121.17
24	a	905	WJP	C17-C16-C18	-20.34	79.92	115.23
24	a	905	WJP	C17-C16-C15	17.18	167.76	123.63
24	a	905	WJP	C07-C06-C08	-15.66	88.04	115.23
24	a	905	WJP	C18-C16-C15	-14.70	88.18	121.17
24	a	905	WJP	C07-C06-C05	-8.10	102.82	123.63
21	A	701	ADP	C5-C4-N3	-5.83	118.69	126.72
21	A	701	ADP	N3-C4-N9	4.53	134.87	127.17
25	a	906	NAG	C2-N2-C7	3.75	127.92	122.90
21	A	701	ADP	C2-N3-C4	3.72	120.91	111.83
21	A	701	ADP	C4-C5-N7	-3.55	106.53	110.58
21	A	701	ADP	N3-C2-N1	-3.38	123.47	128.58
27	h	202	CLR	C16-C17-C20	2.93	116.61	112.18
27	j	203	CLR	C21-C20-C17	2.74	117.00	112.88
27	j	202	CLR	C13-C17-C20	2.74	123.72	119.50
27	h	202	CLR	C22-C20-C17	2.72	115.97	110.33
21	A	701	ADP	C4-N9-C8	2.66	108.53	105.74
27	j	202	CLR	C21-C20-C17	2.66	116.87	112.88
27	o	202	CLR	C16-C17-C20	2.59	116.10	112.18
21	A	701	ADP	C5-N7-C8	2.58	107.51	103.45
22	l	201	PC1	O12-P-O14	2.50	124.06	112.44
27	m	203	CLR	C16-C17-C20	2.45	115.89	112.18
22	a	901	PC1	O12-P-O14	2.44	123.81	112.44
22	P	502	PC1	O12-P-O14	2.42	123.69	112.44
22	P	501	PC1	O12-P-O14	2.41	123.64	112.44
21	A	701	ADP	C3'-C2'-C1'	2.40	106.01	101.46
22	b	301	PC1	O12-P-O14	2.34	123.32	112.44
27	n	201	CLR	C13-C17-C20	2.33	123.10	119.50
27	h	202	CLR	C16-C17-C13	-2.33	101.10	103.84
27	o	202	CLR	C21-C20-C22	2.31	113.91	110.34
27	n	201	CLR	C13-C14-C8	2.30	117.68	114.41
27	o	202	CLR	C21-C20-C17	-2.29	109.44	112.88
27	j	202	CLR	C12-C13-C14	-2.25	103.88	107.25
24	a	905	WJP	C14-C15-C16	-2.24	122.49	127.62
27	i	203	CLR	C16-C17-C20	2.23	115.56	112.18
27	o	201	CLR	C11-C9-C8	-2.17	108.75	111.78
27	i	201	CLR	C22-C20-C17	2.08	114.64	110.33
21	A	701	ADP	N9-C8-N7	-2.07	111.00	113.94
21	A	701	ADP	C6-C5-N7	2.02	135.99	132.09
27	h	202	CLR	C21-C20-C22	-2.02	107.21	110.34
21	A	701	ADP	C2-N1-C6	2.02	122.05	118.73

There are no chirality outliers.

All (451) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	A	701	ADP	C5'-O5'-PA-O1A
21	A	701	ADP	C5'-O5'-PA-O2A
21	A	701	ADP	C5'-O5'-PA-O3A
22	P	501	PC1	C11-O13-P-O11
22	P	501	PC1	C1-O11-P-O13
22	P	501	PC1	C22-C21-O21-C2
22	P	502	PC1	C11-O13-P-O12
22	P	502	PC1	C11-O13-P-O11
22	P	502	PC1	C1-O11-P-O14
22	P	502	PC1	O22-C21-O21-C2
22	a	901	PC1	C11-O13-P-O11
22	a	901	PC1	C1-O11-P-O14
22	a	901	PC1	C22-C21-O21-C2
22	b	301	PC1	C11-O13-P-O12
22	b	301	PC1	C11-O13-P-O11
22	b	301	PC1	O22-C21-O21-C2
22	b	301	PC1	C22-C21-O21-C2
22	l	201	PC1	C11-O13-P-O12
22	l	201	PC1	C11-O13-P-O14
22	l	201	PC1	C11-O13-P-O11
22	l	201	PC1	C1-O11-P-O12
22	l	201	PC1	C2-C1-O11-P
22	l	201	PC1	C22-C21-O21-C2
23	a	902	PTY	C3-O11-P1-O13
23	a	902	PTY	C3-O11-P1-O14
23	a	902	PTY	C5-O14-P1-O11
23	a	902	PTY	C5-O14-P1-O12
23	a	903	PTY	O10-C8-O7-C6
23	a	903	PTY	C5-O14-P1-O11
23	a	904	PTY	C3-O11-P1-O13
23	a	904	PTY	C5-O14-P1-O11
23	a	904	PTY	C5-O14-P1-O12
23	b	302	PTY	N1-C2-C3-O11
23	b	302	PTY	C5-O14-P1-O11
23	b	302	PTY	C5-O14-P1-O13
23	b	303	PTY	N1-C2-C3-O11
23	b	303	PTY	C3-O11-P1-O12
23	b	303	PTY	C3-O11-P1-O13
23	b	303	PTY	C3-O11-P1-O14
23	b	303	PTY	C5-O14-P1-O12
23	p	401	PTY	C2-C3-O11-P1
23	p	401	PTY	C3-O11-P1-O12

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Mol	Chain	Res	Type	Atoms
23	p	401	PTY	C3-O11-P1-O13
23	p	401	PTY	C3-O11-P1-O14
23	p	402	PTY	N1-C2-C3-O11
23	p	402	PTY	C11-C8-O7-C6
23	p	402	PTY	C3-O11-P1-O13
23	p	403	PTY	C11-C8-O7-C6
23	p	403	PTY	C3-O11-P1-O13
23	p	404	PTY	C11-C8-O7-C6
23	p	404	PTY	C3-O11-P1-O13
23	p	404	PTY	C3-O11-P1-O14
24	a	905	WJP	C03-C02-C24-C25
24	a	905	WJP	C02-C03-C04-C05
24	a	905	WJP	P27-O30-P31-O32
26	a	907	LP3	O4P-C4-C5-N
26	a	907	LP3	C1-O3P-P-O2P
26	a	907	LP3	C1-O3P-P-O4P
27	h	202	CLR	C13-C17-C20-C21
22	P	501	PC1	O32-C31-O31-C3
23	p	403	PTY	O30-C30-O4-C1
27	h	202	CLR	C16-C17-C20-C21
27	i	203	CLR	C13-C17-C20-C21
22	P	501	PC1	O22-C21-O21-C2
22	a	901	PC1	O22-C21-O21-C2
22	l	201	PC1	O22-C21-O21-C2
23	p	402	PTY	O10-C8-O7-C6
23	p	403	PTY	O10-C8-O7-C6
23	p	404	PTY	O10-C8-O7-C6
22	P	502	PC1	C22-C21-O21-C2
23	a	903	PTY	C11-C8-O7-C6
27	i	203	CLR	C16-C17-C20-C21
27	h	202	CLR	C16-C17-C20-C22
27	h	202	CLR	C13-C17-C20-C22
22	a	901	PC1	O32-C31-O31-C3
22	b	301	PC1	O32-C31-O31-C3
22	P	501	PC1	C32-C31-O31-C3
22	a	901	PC1	C32-C31-O31-C3
22	b	301	PC1	C32-C31-O31-C3
23	p	402	PTY	C31-C30-O4-C1
23	p	403	PTY	C31-C30-O4-C1
24	a	905	WJP	C04-C05-C06-C08
23	p	402	PTY	O30-C30-O4-C1
27	i	203	CLR	C13-C17-C20-C22

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Mol	Chain	Res	Type	Atoms
27	l	203	CLR	C17-C20-C22-C23
27	i	203	CLR	C16-C17-C20-C22
27	i	204	CLR	C17-C20-C22-C23
27	l	203	CLR	C21-C20-C22-C23
27	m	203	CLR	C13-C17-C20-C22
27	k	201	CLR	C17-C20-C22-C23
27	l	205	CLR	C17-C20-C22-C23
27	m	201	CLR	C17-C20-C22-C23
27	n	205	CLR	C17-C20-C22-C23
27	o	201	CLR	C17-C20-C22-C23
27	m	203	CLR	C16-C17-C20-C21
27	m	203	CLR	C13-C17-C20-C21
27	h	202	CLR	C17-C20-C22-C23
23	p	401	PTY	C40-C41-C42-C43
27	i	204	CLR	C21-C20-C22-C23
27	l	205	CLR	C21-C20-C22-C23
27	n	205	CLR	C21-C20-C22-C23
27	o	201	CLR	C21-C20-C22-C23
27	o	202	CLR	C21-C20-C22-C23
26	a	907	LP3	O3P-C1-C2-O2
23	b	302	PTY	C8-C11-C12-C13
27	b	304	CLR	C17-C20-C22-C23
23	a	904	PTY	O14-C5-C6-O7
27	j	202	CLR	C20-C22-C23-C24
27	n	202	CLR	C22-C23-C24-C25
27	o	202	CLR	C20-C22-C23-C24
25	a	906	NAG	C8-C7-N2-C2
25	a	906	NAG	O7-C7-N2-C2
27	m	203	CLR	C16-C17-C20-C22
27	i	202	CLR	C13-C17-C20-C22
27	j	204	CLR	C17-C20-C22-C23
27	k	202	CLR	C17-C20-C22-C23
27	j	202	CLR	C22-C23-C24-C25
27	h	202	CLR	C21-C20-C22-C23
24	a	905	WJP	C16-C18-C19-C20
22	a	901	PC1	C31-C32-C33-C34
23	p	401	PTY	C8-C11-C12-C13
27	o	202	CLR	C13-C17-C20-C22
27	b	304	CLR	C21-C20-C22-C23
27	k	201	CLR	C21-C20-C22-C23
27	b	304	CLR	C22-C23-C24-C25
27	k	203	CLR	C20-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
23	p	402	PTY	C30-C31-C32-C33
23	p	403	PTY	C30-C31-C32-C33
26	a	907	LP3	C11-C12-C13-C14
27	i	201	CLR	C22-C23-C24-C25
27	m	202	CLR	C22-C23-C24-C25
27	o	201	CLR	C22-C23-C24-C25
27	i	202	CLR	C13-C17-C20-C21
27	j	201	CLR	C13-C17-C20-C21
27	o	202	CLR	C13-C17-C20-C21
23	b	303	PTY	C8-C11-C12-C13
27	m	203	CLR	C22-C23-C24-C25
27	j	201	CLR	C13-C17-C20-C22
27	j	204	CLR	C21-C20-C22-C23
27	n	205	CLR	C22-C23-C24-C25
27	n	201	CLR	C22-C23-C24-C25
22	P	502	PC1	C32-C31-O31-C3
23	a	902	PTY	C31-C30-O4-C1
27	l	206	CLR	C17-C20-C22-C23
27	j	202	CLR	C21-C20-C22-C23
22	P	502	PC1	C21-C22-C23-C24
22	b	301	PC1	C21-C22-C23-C24
27	h	201	CLR	C20-C22-C23-C24
27	k	203	CLR	C22-C23-C24-C25
27	i	202	CLR	C16-C17-C20-C21
27	o	202	CLR	C16-C17-C20-C21
27	l	204	CLR	C22-C23-C24-C25
27	j	203	CLR	C13-C17-C20-C22
27	m	201	CLR	C21-C20-C22-C23
27	k	202	CLR	C21-C20-C22-C23
27	n	203	CLR	C23-C24-C25-C26
27	j	201	CLR	C16-C17-C20-C21
27	n	203	CLR	C23-C24-C25-C27
27	j	202	CLR	C16-C17-C20-C22
27	l	205	CLR	C23-C24-C25-C27
27	j	202	CLR	C13-C17-C20-C22
23	a	902	PTY	O30-C30-O4-C1
23	a	904	PTY	C18-C19-C20-C21
22	P	501	PC1	C23-C24-C25-C26
22	P	501	PC1	C39-C3A-C3B-C3C
23	b	303	PTY	C24-C25-C26-C27
23	p	402	PTY	C38-C39-C40-C41
22	l	201	PC1	C3E-C3F-C3G-C3H

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Mol	Chain	Res	Type	Atoms
22	P	502	PC1	O32-C31-O31-C3
22	P	501	PC1	C37-C38-C39-C3A
22	a	901	PC1	C2B-C2C-C2D-C2E
22	a	901	PC1	C3A-C3B-C3C-C3D
23	b	302	PTY	C20-C21-C22-C23
23	p	403	PTY	C34-C35-C36-C37
27	h	201	CLR	C21-C20-C22-C23
22	P	501	PC1	C2A-C2B-C2C-C2D
23	p	402	PTY	C33-C34-C35-C36
27	j	203	CLR	C16-C17-C20-C22
27	l	203	CLR	C20-C22-C23-C24
23	b	302	PTY	C11-C8-O7-C6
22	l	201	PC1	C36-C37-C38-C39
22	b	301	PC1	C2B-C2C-C2D-C2E
23	b	303	PTY	C16-C17-C18-C19
23	p	403	PTY	C37-C38-C39-C40
26	a	907	LP3	O3P-C1-C2-C3
22	l	201	PC1	C32-C31-O31-C3
23	b	302	PTY	C30-C31-C32-C33
22	P	501	PC1	C26-C27-C28-C29
23	p	402	PTY	C17-C18-C19-C20
23	p	403	PTY	C39-C40-C41-C42
26	a	907	LP3	C12-C13-C14-C15
27	l	206	CLR	C21-C20-C22-C23
23	a	902	PTY	C22-C23-C24-C25
23	p	404	PTY	C32-C33-C34-C35
23	p	401	PTY	C31-C32-C33-C34
23	b	303	PTY	C11-C8-O7-C6
22	P	502	PC1	C25-C26-C27-C28
22	a	901	PC1	C35-C36-C37-C38
22	l	201	PC1	C39-C3A-C3B-C3C
27	l	206	CLR	C22-C23-C24-C25
23	a	903	PTY	C12-C13-C14-C15
22	b	301	PC1	C29-C2A-C2B-C2C
22	P	502	PC1	C28-C29-C2A-C2B
23	p	404	PTY	C15-C16-C17-C18
23	a	903	PTY	C34-C35-C36-C37
23	b	302	PTY	O10-C8-O7-C6
23	p	403	PTY	C35-C36-C37-C38
23	p	404	PTY	C19-C20-C21-C22
23	p	404	PTY	C20-C21-C22-C23
22	b	301	PC1	C3A-C3B-C3C-C3D

