



Full wwPDB EM Validation Report ⓘ

Mar 22, 2026 – 01:58 AM UTC

PDB ID : 2AT9 / pdb_00002at9
Title : STRUCTURE OF BACTERIORHODOPSIN AT 3.0 ANGSTROM BY ELECTRON CRYSTALLOGRAPHY
Authors : Mitsuoka, K.; Hirai, T.; Murata, K.; Miyazawa, A.; Kidera, A.; Kimura, Y.; Fujiyoshi, Y.
Deposited on : 1998-12-17
Resolution : 3.00 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB/EMDB 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:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

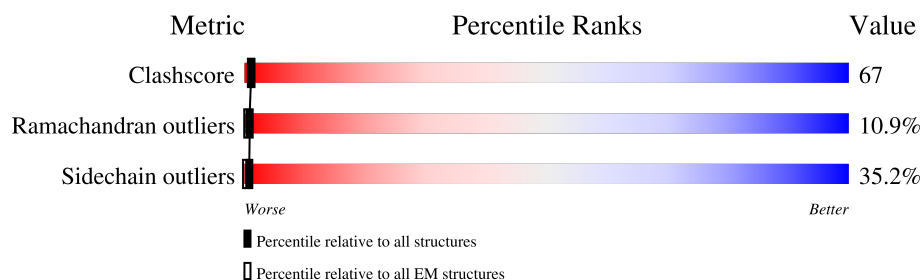
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON CRYSTALLOGRAPHY

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	248	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	2DP	A	261	X	-	-	-
3	2DP	A	262	X	-	-	-
3	2DP	A	263	X	-	-	-
3	2DP	A	264	X	-	-	-
3	2DP	A	265	X	-	-	-
3	2DP	A	267	X	-	-	-
3	2DP	A	268	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	2DP	A	269	X	-	-	-

2 Entry composition [i](#)

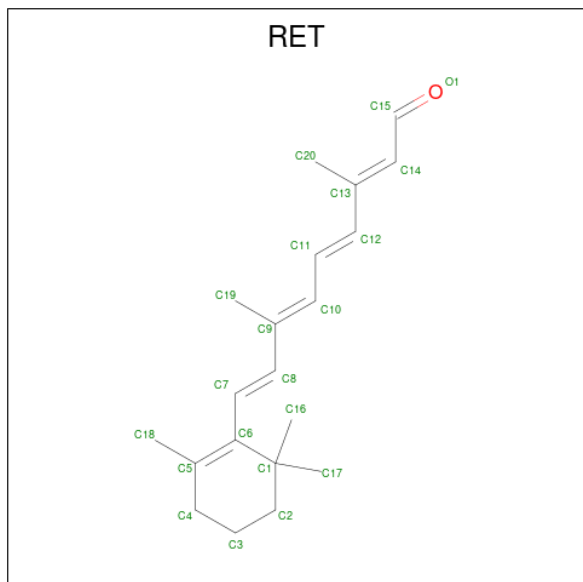
There are 4 unique types of molecules in this entry. The entry contains 2223 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 BACTERIORHODOPSIN.

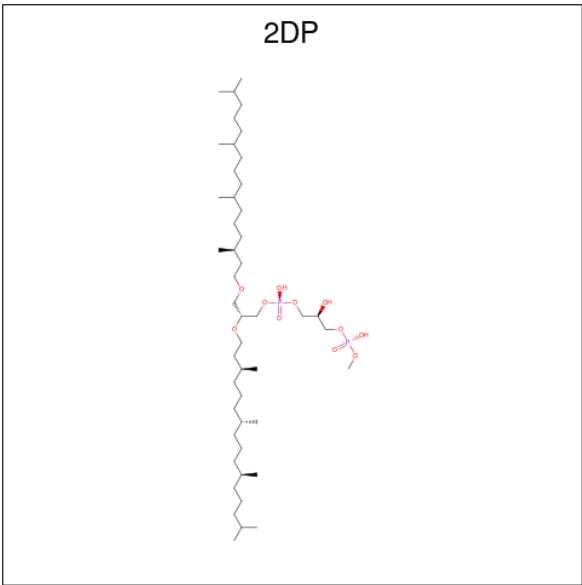
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	222	1721	1156	263	293	9	0	0

- Molecule 2 is RETINAL (CCD ID: RET) (formula: $C_{20}H_{28}O$).



Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	C	0
			20	20	

- Molecule 3 is 3-[[3-METHYLPHOSPHONO-GLYCEROLYL]PHOSPHONYL]-[1,2-DI[2,6,10,14-TETRAMETHYL-HEXADECAN-16-YL]GLYCEROL (CCD ID: 2DP) (formula: $C_{47}H_{98}O_{11}P_2$).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	O	P	0
			60	47	11	2	
3	A	1	Total	C	O	P	0
			60	47	11	2	
3	A	1	Total	C	O	P	0
			60	47	11	2	
3	A	1	Total	C	O	P	0
			60	47	11	2	
3	A	1	Total	C	O	P	0
			60	47	11	2	
3	A	1	Total	C	O	P	0
			60	47	11	2	
3	A	1	Total	C	O	P	0
			60	47	11	2	
3	A	1	Total	C	O	P	0
			60	47	11	2	

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		AltConf
4	A	2	Total	O	0
			2	2	

4 Data and refinement statistics

Xtriage (Phenix) and EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α , β , γ	62.45Å 62.45Å 100.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 3.00	Depositor
% Data completeness (in resolution range)	73.7 (8.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.237 , 0.330	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2223	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: RET, 2DP

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	0.69	1/1768 (0.1%)	1.22	21/2415 (0.9%)

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
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	118	MET	SD-CE	-6.41	1.63	1.79

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	34	VAL	N-CA-C	12.15	122.75	111.45
1	A	9	GLU	N-CA-C	-8.38	103.05	113.28
1	A	225	ARG	N-CA-C	-7.88	102.77	111.36
1	A	163	MET	N-CA-C	7.38	120.98	110.14
1	A	96	ASP	N-CA-C	-7.12	103.53	111.71
1	A	60	MET	N-CA-C	-6.65	103.29	111.40
1	A	148	ILE	N-CA-C	-6.11	104.79	110.53
1	A	76	ASN	CA-C-N	6.11	126.59	119.99
1	A	76	ASN	C-N-CA	6.11	126.59	119.99
1	A	11	ILE	N-CA-C	5.92	116.70	110.72
1	A	187	VAL	N-CA-C	5.82	118.33	111.05
1	A	207	LEU	N-CA-C	-5.78	105.06	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	GLY	N-CA-C	5.78	119.98	110.97
1	A	174	LEU	N-CA-C	-5.54	104.75	112.45
1	A	189	TRP	N-CA-C	-5.30	104.91	111.33
1	A	39	ALA	N-CA-C	-5.29	105.93	112.38
1	A	176	ASN	N-CA-C	-5.20	107.11	113.50
1	A	47	THR	N-CA-C	-5.17	105.34	111.69
1	A	142	THR	N-CA-C	-5.13	104.76	111.02
1	A	69	VAL	CA-C-N	5.09	126.20	119.84
1	A	69	VAL	C-N-CA	5.09	126.20	119.84

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	147	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1721	0	1777	293	0
2	A	20	0	27	6	0
3	A	480	0	752	40	0
4	A	2	0	0	0	0
All	All	2223	0	2556	321	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 67.