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Mol	Chain	Res	Type	Atoms
23	p	402	PTY	C34-C35-C36-C37
27	n	205	CLR	C20-C22-C23-C24
27	l	205	CLR	C23-C24-C25-C26
22	b	301	PC1	C3E-C3F-C3G-C3H
23	p	404	PTY	C13-C14-C15-C16
22	P	502	PC1	C33-C34-C35-C36
22	b	301	PC1	C23-C24-C25-C26
22	b	301	PC1	C38-C39-C3A-C3B
23	b	303	PTY	C19-C20-C21-C22
22	a	901	PC1	C33-C34-C35-C36
27	l	206	CLR	C20-C22-C23-C24
22	a	901	PC1	C24-C25-C26-C27
27	l	205	CLR	C20-C22-C23-C24
27	h	201	CLR	C17-C20-C22-C23
27	n	204	CLR	C23-C24-C25-C27
23	p	402	PTY	C15-C16-C17-C18
23	a	903	PTY	C37-C38-C39-C40
27	l	202	CLR	C13-C17-C20-C22
23	p	401	PTY	C35-C36-C37-C38
22	l	201	PC1	O32-C31-O31-C3
27	j	202	CLR	C16-C17-C20-C21
27	j	203	CLR	C16-C17-C20-C21
23	p	403	PTY	C31-C32-C33-C34
23	a	904	PTY	O14-C5-C6-C1
23	p	403	PTY	C16-C17-C18-C19
27	o	203	CLR	C23-C24-C25-C27
27	j	201	CLR	C22-C23-C24-C25
23	a	902	PTY	C11-C8-O7-C6
22	l	201	PC1	C26-C27-C28-C29
23	b	303	PTY	C31-C30-O4-C1
23	b	303	PTY	O10-C8-O7-C6
23	a	904	PTY	O4-C1-C6-C5
23	a	904	PTY	C12-C13-C14-C15
23	p	403	PTY	C38-C39-C40-C41
23	a	903	PTY	C36-C37-C38-C39
27	n	204	CLR	C23-C24-C25-C26
23	p	404	PTY	C31-C32-C33-C34
27	i	204	CLR	C22-C23-C24-C25
27	o	202	CLR	C22-C23-C24-C25
27	o	203	CLR	C23-C24-C25-C26
22	P	502	PC1	C3C-C3D-C3E-C3F
27	o	203	CLR	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
22	b	301	PC1	C3-C2-O21-C21
22	l	201	PC1	C3-C2-O21-C21
23	b	302	PTY	C19-C20-C21-C22
23	p	401	PTY	C25-C26-C27-C28
23	b	303	PTY	C34-C35-C36-C37
27	l	202	CLR	C16-C17-C20-C21
23	b	303	PTY	O14-C5-C6-O7
23	p	402	PTY	O14-C5-C6-O7
27	l	202	CLR	C13-C17-C20-C21
22	P	501	PC1	C2C-C2D-C2E-C2F
23	b	302	PTY	C40-C41-C42-C43
23	p	403	PTY	C32-C33-C34-C35
23	a	904	PTY	C34-C35-C36-C37
23	p	402	PTY	C36-C37-C38-C39
27	m	201	CLR	C23-C24-C25-C27
22	P	501	PC1	C28-C29-C2A-C2B
22	l	201	PC1	C3F-C3G-C3H-C3I
23	a	902	PTY	C14-C15-C16-C17
23	p	404	PTY	C24-C25-C26-C27
23	p	404	PTY	C37-C38-C39-C40
23	a	904	PTY	C31-C30-O4-C1
27	b	304	CLR	C20-C22-C23-C24
22	l	201	PC1	C37-C38-C39-C3A
23	b	302	PTY	C12-C13-C14-C15
22	l	201	PC1	C22-C23-C24-C25
23	p	404	PTY	O14-C5-C6-C1
24	a	905	WJP	C12-C11-C13-C14
27	j	203	CLR	C20-C22-C23-C24
23	p	403	PTY	C23-C24-C25-C26
23	b	303	PTY	O30-C30-O4-C1
23	b	303	PTY	C20-C21-C22-C23
22	P	501	PC1	C2B-C2C-C2D-C2E
24	a	905	WJP	C10-C11-C13-C14
23	p	404	PTY	O14-C5-C6-O7
27	l	202	CLR	C16-C17-C20-C22
22	a	901	PC1	C2F-C2G-C2H-C2I
22	l	201	PC1	C3A-C3B-C3C-C3D
27	i	204	CLR	C23-C24-C25-C26
24	a	905	WJP	C07-C06-C08-C09
24	a	905	WJP	C05-C06-C08-C09
22	b	301	PC1	C2D-C2E-C2F-C2G
26	a	907	LP3	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
27	m	201	CLR	C23-C24-C25-C26
23	b	302	PTY	C24-C25-C26-C27
23	p	404	PTY	C23-C24-C25-C26
24	a	905	WJP	P31-O30-P27-O26
23	a	904	PTY	C19-C20-C21-C22
23	a	904	PTY	C31-C32-C33-C34
23	a	904	PTY	O30-C30-O4-C1
23	p	402	PTY	C20-C21-C22-C23
23	p	403	PTY	O14-C5-C6-C1
23	p	404	PTY	C33-C34-C35-C36
27	i	203	CLR	C22-C23-C24-C25
27	i	202	CLR	C20-C22-C23-C24
23	a	902	PTY	O10-C8-O7-C6
23	b	303	PTY	C14-C15-C16-C17
27	j	202	CLR	C17-C20-C22-C23
22	a	901	PC1	C3E-C3F-C3G-C3H
23	p	403	PTY	O14-C5-C6-O7
26	a	907	LP3	C25-C26-C27-C28
23	p	402	PTY	O4-C1-C6-C5
23	a	904	PTY	O4-C1-C6-O7
26	a	907	LP3	C14-C15-C16-C17
23	p	404	PTY	C14-C15-C16-C17
23	a	904	PTY	C11-C8-O7-C6
22	b	301	PC1	C22-C23-C24-C25
22	a	901	PC1	C2-C1-O11-P
23	p	401	PTY	C15-C16-C17-C18
22	a	901	PC1	O13-C11-C12-N
22	b	301	PC1	O13-C11-C12-N
22	l	201	PC1	O13-C11-C12-N
27	i	201	CLR	C17-C20-C22-C23
23	b	302	PTY	C37-C38-C39-C40
23	b	303	PTY	O14-C5-C6-C1
23	p	402	PTY	O14-C5-C6-C1
23	a	904	PTY	O10-C8-O7-C6
22	P	502	PC1	C2E-C2F-C2G-C2H
23	p	404	PTY	C25-C26-C27-C28
27	i	204	CLR	C23-C24-C25-C27
26	a	907	LP3	C24-C25-C26-C27
23	a	903	PTY	O14-C5-C6-O7
23	p	402	PTY	O4-C1-C6-O7
24	a	905	WJP	C01-C02-C24-C25
23	a	903	PTY	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
22	P	501	PC1	C11-O13-P-O14
22	P	501	PC1	C1-O11-P-O14
22	P	502	PC1	C1-O11-P-O13
22	a	901	PC1	C11-O13-P-O14
22	b	301	PC1	C11-O13-P-O14
23	a	902	PTY	C3-O11-P1-O12
23	a	903	PTY	C5-O14-P1-O13
23	b	302	PTY	C3-O11-P1-O13
23	b	303	PTY	C5-O14-P1-O11
23	b	303	PTY	C5-O14-P1-O13
23	p	401	PTY	N1-C2-C3-O11
23	p	403	PTY	N1-C2-C3-O11
23	p	403	PTY	C3-O11-P1-O14
23	p	404	PTY	C5-O14-P1-O13
26	a	907	LP3	C1-O3P-P-O1P
27	n	204	CLR	C22-C23-C24-C25
23	a	903	PTY	C24-C25-C26-C27
23	a	902	PTY	C23-C24-C25-C26
23	a	904	PTY	C6-C5-O14-P1
23	a	903	PTY	C41-C42-C43-C44
22	P	501	PC1	C29-C2A-C2B-C2C
23	a	904	PTY	C8-C11-C12-C13
22	a	901	PC1	C21-C22-C23-C24
23	p	403	PTY	C20-C21-C22-C23
22	P	501	PC1	C3-C2-O21-C21
22	b	301	PC1	C32-C33-C34-C35
23	a	904	PTY	C30-C31-C32-C33
23	p	402	PTY	C35-C36-C37-C38
23	b	302	PTY	C34-C35-C36-C37
23	p	403	PTY	C15-C16-C17-C18
23	p	402	PTY	C25-C26-C27-C28
23	a	903	PTY	C39-C40-C41-C42
27	j	204	CLR	C20-C22-C23-C24
23	a	903	PTY	C6-C5-O14-P1
26	a	907	LP3	C2-C1-O3P-P
22	a	901	PC1	C38-C39-C3A-C3B
23	a	903	PTY	C38-C39-C40-C41
23	b	302	PTY	O4-C1-C6-O7
23	p	404	PTY	C35-C36-C37-C38
23	a	903	PTY	C15-C16-C17-C18
23	b	303	PTY	C23-C24-C25-C26
23	p	402	PTY	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
27	o	201	CLR	C16-C17-C20-C22
22	P	502	PC1	C3-C2-O21-C21
23	p	403	PTY	C5-C6-O7-C8
22	l	201	PC1	C2A-C2B-C2C-C2D
22	P	501	PC1	C32-C33-C34-C35
23	a	902	PTY	C18-C19-C20-C21
22	P	501	PC1	C35-C36-C37-C38
27	o	201	CLR	C13-C17-C20-C21
22	a	901	PC1	C32-C33-C34-C35
23	a	903	PTY	O14-C5-C6-C1
27	j	203	CLR	C22-C23-C24-C25
23	p	401	PTY	C24-C25-C26-C27
22	P	502	PC1	C3B-C3C-C3D-C3E
23	a	902	PTY	C17-C18-C19-C20
23	b	302	PTY	C35-C36-C37-C38
26	a	907	LP3	C2-C3-O3-C11
27	l	204	CLR	C20-C22-C23-C24
27	k	201	CLR	C22-C23-C24-C25
23	p	403	PTY	C13-C14-C15-C16
22	P	501	PC1	C3D-C3E-C3F-C3G
23	p	402	PTY	C11-C12-C13-C14
22	P	502	PC1	C37-C38-C39-C3A
23	a	902	PTY	C19-C20-C21-C22
27	o	201	CLR	C13-C17-C20-C22
22	b	301	PC1	C26-C27-C28-C29
24	a	905	WJP	P27-O30-P31-O34
22	P	501	PC1	C2D-C2E-C2F-C2G
22	b	301	PC1	C39-C3A-C3B-C3C
27	j	203	CLR	C23-C24-C25-C27
23	b	302	PTY	C21-C22-C23-C24
23	p	402	PTY	C14-C15-C16-C17
23	b	302	PTY	C32-C33-C34-C35
22	b	301	PC1	C25-C26-C27-C28
22	P	501	PC1	C3F-C3G-C3H-C3I
23	p	401	PTY	C26-C27-C28-C29
22	b	301	PC1	C3C-C3D-C3E-C3F
23	b	303	PTY	C17-C18-C19-C20
24	a	905	WJP	C14-C15-C16-C17
23	b	302	PTY	O4-C30-C31-C32
27	i	201	CLR	C21-C20-C22-C23
24	a	905	WJP	C11-C13-C14-C15
23	a	902	PTY	O4-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
23	p	402	PTY	C26-C27-C28-C29
22	l	201	PC1	C32-C33-C34-C35
23	p	404	PTY	C12-C11-C8-O7
23	b	302	PTY	C41-C42-C43-C44
22	a	901	PC1	C3D-C3E-C3F-C3G
27	h	202	CLR	C20-C22-C23-C24
22	P	502	PC1	C31-C32-C33-C34
24	a	905	WJP	C17-C16-C18-C19
22	P	501	PC1	C34-C35-C36-C37
23	a	904	PTY	C25-C26-C27-C28
24	a	905	WJP	P27-O30-P31-O33
27	l	203	CLR	C23-C24-C25-C26
27	i	204	CLR	C13-C17-C20-C21
23	a	903	PTY	C12-C11-C8-O7
23	b	302	PTY	O30-C30-C31-C32
23	b	303	PTY	C36-C37-C38-C39
22	P	502	PC1	C3D-C3E-C3F-C3G
23	p	401	PTY	C19-C20-C21-C22
23	p	401	PTY	C22-C23-C24-C25
23	a	902	PTY	O30-C30-C31-C32
23	a	902	PTY	C12-C11-C8-O7
23	p	404	PTY	C12-C11-C8-O10
27	j	204	CLR	C16-C17-C20-C22
23	p	403	PTY	C11-C12-C13-C14
23	p	401	PTY	C12-C11-C8-O7
22	P	502	PC1	C34-C35-C36-C37
23	p	401	PTY	O14-C5-C6-C1
23	p	404	PTY	C36-C37-C38-C39
23	a	903	PTY	C12-C11-C8-O10
23	a	902	PTY	C12-C11-C8-O10
27	l	205	CLR	C13-C17-C20-C21

There are no ring outliers.

30 monomers are involved in 55 short contacts:

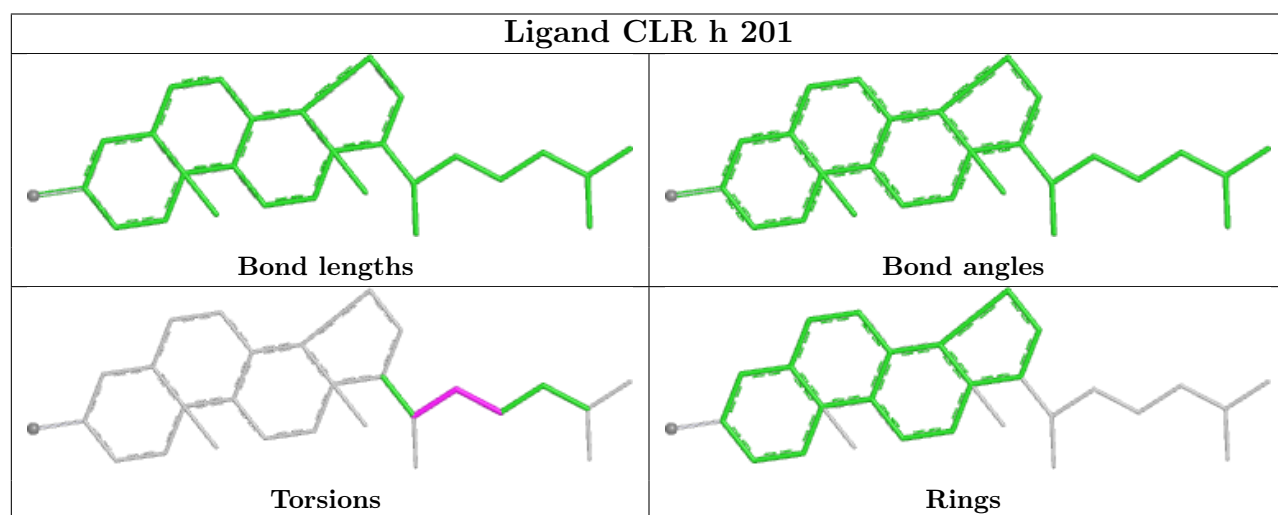
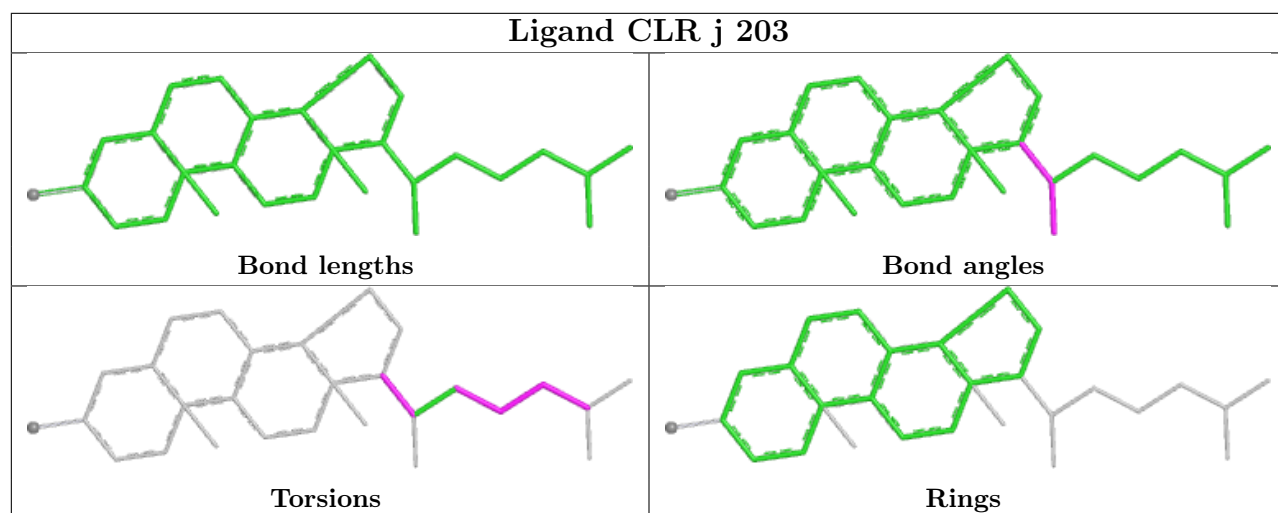
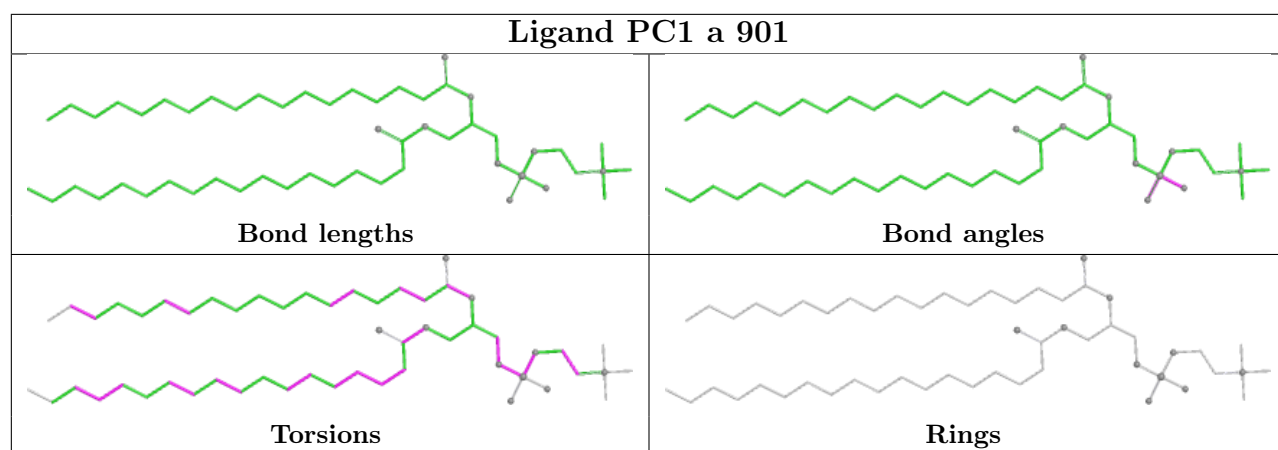
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	a	901	PC1	1	0
27	j	203	CLR	5	0
27	h	201	CLR	3	0
27	m	202	CLR	1	0
25	a	906	NAG	3	0
21	A	701	ADP	2	0

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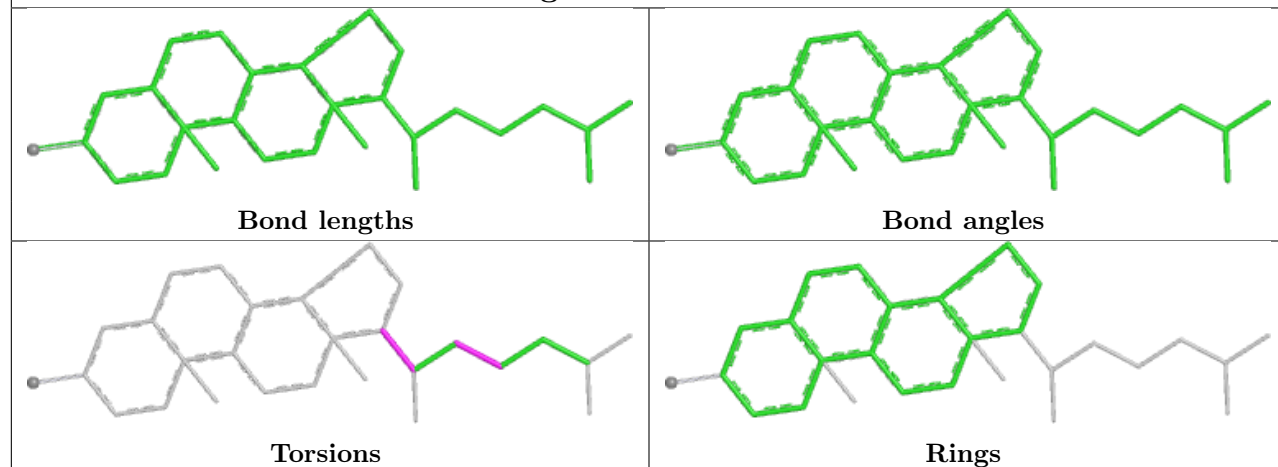
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	o	201	CLR	3	0
27	i	204	CLR	1	0
27	j	201	CLR	1	0
27	j	204	CLR	1	0
27	n	204	CLR	2	0
23	a	903	PTY	1	0
27	o	202	CLR	4	0
23	b	302	PTY	1	0
27	n	205	CLR	2	0
23	p	403	PTY	2	0
27	n	202	CLR	2	0
27	o	203	CLR	2	0
27	j	202	CLR	2	0
27	h	202	CLR	1	0
23	p	401	PTY	4	0
22	P	502	PC1	2	0
27	k	201	CLR	2	0
27	b	304	CLR	1	0
22	P	501	PC1	2	0
27	l	203	CLR	1	0
24	a	905	WJP	1	0
27	i	203	CLR	7	0
27	n	201	CLR	3	0
23	a	904	PTY	1	0

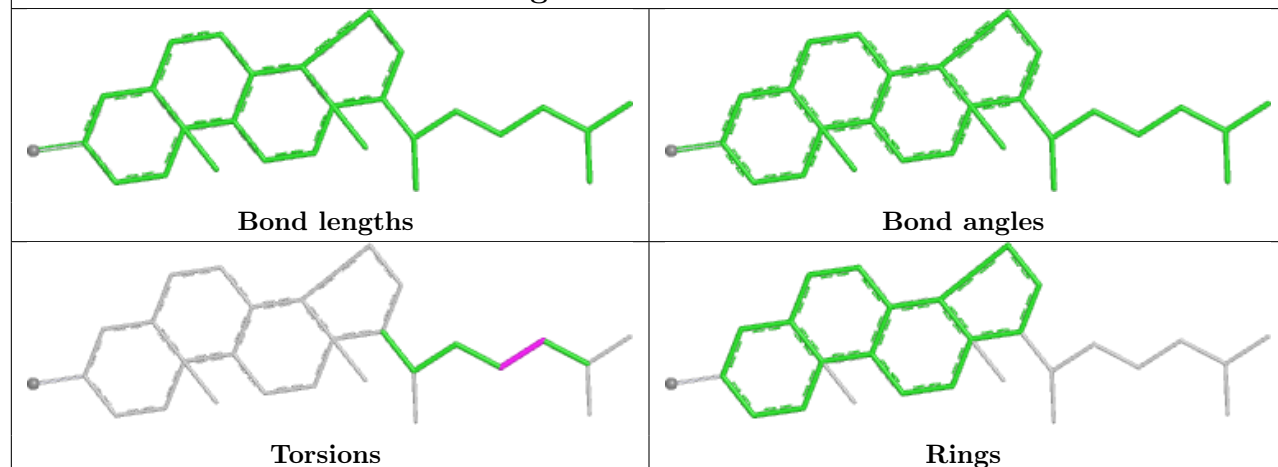
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



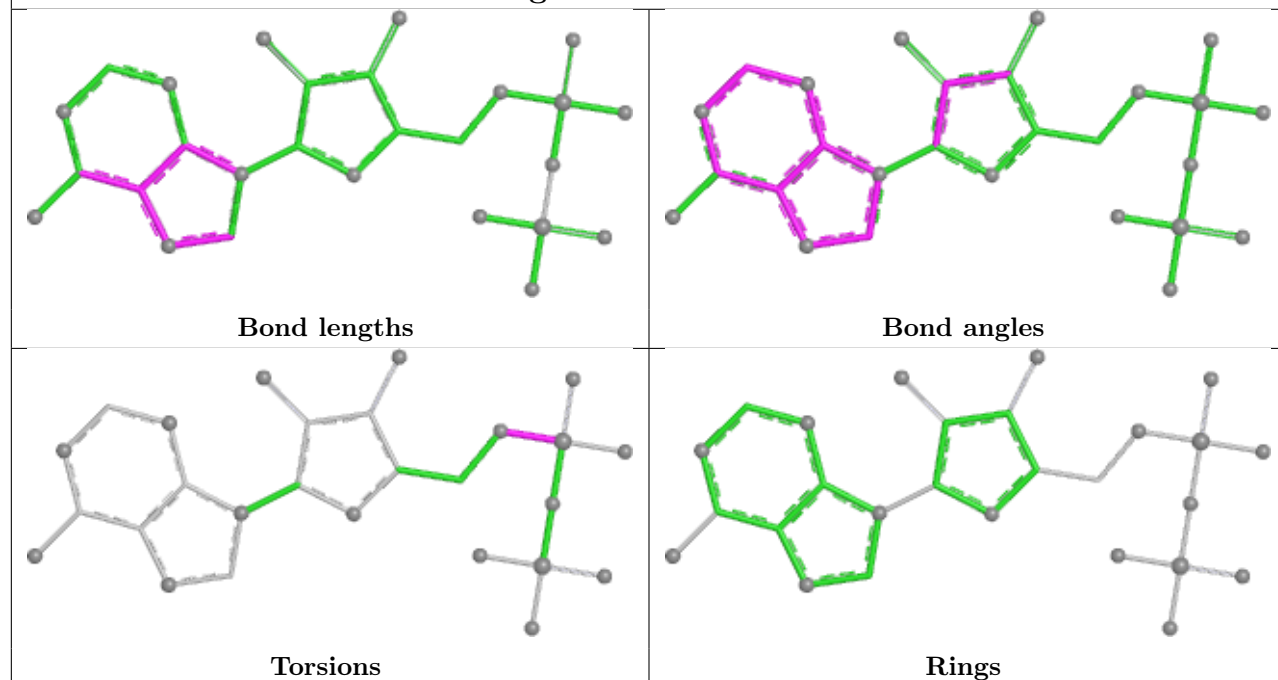
Ligand CLR i 202

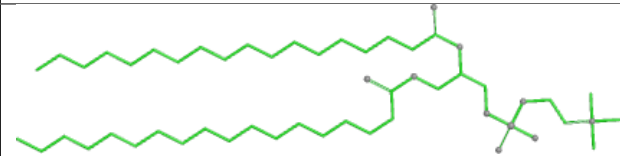
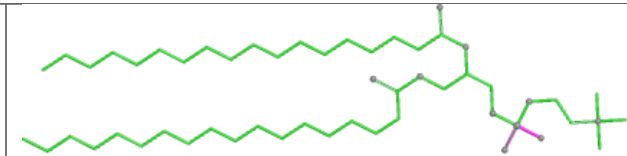
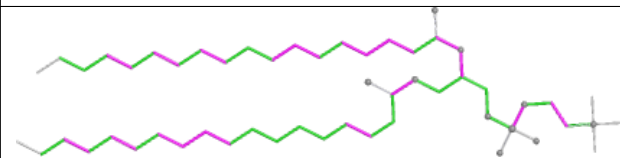
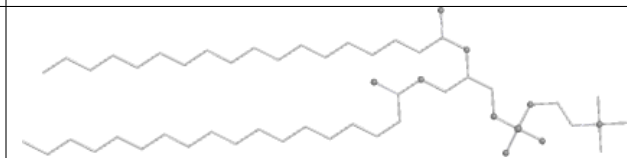


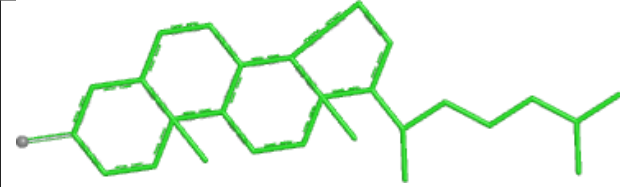
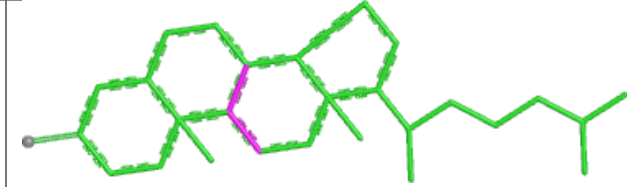
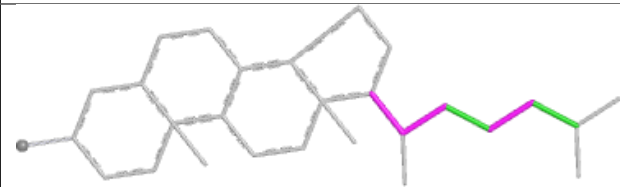
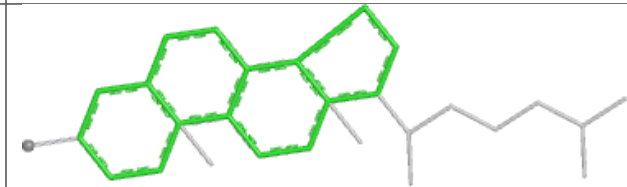
Ligand CLR m 202

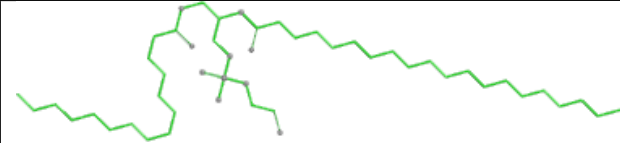
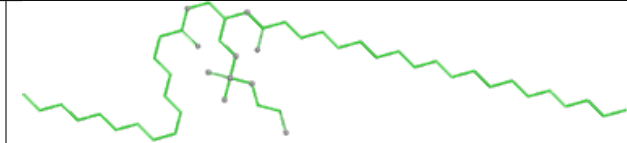
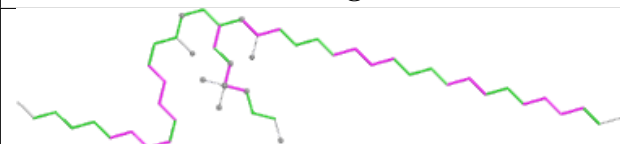
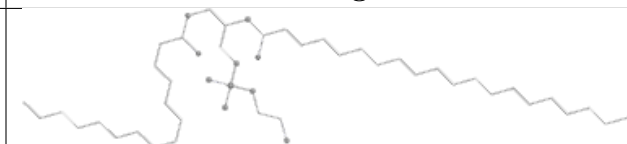


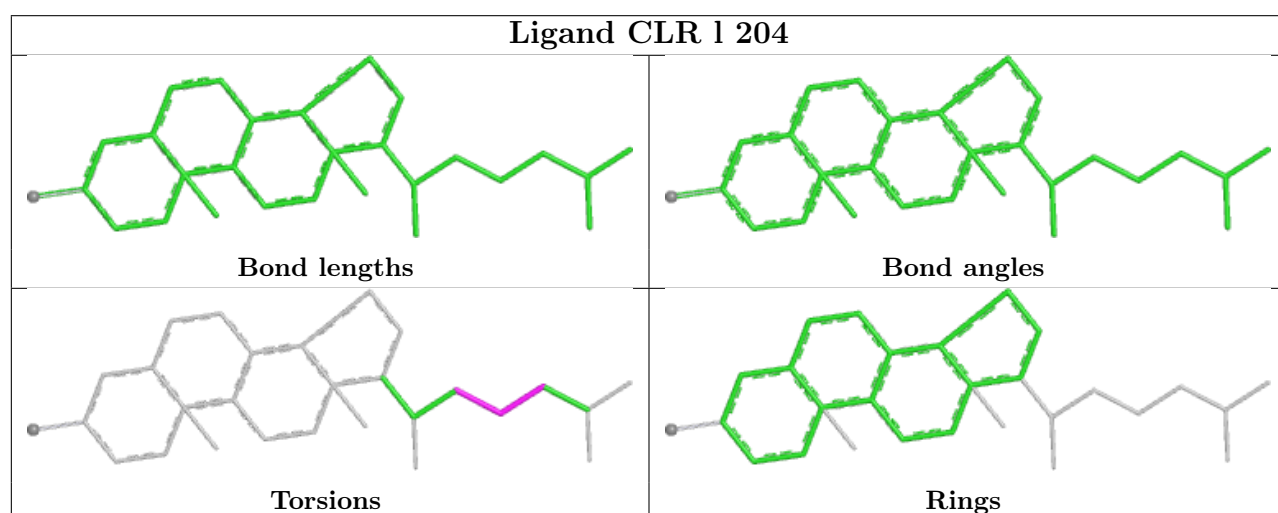
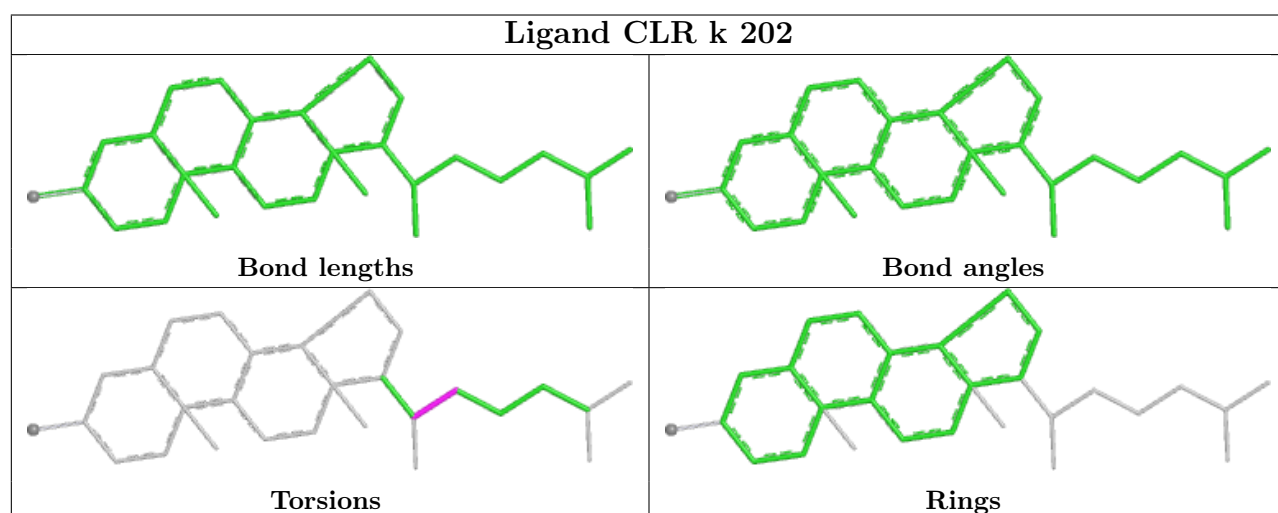
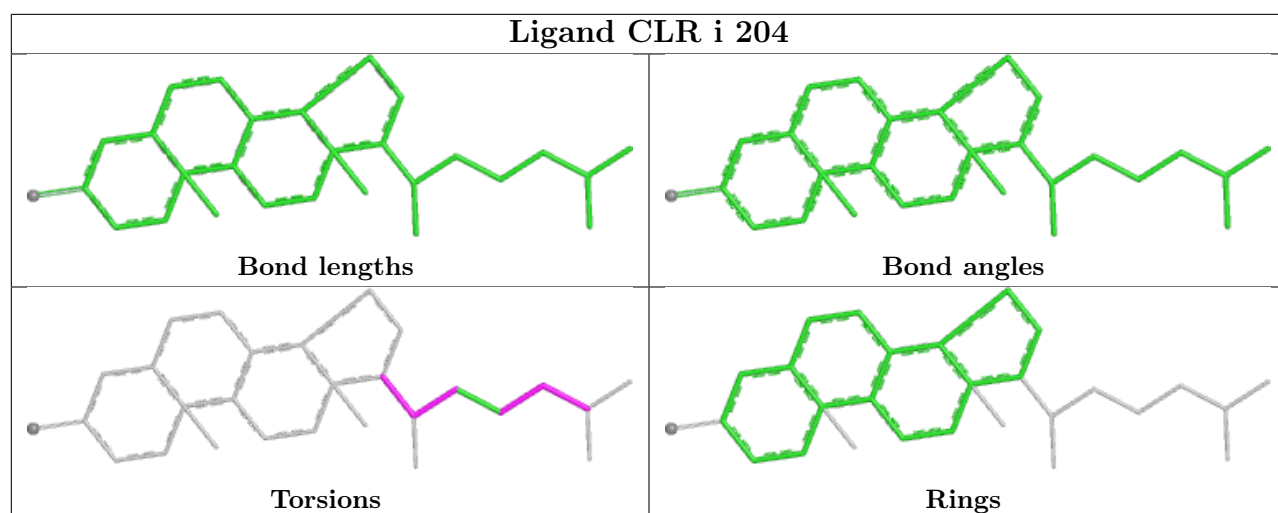
Ligand ADP A 701



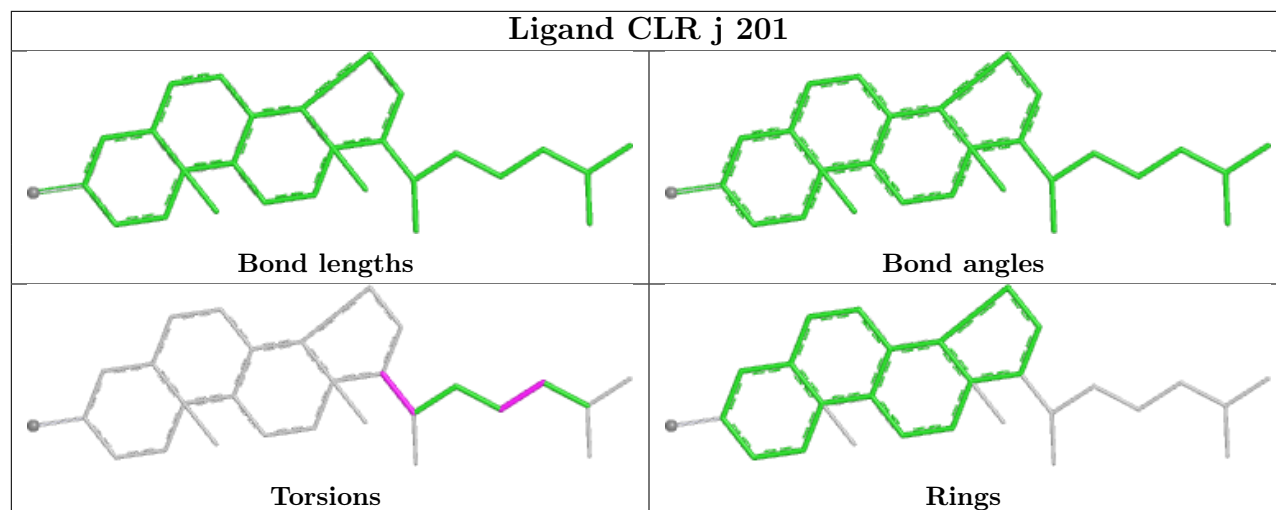
Ligand PC1 b 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLR o 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