All (321) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:MET:HE3	1:A:145:MET:HB2	1.38	1.06
1:A:56:MET:HG3	1:A:85:ASP:HB2	1.44	0.99
1:A:168:ALA:O	1:A:172:LYS:HD2	1.64	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:ALA:C	1:A:172:LYS:HD2	1.91	0.95
1:A:67:THR:HG22	1:A:80:TRP:HD1	1.34	0.92
1:A:169:SER:O	1:A:173:VAL:HG22	1.73	0.89
1:A:37:PRO:HB3	1:A:40:LYS:NZ	1.90	0.87
2:A:249(A):RET:H161	2:A:249(A):RET:H8	1.53	0.86
1:A:37:PRO:HA	1:A:40:LYS:HG3	1.58	0.83
3:A:267:2DP:H221	3:A:267:2DP:H512	1.61	0.81
1:A:37:PRO:HB3	1:A:40:LYS:HZ2	1.45	0.81
1:A:82:ARG:NH2	1:A:205:THR:HG23	1.96	0.81
1:A:82:ARG:HH22	1:A:205:THR:HG23	1.43	0.81
3:A:262:2DP:H53	3:A:263:2DP:H541	1.63	0.81
1:A:76:ASN:HB2	1:A:77:PRO:HD2	1.64	0.80
1:A:185:TYR:HD1	1:A:208:PHE:HE1	1.28	0.80
1:A:215:ALA:O	1:A:219:PHE:HB2	1.82	0.79
1:A:130:VAL:HG12	1:A:132:SER:H	1.48	0.79
1:A:71:PHE:HE2	1:A:76:ASN:HD21	1.30	0.79
1:A:145:MET:HE1	1:A:183:SER:HA	1.62	0.79
3:A:269:2DP:H492	3:A:269:2DP:H441	1.62	0.79
1:A:199:VAL:HG13	3:A:262:2DP:H451	1.66	0.78
1:A:213:VAL:HG23	1:A:214:SER:H	1.47	0.78
1:A:31:GLY:O	1:A:32:MET:SD	2.42	0.77
1:A:151:VAL:O	1:A:155:GLY:HA3	1.84	0.77
1:A:45:ILE:HG22	1:A:46:THR:N	1.98	0.77
1:A:164:ARG:C	1:A:166:GLU:H	1.92	0.76
1:A:186:PRO:O	1:A:190:LEU:HB2	1.86	0.76
1:A:191:ILE:HG22	1:A:198:ILE:HG13	1.65	0.76
1:A:220:GLY:O	1:A:224:LEU:HG	1.86	0.75
1:A:222:ILE:HD11	3:A:268:2DP:H122	1.68	0.75
1:A:133:TYR:O	1:A:136:VAL:HG13	1.87	0.75
3:A:262:2DP:H222	3:A:267:2DP:H28	1.69	0.75
1:A:19:LEU:HD13	3:A:268:2DP:H552	1.68	0.75
3:A:263:2DP:H243	3:A:263:2DP:H191	1.69	0.74
3:A:261:2DP:H162	3:A:261:2DP:H551	1.71	0.73
1:A:78:ILE:HD11	1:A:194:GLU:HB3	1.71	0.72
1:A:48:LEU:HD13	1:A:92:LEU:HD11	1.71	0.72
1:A:56:MET:CG	1:A:85:ASP:HB2	2.17	0.72
1:A:71:PHE:HZ	1:A:134:ARG:NH1	1.87	0.72
1:A:181:LEU:HD21	1:A:214:SER:OG	1.89	0.72
1:A:20:MET:HE2	1:A:20:MET:HA	1.71	0.72
1:A:17:THR:HG22	1:A:54:PHE:CE1	2.25	0.71
1:A:56:MET:HG3	1:A:85:ASP:CB	2.19	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:TRP:CD1	2:A:249(A):RET:H14	2.25	0.71