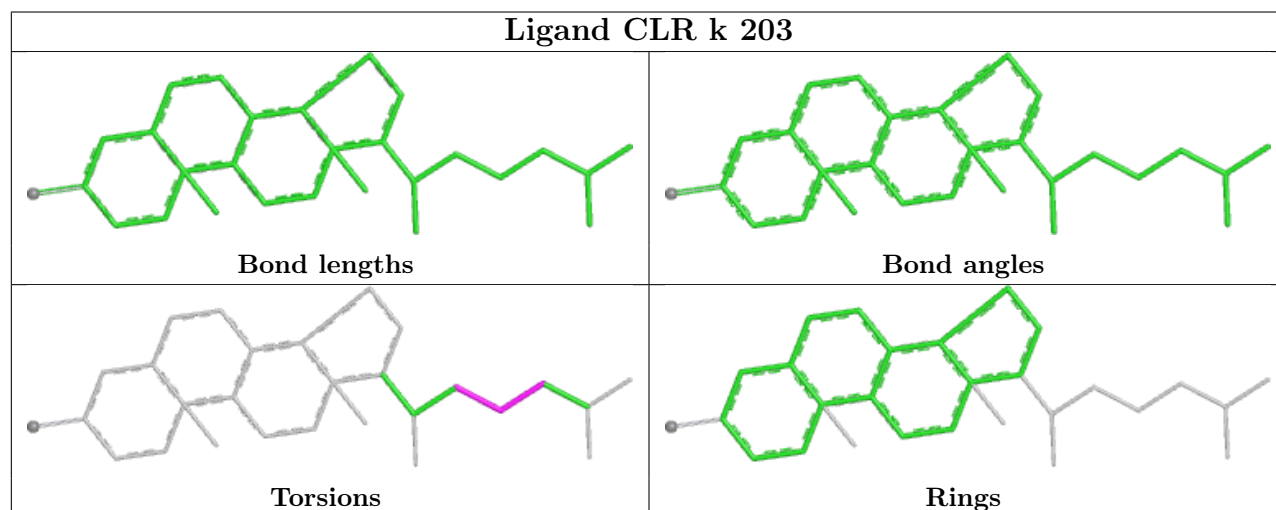
Ligand PTY p 404	
	
Bond lengths	Bond angles
	
Torsions	Rings



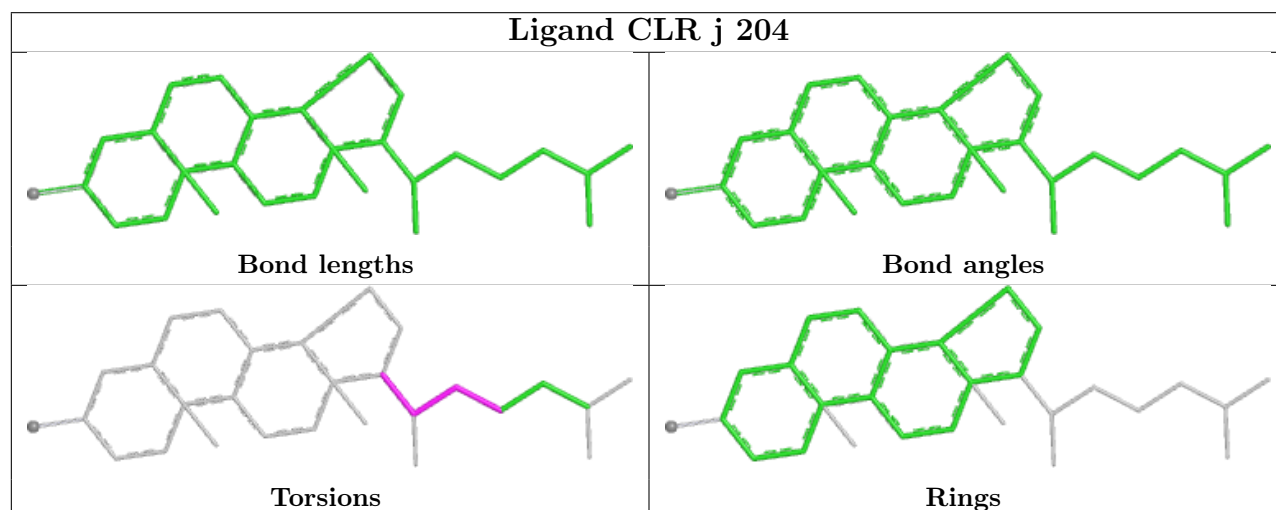
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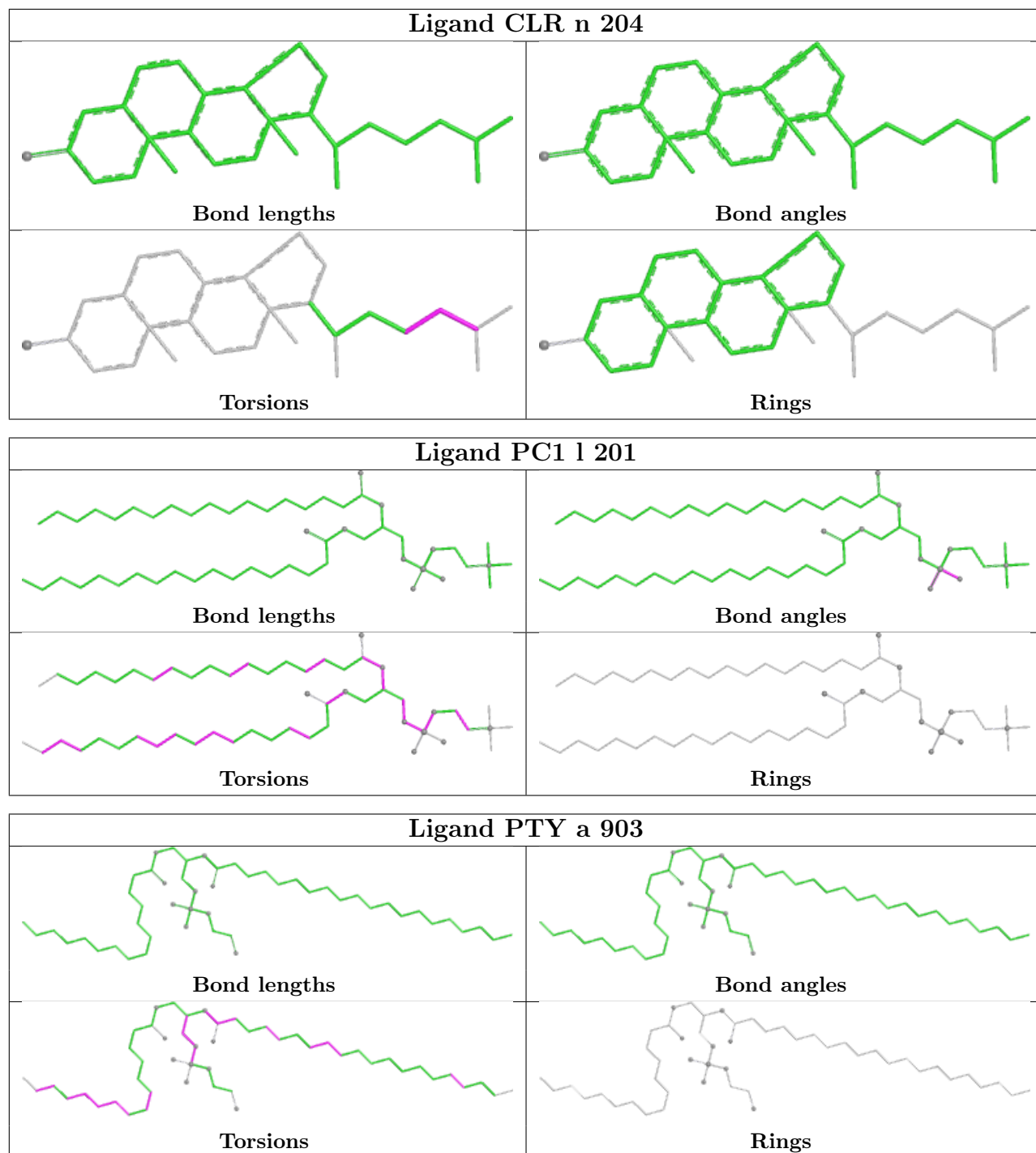


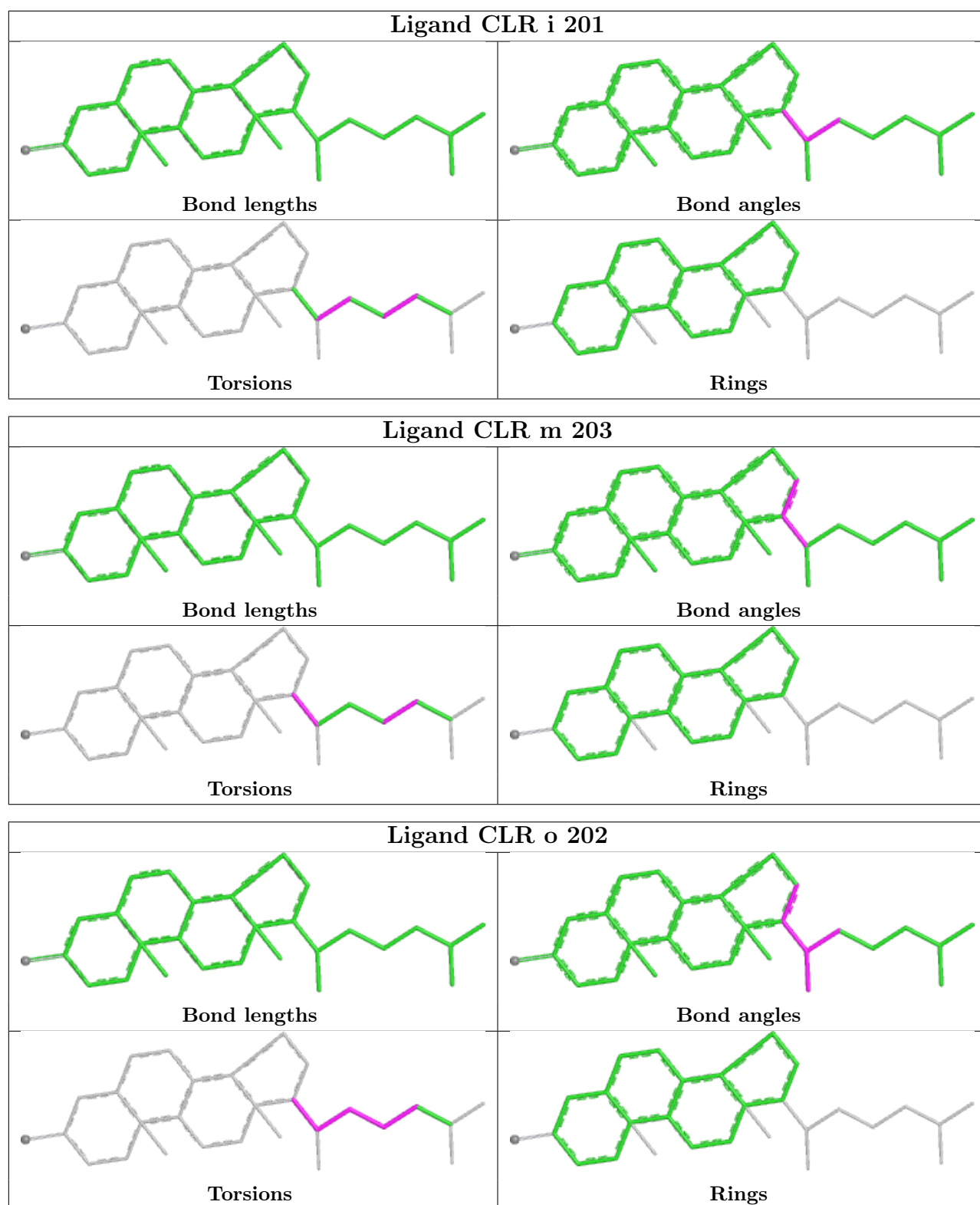
Ligand CLR k 203



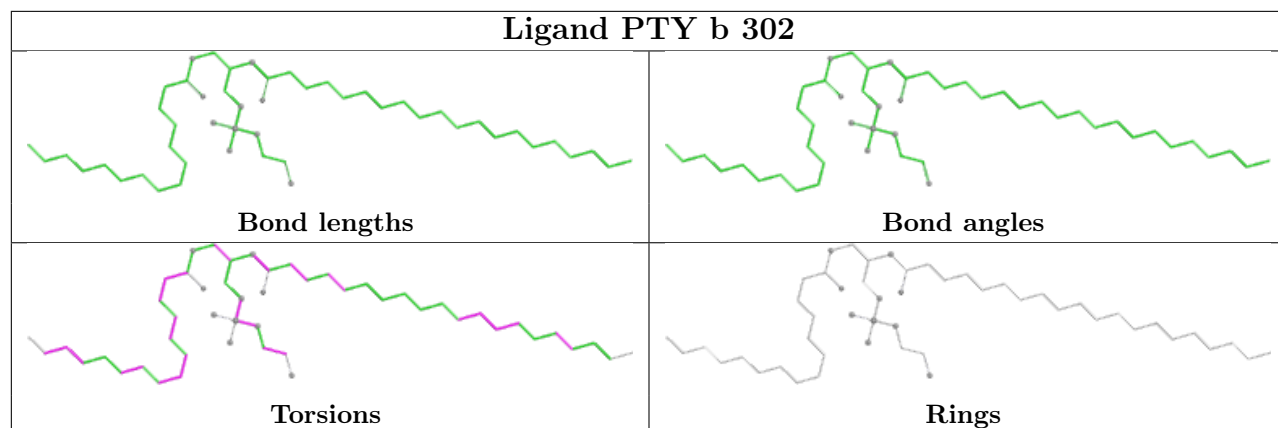
Ligand CLR j 204



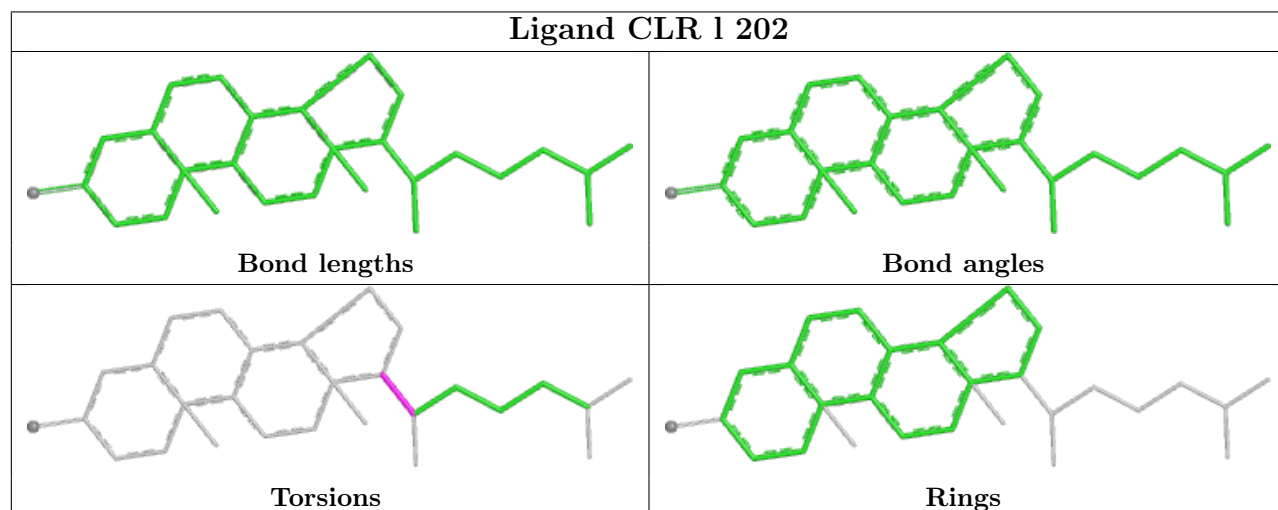




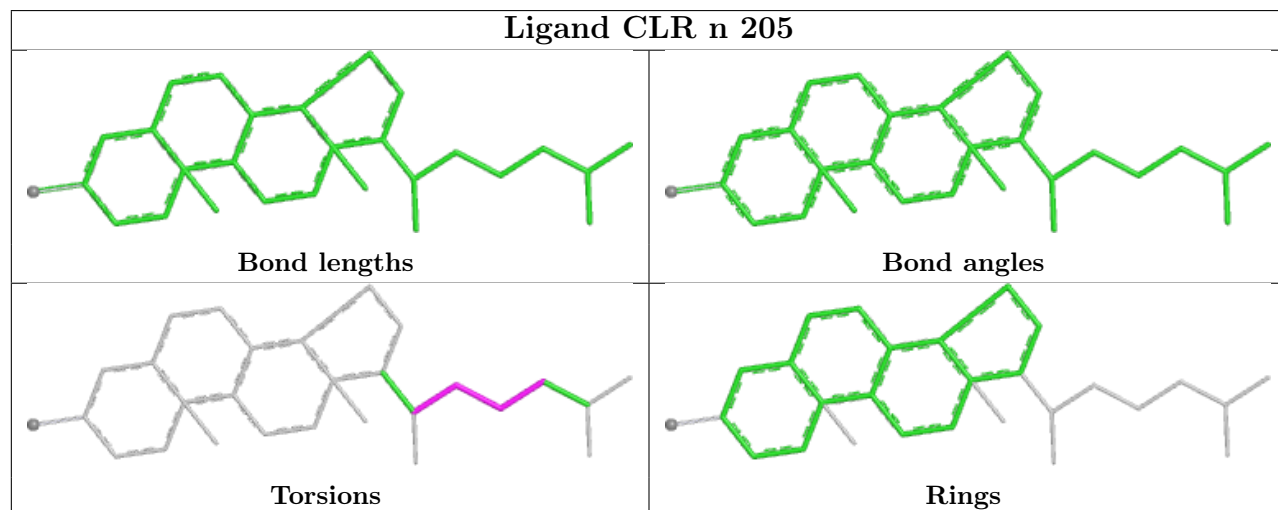
Ligand PTY b 302

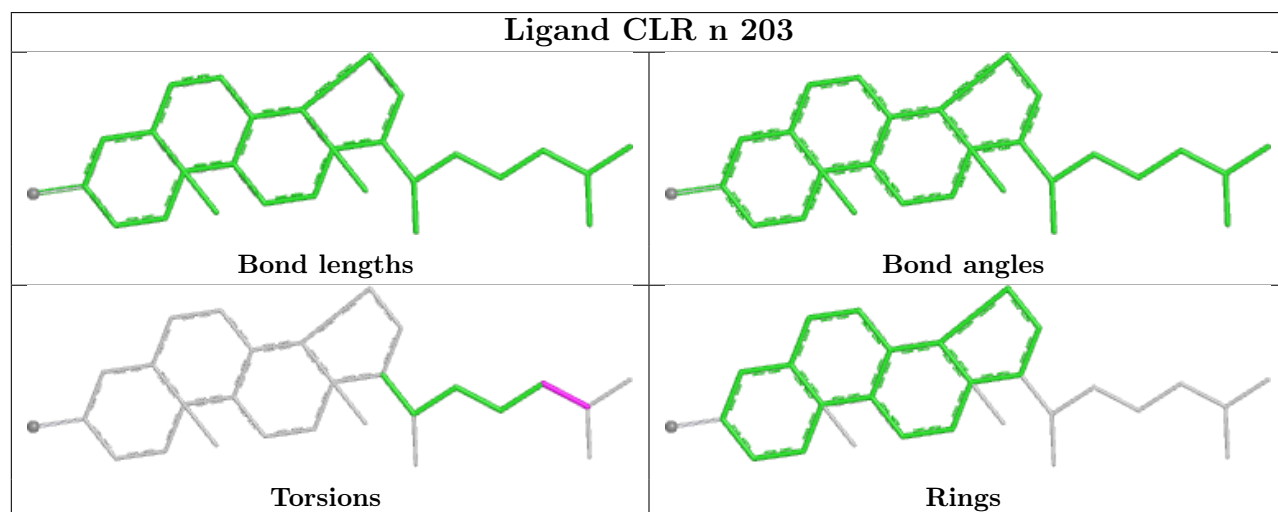
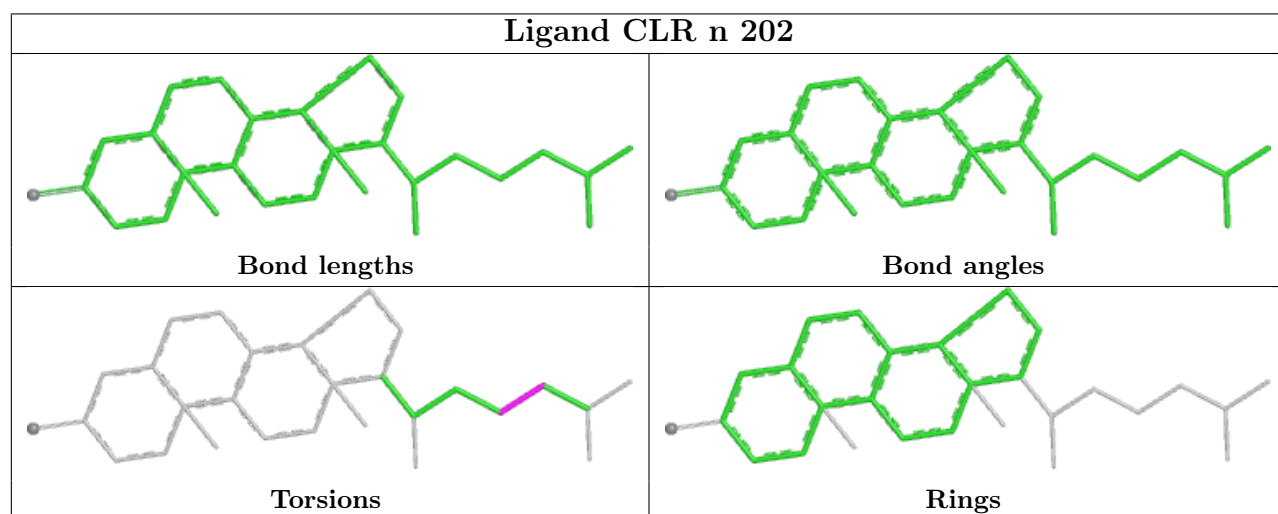
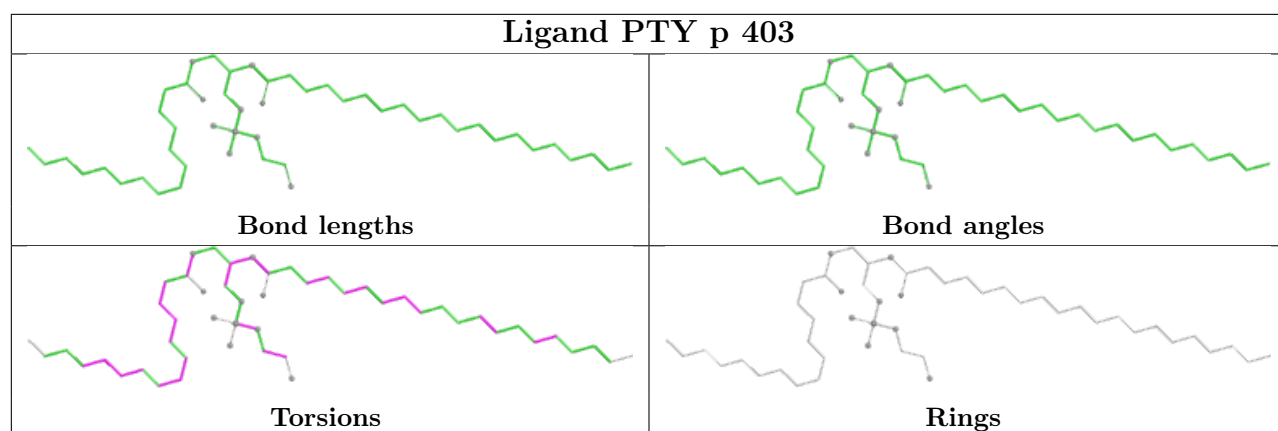


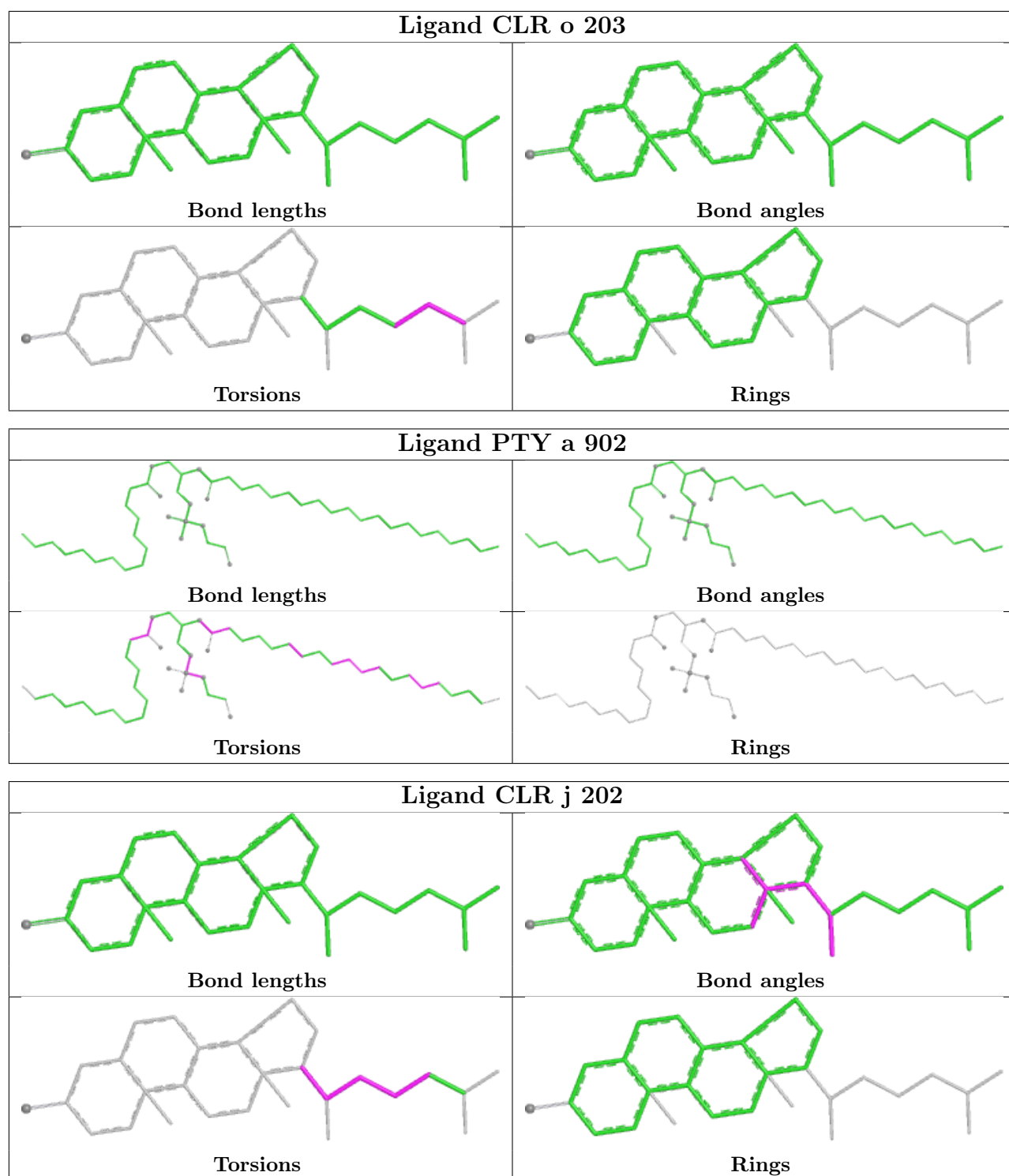
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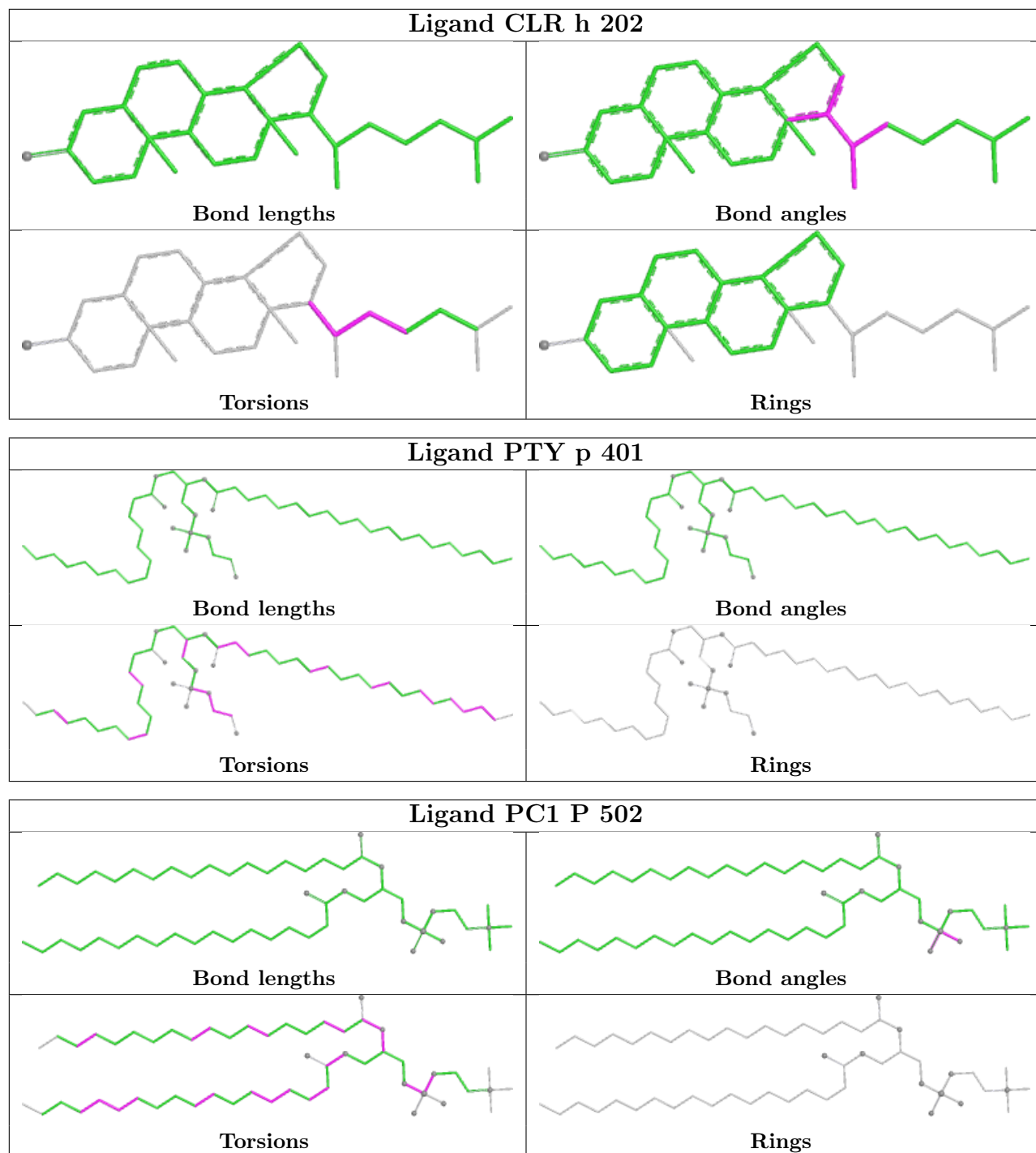