1:A:71:PHE:CZ	1:A:134:ARG:CZ	2.74	0.70
1:A:153:PHE:HZ	1:A:179:VAL:HG11	1.56	0.69
1:A:190:LEU:O	1:A:195:GLY:HA3	1.91	0.69
1:A:185:TYR:CD1	1:A:208:PHE:HE1	2.08	0.69
1:A:71:PHE:HZ	1:A:134:ARG:CZ	2.05	0.69
1:A:36:ASP:C	1:A:38:ASP:H	2.01	0.69
1:A:112:VAL:O	1:A:115:ASP:HB2	1.92	0.69
1:A:134:ARG:O	1:A:136:VAL:N	2.26	0.69
1:A:45:ILE:CG2	1:A:46:THR:N	2.56	0.69
1:A:191:ILE:CG2	1:A:198:ILE:HG13	2.23	0.68
1:A:175:ARG:O	1:A:179:VAL:HG23	1.94	0.68
1:A:71:PHE:CZ	1:A:134:ARG:NH1	2.63	0.67
1:A:152:LEU:HD23	1:A:156:PHE:CD2	2.30	0.67
1:A:94:LEU:HD13	1:A:111:LEU:CD1	2.26	0.66
1:A:209:MET:O	1:A:213:VAL:HG22	1.96	0.66
1:A:221:LEU:O	1:A:223:LEU:N	2.29	0.66
1:A:212:ASP:O	1:A:215:ALA:HB3	1.94	0.66
1:A:213:VAL:HG23	1:A:214:SER:N	2.11	0.65
1:A:112:VAL:HG22	1:A:113:GLY:N	2.12	0.65
1:A:130:VAL:HG12	1:A:132:SER:N	2.12	0.65
1:A:164:ARG:CD	1:A:166:GLU:HG3	2.26	0.65
1:A:180:VAL:HG21	3:A:267:2DP:H441	1.78	0.65
1:A:24:THR:C	1:A:26:TYR:H	2.05	0.65
1:A:95:LEU:O	1:A:99:LEU:HG	1.97	0.64
1:A:149:LEU:CD1	1:A:179:VAL:HG13	2.27	0.64
1:A:167:VAL:O	1:A:168:ALA:C	2.41	0.64
1:A:94:LEU:HD11	1:A:115:ASP:OD1	1.98	0.64
1:A:101:VAL:O	1:A:102:ASP:C	2.40	0.64
1:A:94:LEU:HD13	1:A:111:LEU:HD13	1.81	0.63
1:A:77:PRO:HG2	1:A:201:LEU:HD11	1.81	0.63
1:A:164:ARG:HG3	1:A:166:GLU:HG3	1.79	0.63
3:A:264:2DP:H111	3:A:264:2DP:H421	1.80	0.63
1:A:130:VAL:CG1	1:A:132:SER:H	2.11	0.63
1:A:168:ALA:HB1	1:A:172:LYS:NZ	2.14	0.63
1:A:83:TYR:HB2	1:A:123:LEU:HD13	1.80	0.62
1:A:185:TYR:HD1	1:A:208:PHE:CE1	2.15	0.62
1:A:196:ALA:HB3	1:A:198:ILE:HG12	1.82	0.62
1:A:101:VAL:O	1:A:101:VAL:HG12	1.97	0.62
1:A:142:THR:HG22	1:A:146:LEU:HD12	1.82	0.62
1:A:105:GLN:HA	1:A:108:ILE:HG13	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:SER:HB2	3:A:268:2DP:HM2	1.81	0.61
1:A:217:VAL:O	1:A:221:LEU:HG	2.00	0.61
1:A:98:ALA:O	1:A:101:VAL:O	2.17	0.61
1:A:24:THR:C	1:A:26:TYR:N	2.57	0.61
1:A:49:VAL:HB	1:A:50:PRO:HD3	1.83	0.61
1:A:168:ALA:HA	1:A:172:LYS:HE3	1.82	0.61
1:A:118:MET:HE3	1:A:145:MET:CB	2.25	0.61
1:A:47:THR:O	1:A:50:PRO:HD2	2.01	0.61
1:A:9:GLU:OE1	1:A:9:GLU:N	2.33	0.61