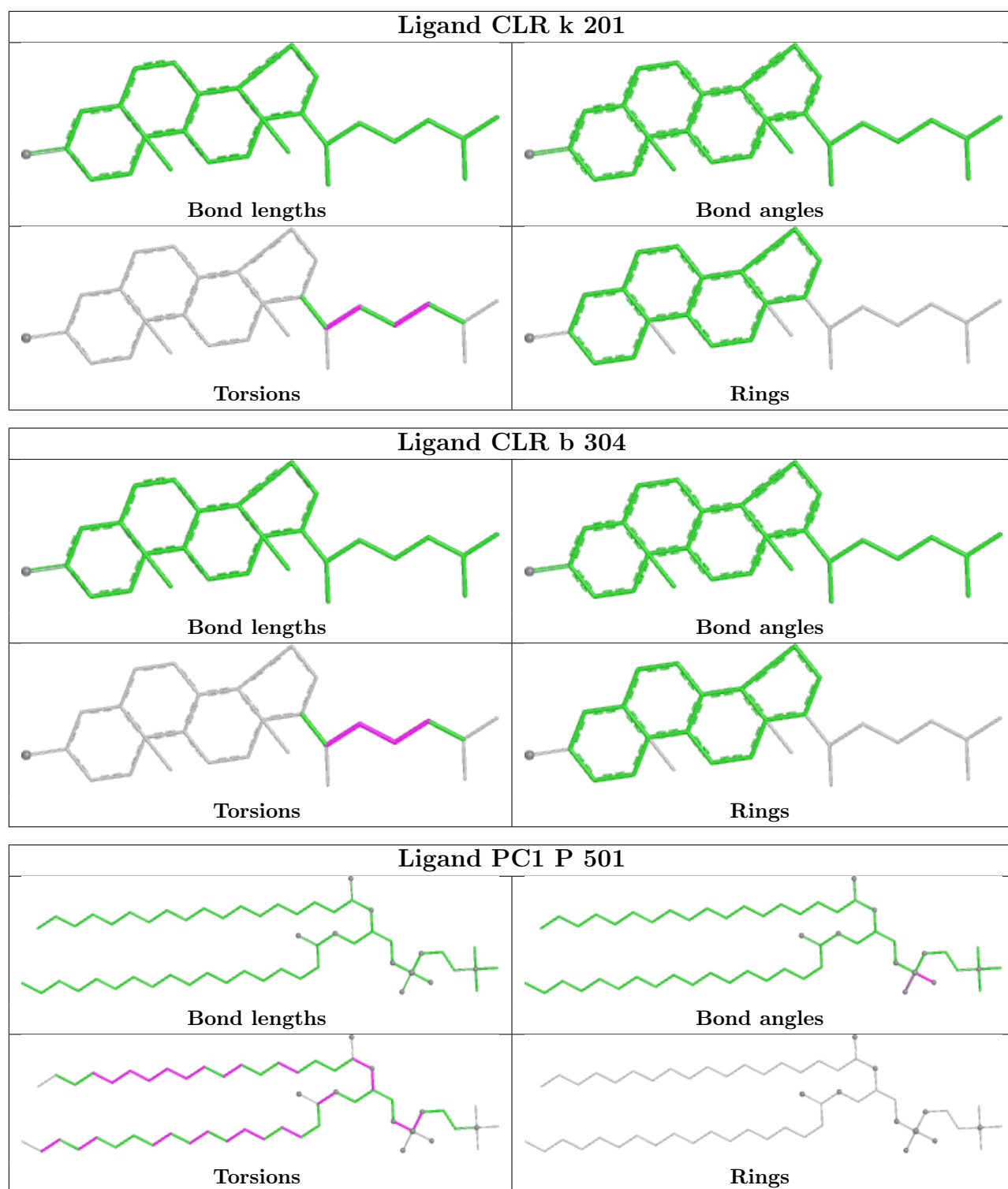
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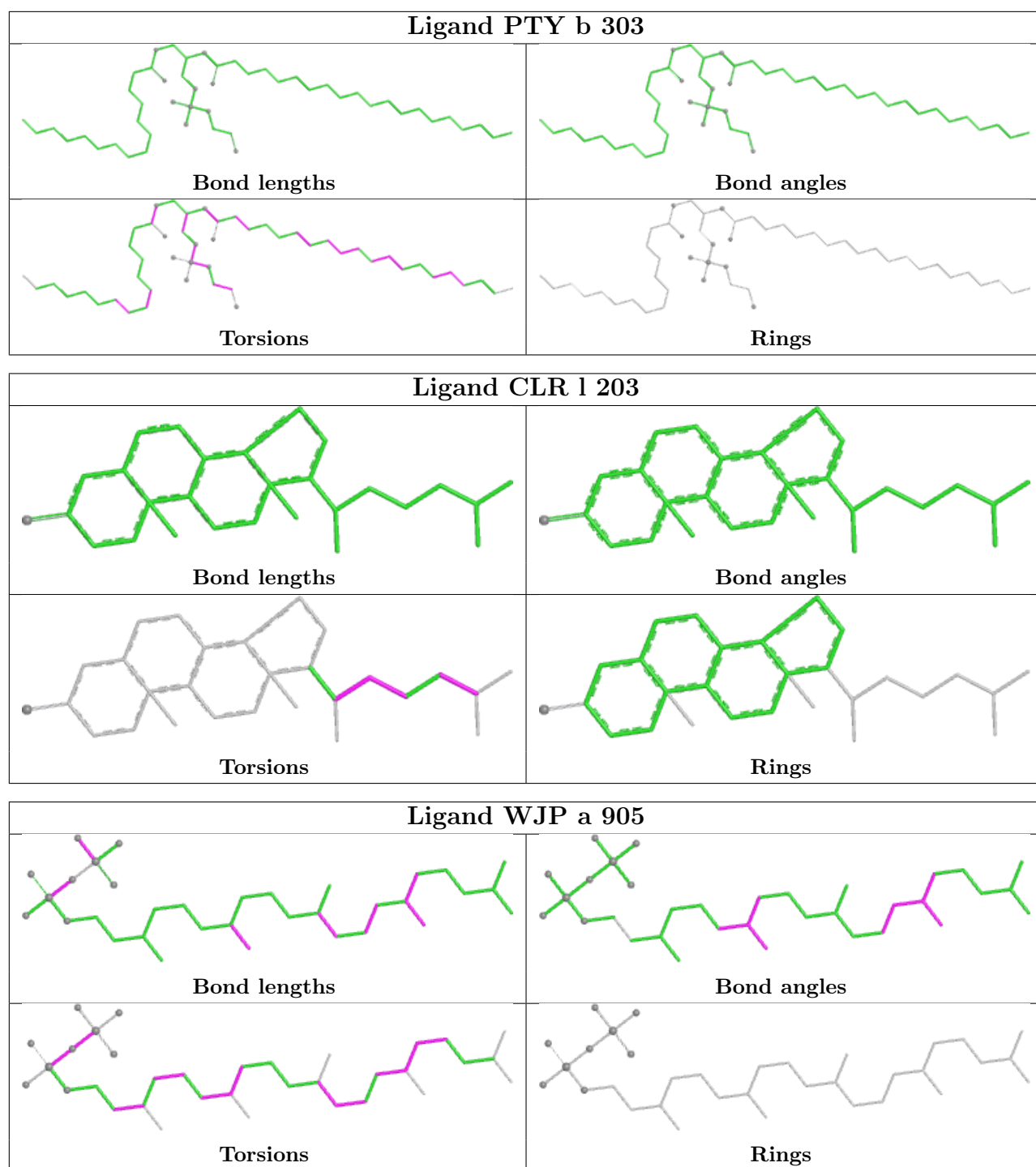


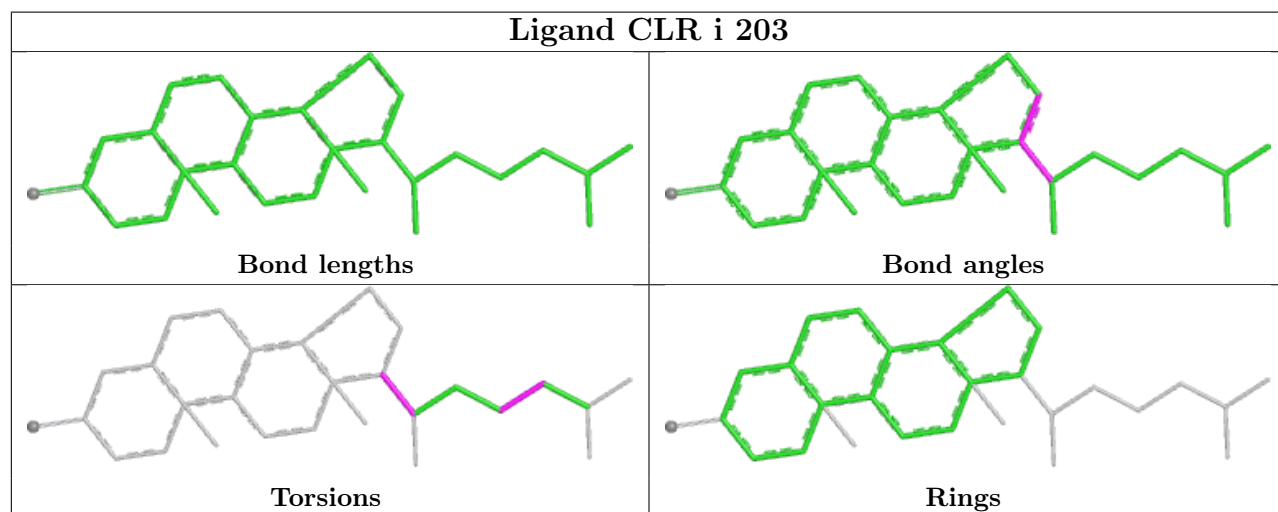
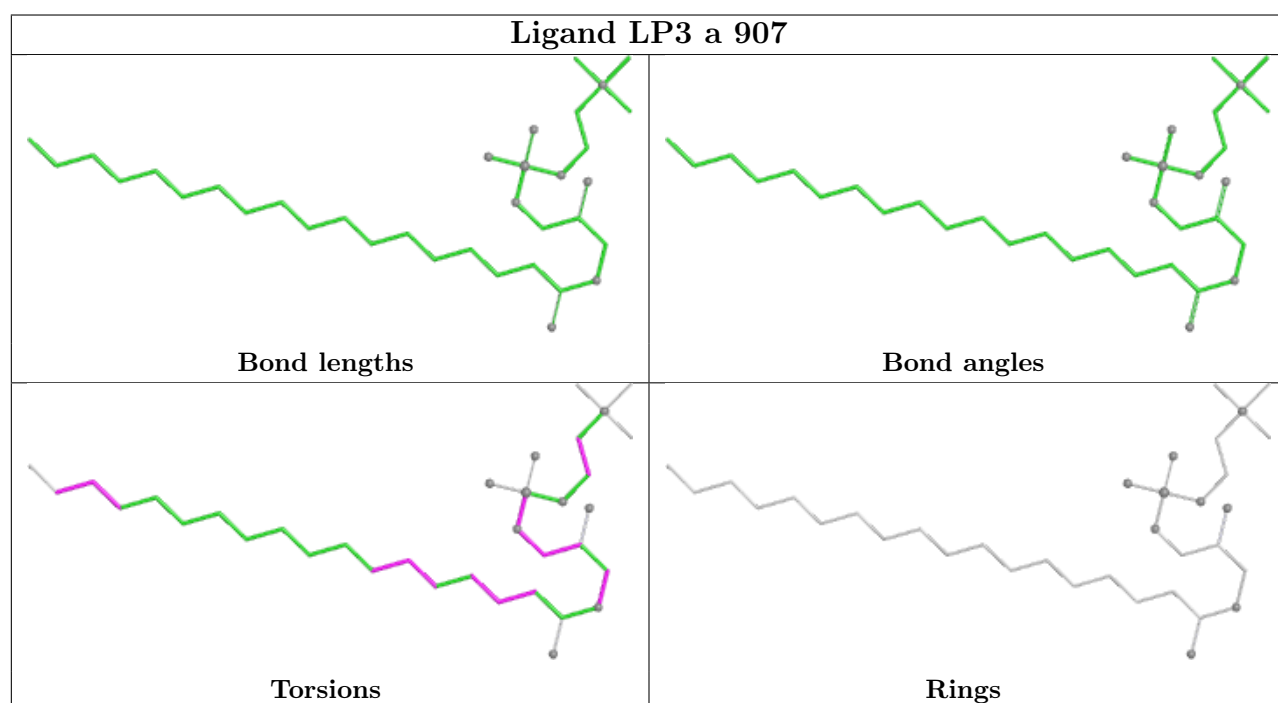
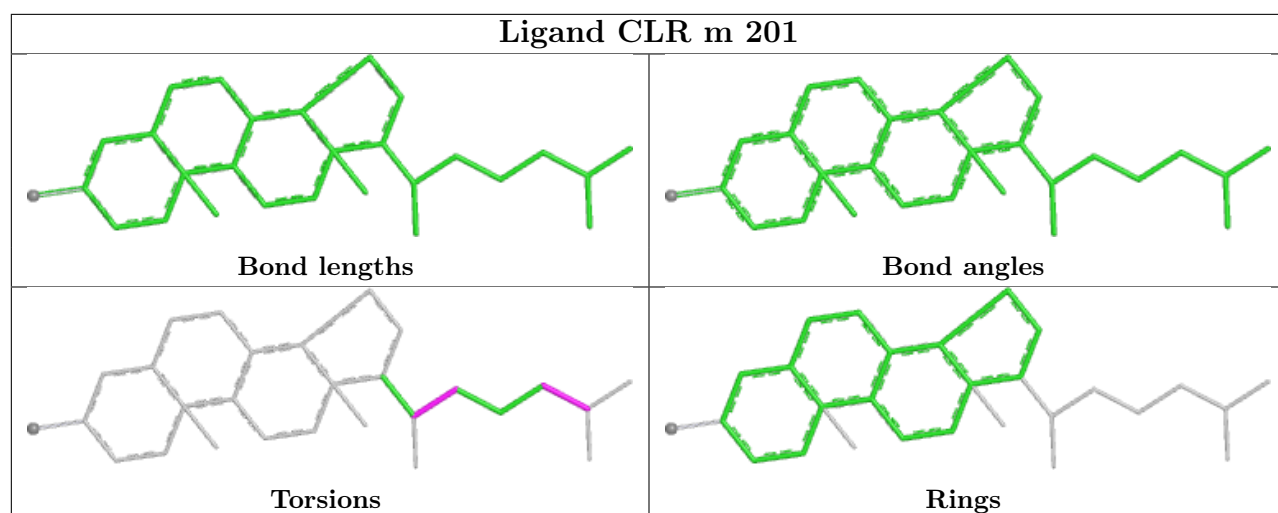


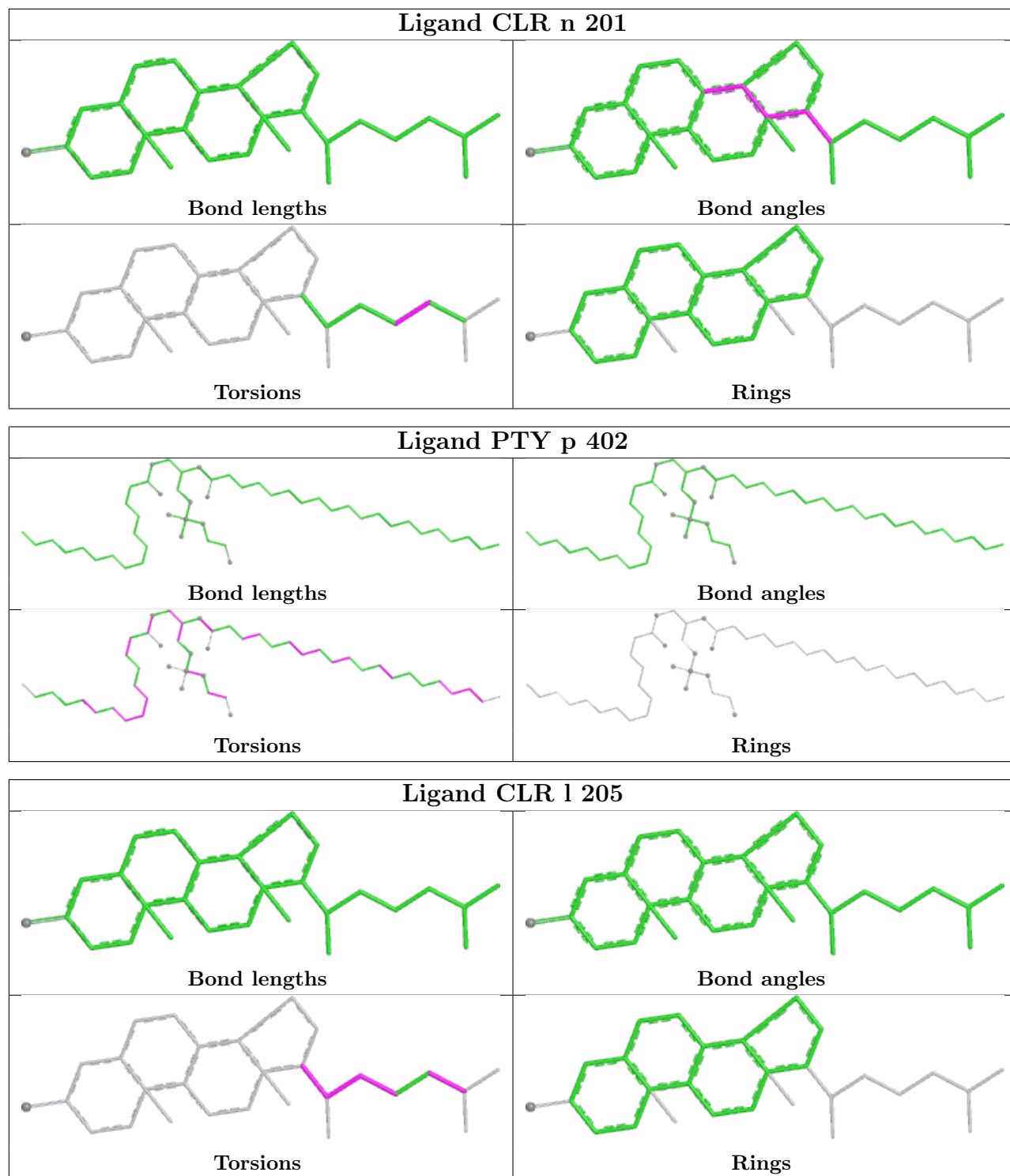


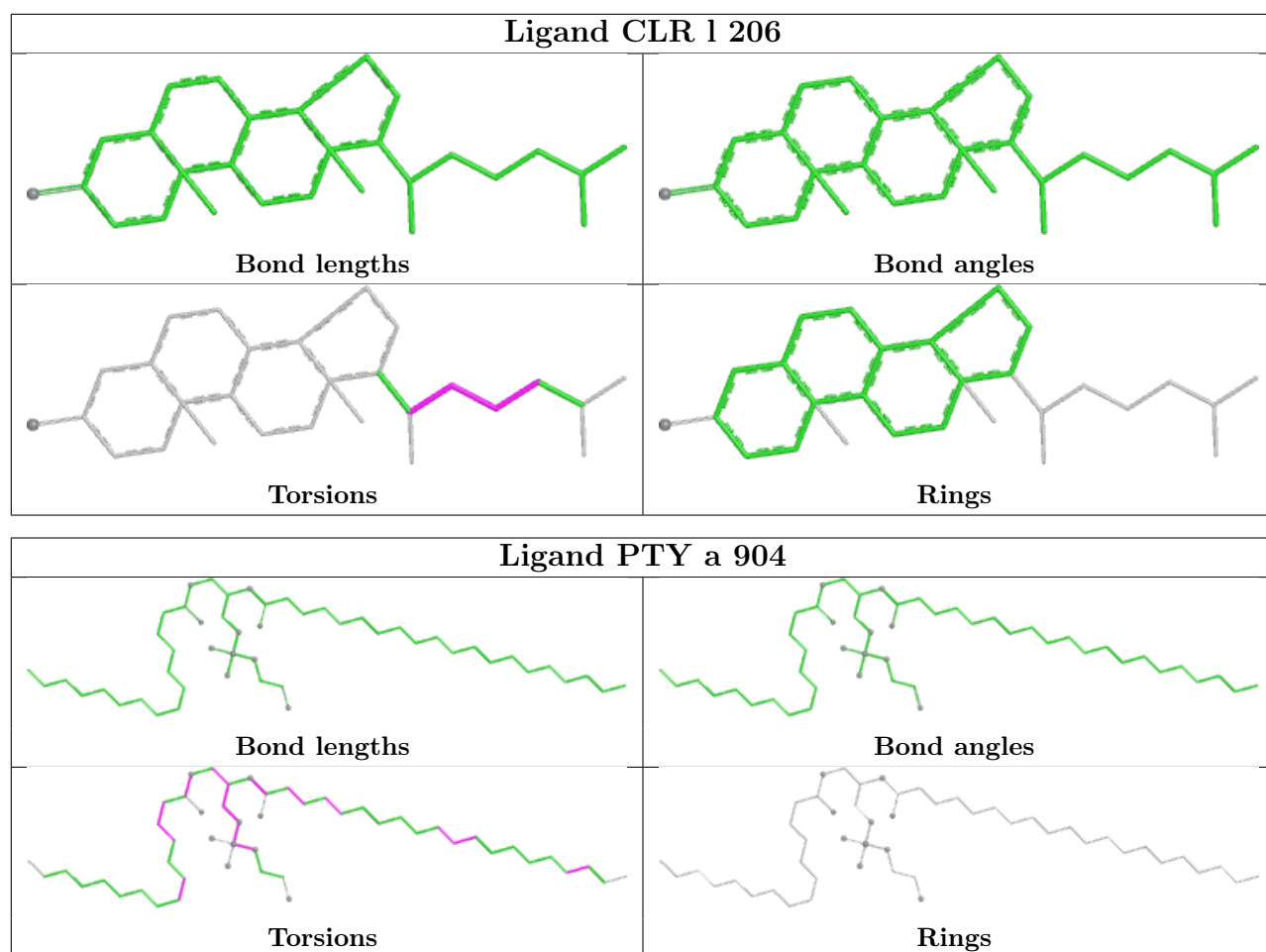












4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

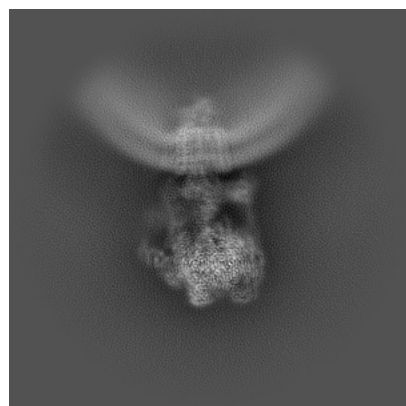
5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44353. These allow visual inspection of the internal detail of the map and identification of artifacts.