1:A:216:LYS:O	1:A:217:VAL:C	2.43	0.61
1:A:78:ILE:HG21	1:A:126:ALA:O	2.01	0.60
1:A:24:THR:HG21	1:A:51:ALA:HB2	1.84	0.60
1:A:45:ILE:HG22	1:A:46:THR:H	1.64	0.60
1:A:49:VAL:HG12	1:A:216:LYS:HG2	1.84	0.60
1:A:118:MET:HE2	2:A:249(A):RET:H181	1.84	0.60
1:A:42:PHE:O	1:A:44:ALA:N	2.34	0.60
1:A:153:PHE:C	1:A:155:GLY:N	2.58	0.60
1:A:44:ALA:HA	3:A:269:2DP:H152	1.84	0.59
1:A:98:ALA:HB1	1:A:103:ALA:HB3	1.84	0.59
1:A:99:LEU:O	1:A:100:LEU:C	2.44	0.59
1:A:171:PHE:CZ	1:A:175:ARG:HG3	2.37	0.59
1:A:211:LEU:HD21	3:A:262:2DP:H591	1.85	0.59
1:A:56:MET:HE2	1:A:81:ALA:O	2.02	0.59
1:A:111:LEU:HD21	1:A:151:VAL:HG11	1.85	0.59
1:A:168:ALA:CA	1:A:172:LYS:HE3	2.33	0.58
1:A:152:LEU:HD23	1:A:156:PHE:HD2	1.68	0.58
1:A:60:MET:HG2	1:A:79:TYR:CD2	2.38	0.58
1:A:221:LEU:C	1:A:223:LEU:H	2.12	0.58
2:A:249(A):RET:H161	2:A:249(A):RET:C8	2.29	0.58
1:A:213:VAL:C	1:A:215:ALA:H	2.11	0.58
1:A:153:PHE:CZ	1:A:179:VAL:HG21	2.39	0.58
1:A:60:MET:HG2	1:A:79:TYR:HD2	1.69	0.58
1:A:17:THR:HG22	1:A:54:PHE:HE1	1.66	0.58
1:A:97:LEU:HD13	1:A:152:LEU:HD21	1.85	0.58
1:A:164:ARG:CG	1:A:166:GLU:HG3	2.35	0.57
1:A:149:LEU:HD13	1:A:179:VAL:HG13	1.86	0.57
1:A:206:LEU:O	1:A:210:VAL:HG22	2.04	0.57
1:A:10:TRP:O	1:A:14:ALA:HB2	2.04	0.57
1:A:42:PHE:C	1:A:44:ALA:N	2.62	0.57
1:A:217:VAL:HG23	1:A:218:GLY:H	1.68	0.57
1:A:167:VAL:HG12	1:A:168:ALA:N	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:VAL:CG2	1:A:113:GLY:N	2.68	0.57
1:A:115:ASP:O	1:A:118:MET:HB3	2.04	0.57
1:A:20:MET:HG3	1:A:57:TYR:CE2	2.40	0.56
1:A:67:THR:HG22	1:A:80:TRP:CD1	2.27	0.56
1:A:213:VAL:C	1:A:215:ALA:N	2.62	0.56
1:A:103:ALA:HB1	1:A:156:PHE:HE1	1.70	0.56
1:A:24:THR:O	1:A:26:TYR:N	2.39	0.56
1:A:164:ARG:C	1:A:166:GLU:N	2.59	0.55
1:A:130:VAL:HG12	1:A:133:TYR:H	1.70	0.55
1:A:37:PRO:CB	1:A:40:LYS:HZ2	2.17	0.55
1:A:142:THR:O	1:A:145:MET:N	2.40	0.55
1:A:142:THR:O	1:A:143:ALA:C	2.48	0.55
1:A:176:ASN:O	1:A:180:VAL:HG23	2.07	0.55
1:A:36:ASP:O	1:A:38:ASP:N	2.35	0.54
1:A:87:LEU:HD11	3:A:261:2DP:H603	1.89	0.54
1:A:221:LEU:C	1:A:223:LEU:N	2.66	0.54
1:A:76:ASN:HB2	1:A:77:PRO:CD	2.36	0.54
1:A:168:ALA:HB1	1:A:172:LYS:CE	2.36	0.54
1:A:177:VAL:O	1:A:177:VAL:CG1	2.55	0.54
1:A:164:ARG:O	1:A:166:GLU:N	2.40	0.53
1:A:36:ASP:C	1:A:38:ASP:N	2.67	0.53
3:A:262:2DP:H541	3:A:268:2DP:H291	1.89	0.53
1:A:134:ARG:HH12	1:A:194:GLU:HB3	1.74	0.53
1:A:49:VAL:CG1	1:A:216:LYS:HG2	2.38	0.53
1:A:171:PHE:CE2	1:A:175:ARG:HG3	2.43	0.53
1:A:153:PHE:HZ	1:A:179:VAL:CG1	2.22	0.53
1:A:169:SER:O	1:A:170:THR:C	2.51	0.53
1:A:45:ILE:HG13	1:A:92:LEU:HD13	1.91	0.53
1:A:45:ILE:O	1:A:48:LEU:HB2	2.10	0.52
1:A:138:TRP:CZ2	1:A:190:LEU:HD22	2.44	0.52
1:A:20:MET:HA	1:A:20:MET:CE	2.39	0.52
3:A:261:2DP:H172	3:A:261:2DP:H602	1.92	0.52
3:A:262:2DP:C22	3:A:267:2DP:H28	2.39	0.52
1:A:123:LEU:O	1:A:126:ALA:HB3	2.10	0.52
1:A:20:MET:HG3	1:A:57:TYR:CD2	2.45	0.52
1:A:118:MET:HE2	2:A:249(A):RET:H7	1.91	0.52
1:A:126:ALA:O	1:A:127:LEU:HD23	2.10	0.52
1:A:78:ILE:CD1	1:A:194:GLU:HG2	2.40	0.51
1:A:71:PHE:O	1:A:72:GLY:C	2.53	0.51
3:A:262:2DP:H53	3:A:263:2DP:C54	2.39	0.51
1:A:118:MET:HE1	2:A:249(A):RET:H192	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:ILE:CD1	3:A:268:2DP:H122	2.38	0.51
1:A:180:VAL:HG22	3:A:267:2DP:H172	1.93	0.51
1:A:103:ALA:CB	1:A:156:PHE:CE1	2.94	0.51
1:A:53:ALA:O	1:A:56:MET:HB2	2.11	0.50
1:A:115:ASP:OD1	1:A:148:ILE:HD13	2.11	0.50
1:A:130:VAL:HG12	1:A:133:TYR:N	2.26	0.50
1:A:218:GLY:O	1:A:219:PHE:C	2.54	0.50
1:A:79:TYR:O	1:A:82:ARG:HB2	2.12	0.50
1:A:108:ILE:O	1:A:109:LEU:C	2.52	0.50
1:A:164:ARG:HG3	1:A:166:GLU:CB	2.41	0.50
1:A:223:LEU:C	1:A:223:LEU:HD12	2.37	0.50
1:A:37:PRO:HB3	1:A:40:LYS:HZ1	1.73	0.50
1:A:56:MET:CE	1:A:81:ALA:O	2.60	0.50
1:A:164:ARG:HD2	1:A:166:GLU:HG3	1.92	0.50
1:A:56:MET:CE	1:A:81:ALA:HB1	2.42	0.50
1:A:168:ALA:C	1:A:172:LYS:CD	2.78	0.50
1:A:170:THR:O	1:A:174:LEU:HG	2.12	0.50
1:A:196:ALA:HB3	1:A:198:ILE:CG1	2.41	0.50
1:A:209:MET:SD	1:A:209:MET:C	2.95	0.50
1:A:164:ARG:HG3	1:A:166:GLU:CG	2.42	0.50
1:A:219:PHE:O	1:A:220:GLY:C	2.54	0.50
1:A:83:TYR:CD1	1:A:83:TYR:N	2.77	0.49
1:A:44:ALA:O	1:A:45:ILE:C	2.54	0.49
1:A:212:ASP:O	1:A:215:ALA:N	2.42	0.49
1:A:168:ALA:HB1	1:A:172:LYS:HE3	1.95	0.49