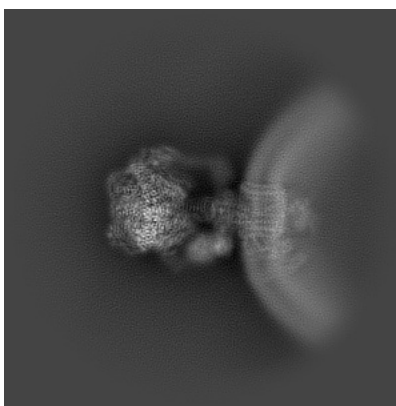
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

5.1 Orthogonal projections [i](#)

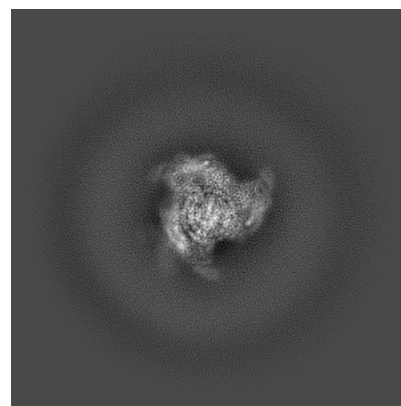
5.1.1 Primary map



X

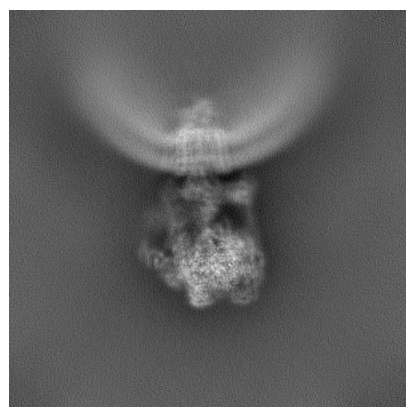


Y

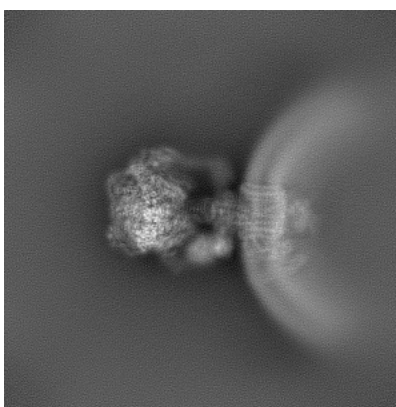


Z

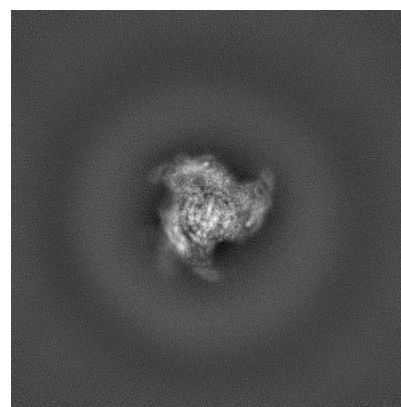
5.1.2 Raw map



X



Y



Z

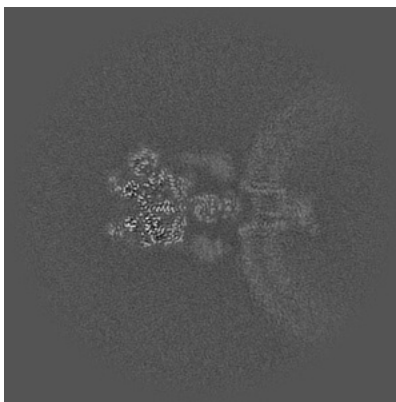
The images above show the map projected in three orthogonal directions.

5.2 Central slices [i](#)

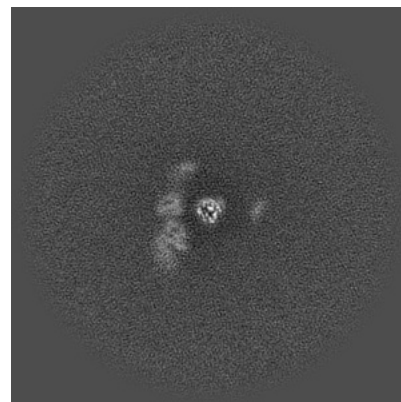
5.2.1 Primary map



X Index: 192

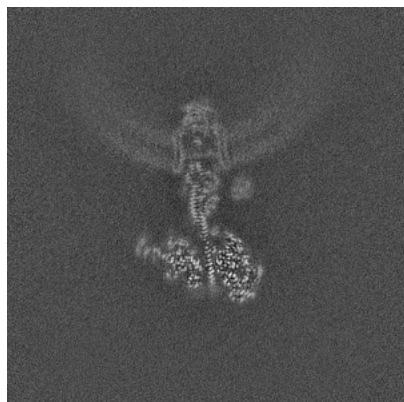


Y Index: 192

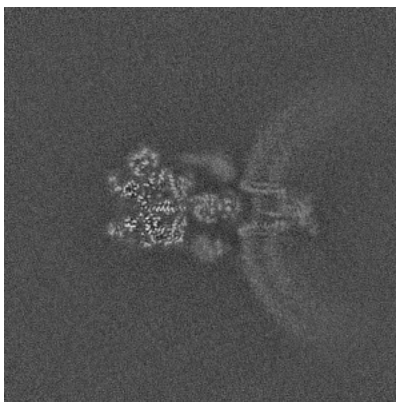


Z Index: 192

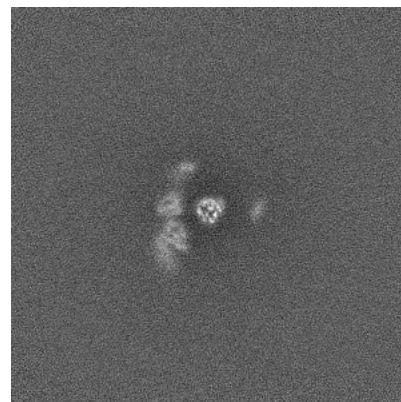
5.2.2 Raw map



X Index: 192



Y Index: 192



Z Index: 192

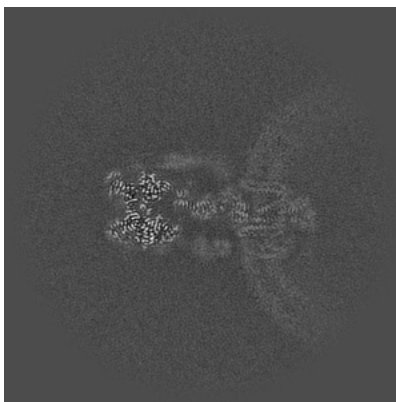
The images above show central slices of the map in three orthogonal directions.

5.3 Largest variance slices [i](#)

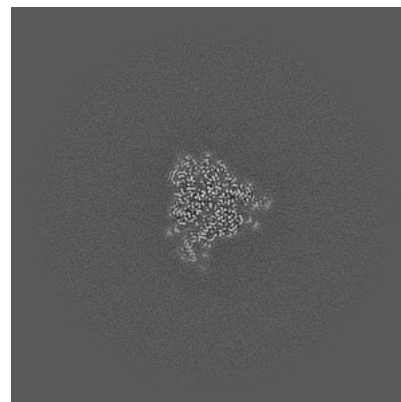
5.3.1 Primary map



X Index: 191



Y Index: 185



Z Index: 136

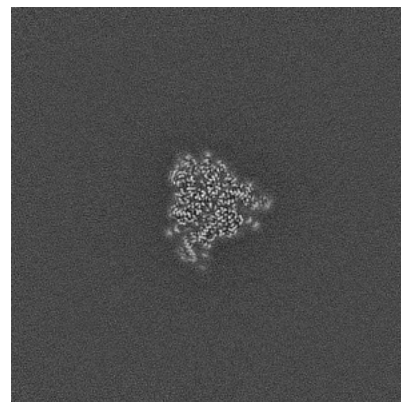
5.3.2 Raw map



X Index: 191



Y Index: 179

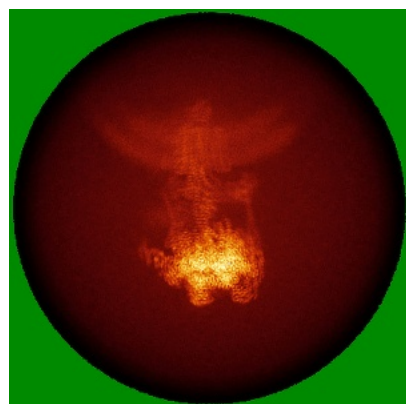


Z Index: 136

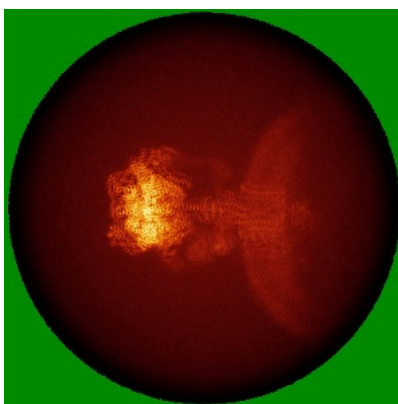
The images above show the largest variance slices of the map in three orthogonal directions.

5.4 Orthogonal standard-deviation projections (False-color) [i](#)

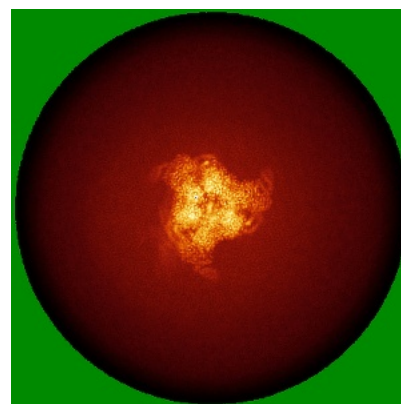
5.4.1 Primary map



X

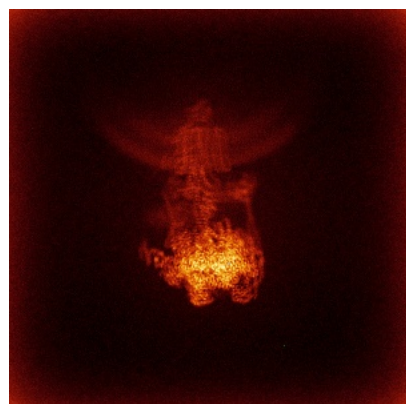


Y

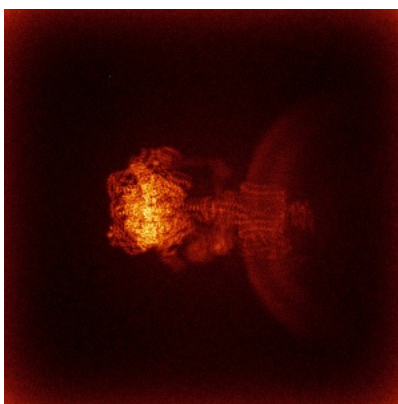


Z

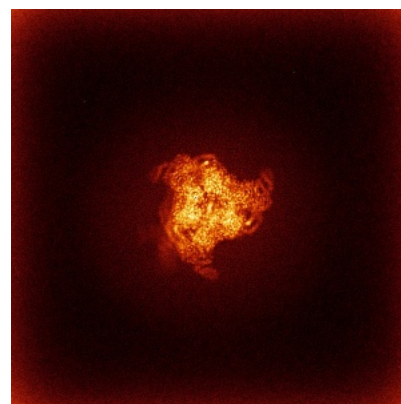
5.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

5.5 Orthogonal surface views [i](#)

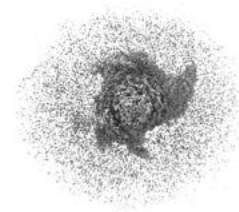
5.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.185. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

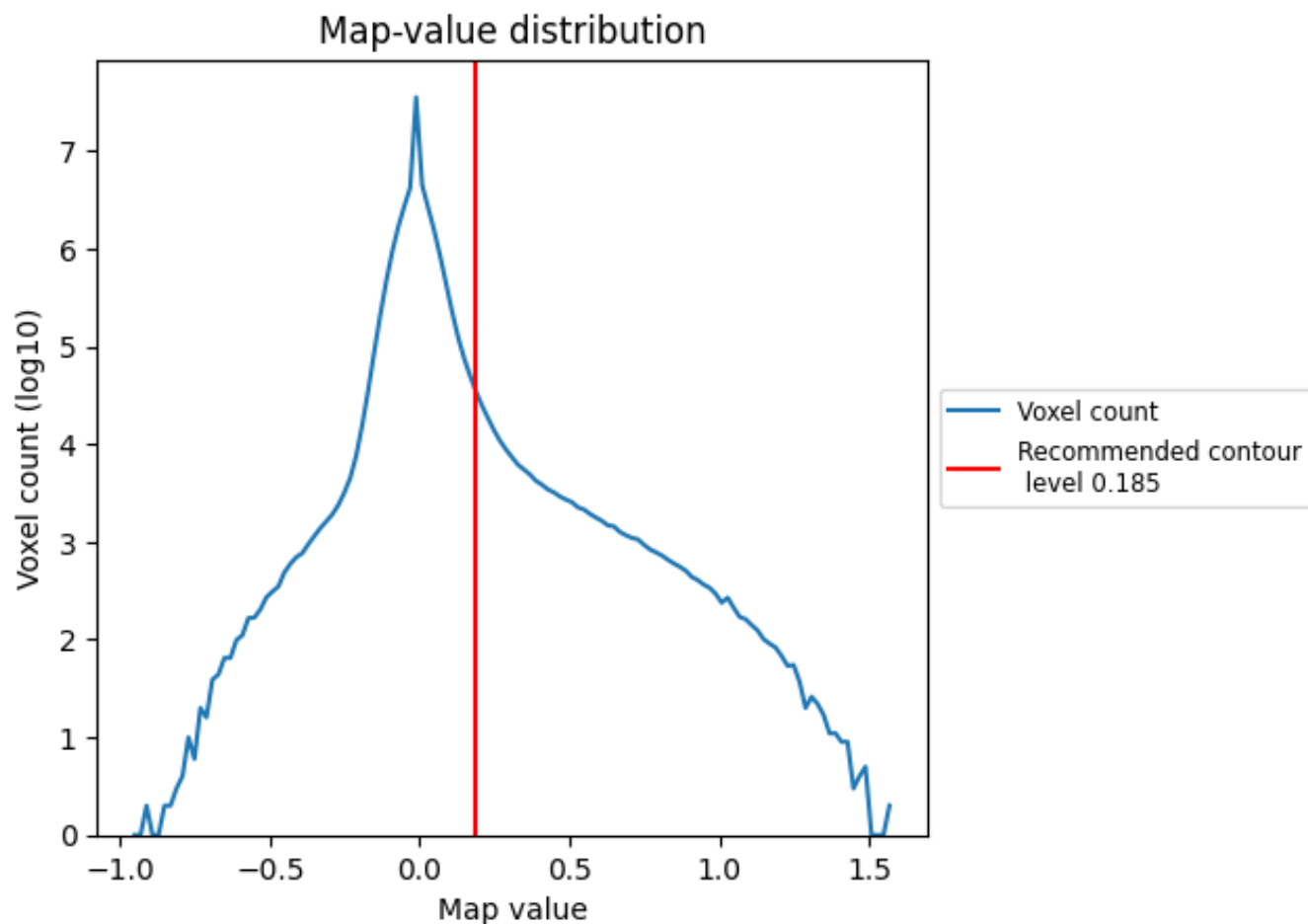
5.6 Mask visualisation [i](#)