1:A:94:LEU:HD13	1:A:111:LEU:HD12	1.94	0.49
1:A:188:VAL:O	1:A:192:GLY:N	2.46	0.49
1:A:19:LEU:HD12	1:A:213:VAL:HG11	1.95	0.49
1:A:103:ALA:O	1:A:104:ASP:C	2.54	0.49
3:A:262:2DP:H422	3:A:262:2DP:H112	1.93	0.49
3:A:263:2DP:H462	3:A:263:2DP:H143	1.95	0.49
1:A:40:LYS:HE2	3:A:269:2DP:O4	2.13	0.48
1:A:10:TRP:CG	1:A:11:ILE:N	2.82	0.48
1:A:185:TYR:CD1	1:A:208:PHE:CE1	2.96	0.48
1:A:110:ALA:O	1:A:111:LEU:C	2.57	0.48
1:A:56:MET:HE1	1:A:81:ALA:HB1	1.95	0.48
1:A:28:LEU:HD23	1:A:47:THR:HG21	1.96	0.48
1:A:90:THR:OG1	1:A:91:PRO:HD3	2.14	0.48
1:A:169:SER:C	1:A:171:PHE:N	2.71	0.48
3:A:262:2DP:H443	3:A:263:2DP:H442	1.95	0.48
1:A:65:GLY:O	1:A:79:TYR:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ILE:O	1:A:80:TRP:N	2.47	0.48
1:A:159:LYS:O	1:A:161:GLU:N	2.47	0.47
1:A:168:ALA:CB	1:A:172:LYS:HE3	2.44	0.47
1:A:169:SER:O	1:A:171:PHE:N	2.47	0.47
1:A:196:ALA:HB1	1:A:198:ILE:HD11	1.97	0.47
1:A:213:VAL:O	1:A:215:ALA:N	2.47	0.47
1:A:142:THR:HG22	1:A:146:LEU:CD1	2.43	0.47
3:A:262:2DP:H602	3:A:267:2DP:H241	1.97	0.47
1:A:76:ASN:CB	1:A:77:PRO:HD2	2.42	0.47
1:A:221:LEU:HD11	3:A:268:2DP:H511	1.95	0.47
1:A:24:THR:CG2	1:A:51:ALA:HB2	2.44	0.46
1:A:101:VAL:O	1:A:103:ALA:N	2.47	0.46
1:A:168:ALA:O	1:A:171:PHE:HB3	2.16	0.46
1:A:219:PHE:O	1:A:222:ILE:N	2.48	0.46
1:A:13:LEU:HD13	1:A:60:MET:HB3	1.98	0.46
1:A:24:THR:HG21	3:A:269:2DP:H271	1.96	0.46
1:A:46:THR:O	1:A:46:THR:HG22	2.15	0.46
1:A:207:LEU:HD23	1:A:207:LEU:HA	1.67	0.46
1:A:42:PHE:O	1:A:43:TYR:C	2.57	0.46
1:A:188:VAL:HA	1:A:191:ILE:HD11	1.96	0.46
1:A:191:ILE:HG22	1:A:198:ILE:CG1	2.39	0.46
3:A:264:2DP:H141	3:A:265:2DP:H43	1.97	0.46
1:A:111:LEU:CD2	1:A:151:VAL:HG11	2.46	0.46
3:A:269:2DP:H121	3:A:269:2DP:H162	1.78	0.46
1:A:77:PRO:CG	1:A:201:LEU:HD11	2.44	0.46
1:A:153:PHE:CE1	1:A:179:VAL:HG21	2.50	0.46
1:A:27:PHE:CZ	1:A:221:LEU:HD23	2.51	0.46
1:A:28:LEU:CD2	1:A:47:THR:HG21	2.46	0.46
3:A:264:2DP:H511	3:A:264:2DP:H441	1.98	0.46
3:A:267:2DP:H151	3:A:267:2DP:H452	1.98	0.46
1:A:111:LEU:HD21	1:A:151:VAL:CG1	2.46	0.45
1:A:80:TRP:C	1:A:82:ARG:H	2.24	0.45