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

6 Map analysis [i](#)

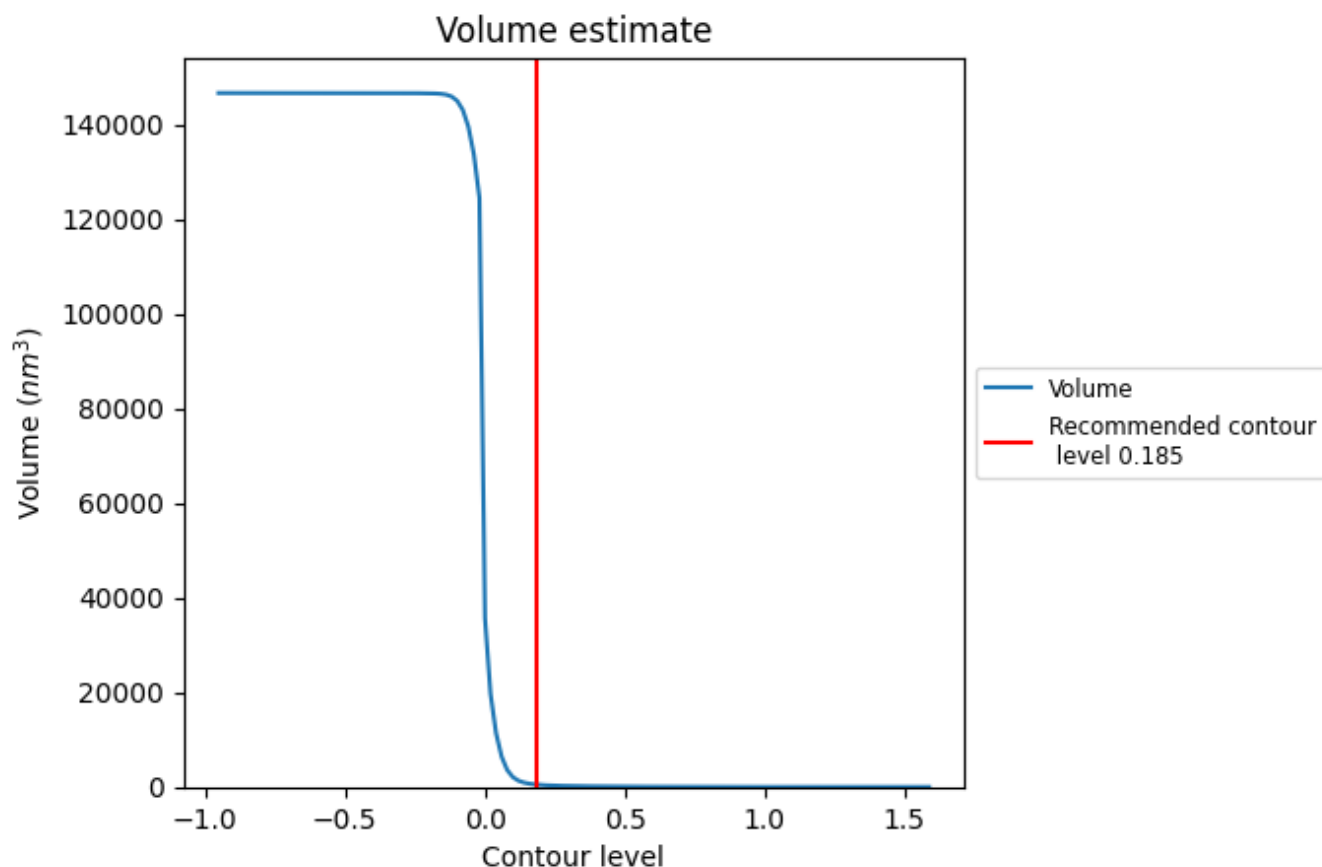
This section contains the results of statistical analysis of the map.

6.1 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.

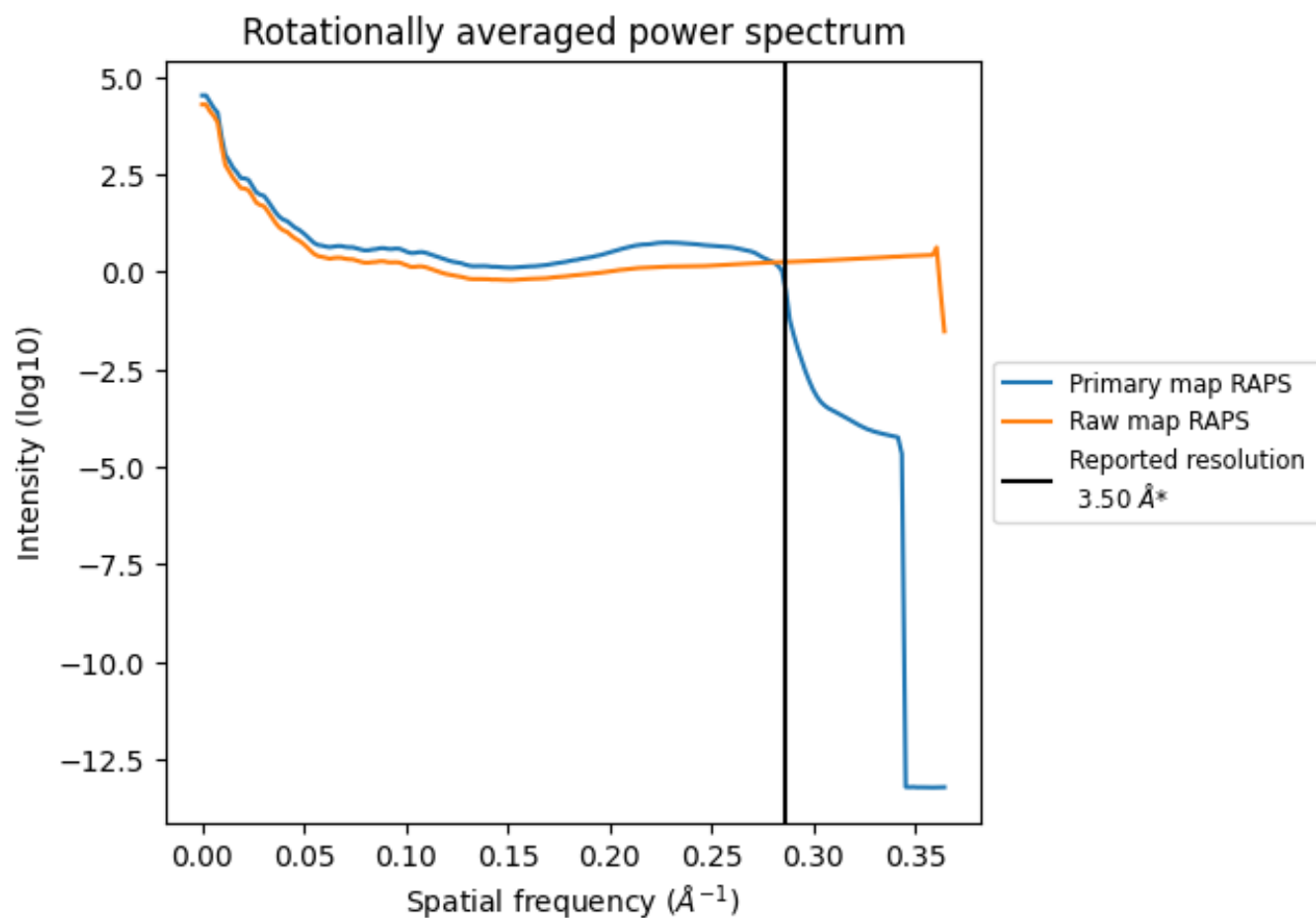
6.2 Volume estimate [i](#)



The volume at the recommended contour level is 499 nm^3 ; this corresponds to an approximate mass of 450 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.

6.3 Rotationally averaged power spectrum ⓘ

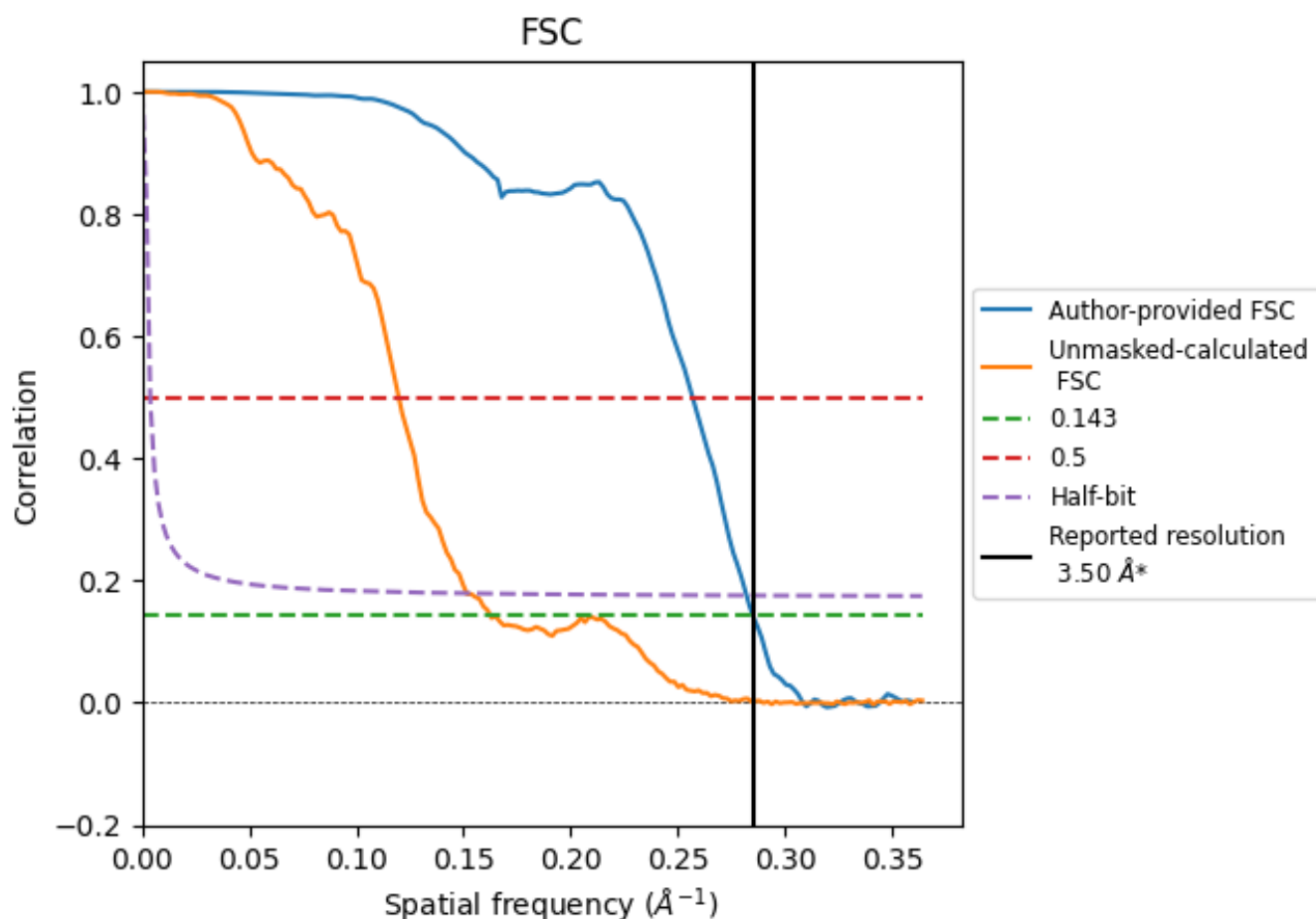


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

7 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

7.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.286 \text{ \AA}^{-1}$

7.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.51	3.89	3.54
Unmasked-calculated*	6.16	8.36	6.60

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.16 differs from the reported value 3.5 by more than 10 %

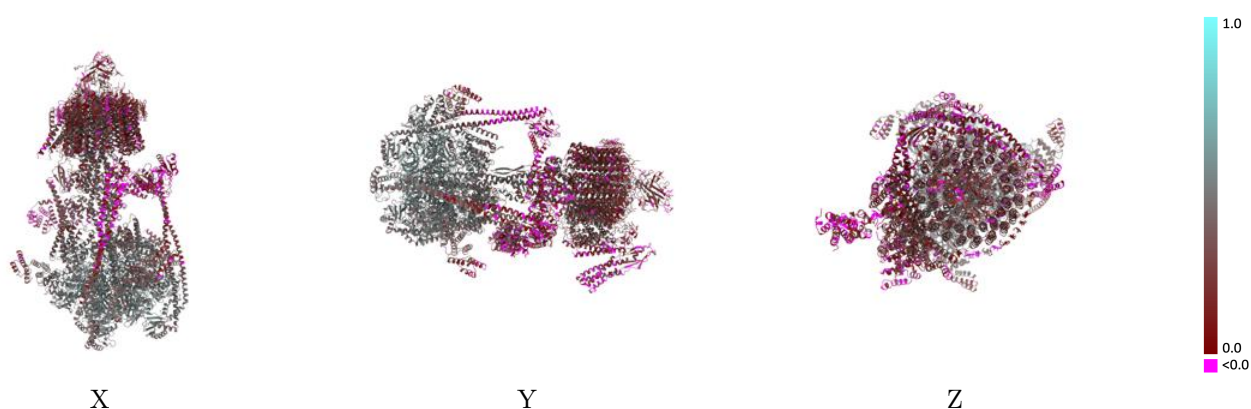
8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44353 and PDB model 9BRD. Per-residue inclusion information can be found in section ?? on page ??.

8.1 Map-model overlay [i](#)

This section was not generated.

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

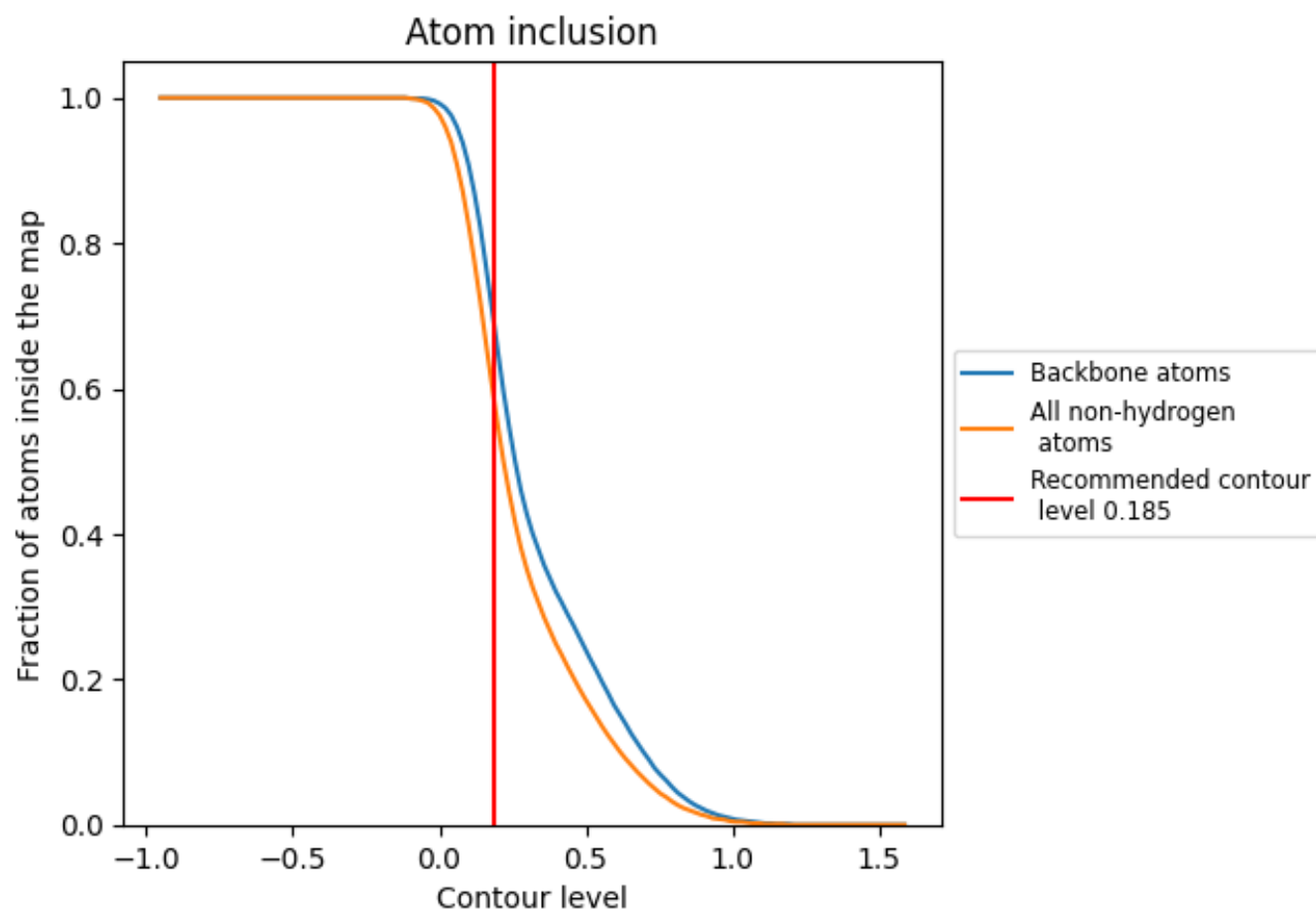


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

8.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

8.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 59% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.185) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5880	 0.3510
A	 0.8430	 0.4940
B	 0.8120	 0.4820
C	 0.8080	 0.4710
D	 0.8530	 0.5110
E	 0.8690	 0.5140
F	 0.8690	 0.5120
G	 0.2150	 0.0830
H	 0.7390	 0.4320
I	 0.7180	 0.4000
J	 0.7200	 0.3680
K	 0.6980	 0.3660
L	 0.6570	 0.3720
M	 0.6310	 0.3150
N	 0.6620	 0.3080
O	 0.5510	 0.2490
P	 0.4210	 0.2740
Q	 0.7020	 0.3570
R	 0.7140	 0.3500
S	 0.7480	 0.3820
T	 0.2470	 0.1220
U	 0.0570	 0.0590
V	 0.1430	 0.0320
W	 0.0710	 0.0100
X	 0.2500	 0.1750
Y	 0.3930	 0.3350
Z	 0.2140	 0.2230
a	 0.3280	 0.2100
b	 0.4910	 0.3580
c	 0.3210	 0.1100
d	 0.5210	 0.3490
e	 0.2770	 0.2280
f	 0.2080	 0.1400
g	 0.5340	 0.3640
h	 0.3820	 0.3030



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Chain	Atom inclusion	Q-score
i	 0.2390	 0.2180
j	 0.2220	 0.2160
k	 0.2700	 0.2060
l	 0.2890	 0.2180
m	 0.2850	 0.2180
n	 0.3060	 0.2520
o	 0.4130	 0.3080
p	 0.2610	 0.2900
q	 0.1070	 0.0340
r	 0.1790	 0.0680
s	 0.3460	 0.2230