1:A:119:ILE:O	1:A:120:GLY:C	2.58	0.45
3:A:261:2DP:H593	3:A:261:2DP:H541	1.98	0.45
1:A:56:MET:CB	1:A:85:ASP:HB2	2.46	0.45
1:A:136:VAL:HG22	1:A:137:TRP:N	2.31	0.45
1:A:42:PHE:C	1:A:44:ALA:H	2.23	0.45
1:A:115:ASP:O	1:A:116:GLY:C	2.60	0.45
1:A:174:LEU:CD2	1:A:222:ILE:HG22	2.47	0.45
3:A:267:2DP:H512	3:A:267:2DP:H551	1.81	0.45
1:A:135:PHE:O	1:A:138:TRP:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:PHE:O	1:A:154:PHE:C	2.59	0.45
1:A:29:VAL:HA	3:A:269:2DP:H472	1.99	0.45
1:A:26:TYR:O	1:A:26:TYR:CD1	2.71	0.44
1:A:153:PHE:C	1:A:155:GLY:H	2.24	0.44
1:A:39:ALA:O	1:A:42:PHE:HB2	2.17	0.44
1:A:52:ILE:HG22	1:A:53:ALA:N	2.31	0.44
1:A:10:TRP:O	1:A:14:ALA:CB	2.65	0.44
1:A:48:LEU:CD1	1:A:92:LEU:HD11	2.42	0.44
1:A:103:ALA:HB1	1:A:156:PHE:CE1	2.51	0.44
1:A:181:LEU:HD12	1:A:181:LEU:HA	1.80	0.44
3:A:264:2DP:H13	3:A:264:2DP:H171	1.86	0.44
1:A:150:TYR:CE2	1:A:154:PHE:CD1	3.06	0.44
1:A:178:THR:HG22	1:A:182:TRP:CE2	2.52	0.44
1:A:83:TYR:HB2	1:A:123:LEU:CD1	2.48	0.44
1:A:134:ARG:HH12	1:A:194:GLU:CB	2.30	0.44
1:A:153:PHE:O	1:A:155:GLY:N	2.50	0.43
1:A:119:ILE:H	1:A:119:ILE:HG12	1.37	0.43
1:A:196:ALA:CB	1:A:198:ILE:HD11	2.48	0.43
1:A:164:ARG:HG3	1:A:166:GLU:H	1.82	0.43
1:A:38:ASP:HA	1:A:41:LYS:HD2	2.01	0.43
1:A:168:ALA:O	1:A:169:SER:C	2.62	0.43
1:A:164:ARG:HG3	1:A:166:GLU:HB2	1.99	0.43
3:A:263:2DP:H261	3:A:263:2DP:H241	1.87	0.43
1:A:29:VAL:HG12	1:A:30:LYS:N	2.33	0.43
1:A:134:ARG:O	1:A:137:TRP:N	2.50	0.43
1:A:212:ASP:O	1:A:215:ALA:CB	2.66	0.43
1:A:134:ARG:NH1	1:A:194:GLU:CB	2.82	0.43
1:A:10:TRP:O	1:A:14:ALA:N	2.52	0.43
1:A:76:ASN:CB	1:A:77:PRO:CD	2.97	0.43
1:A:145:MET:O	1:A:148:ILE:HG13	2.19	0.43
1:A:10:TRP:CZ2	1:A:11:ILE:HD13	2.54	0.42
1:A:45:ILE:HG21	1:A:96:ASP:CG	2.44	0.42
1:A:31:GLY:C	1:A:32:MET:HG2	2.44	0.42
1:A:37:PRO:C	1:A:40:LYS:HB2	2.44	0.42
1:A:124:VAL:C	1:A:126:ALA:H	2.27	0.42
1:A:26:TYR:CD1	1:A:26:TYR:C	2.97	0.42
1:A:198:ILE:HG12	1:A:198:ILE:H	1.66	0.42
1:A:202:ASN:OD1	1:A:202:ASN:N	2.51	0.42
1:A:107:THR:O	1:A:111:LEU:HD23	2.19	0.42
1:A:115:ASP:O	1:A:118:MET:N	2.45	0.42
1:A:124:VAL:O	1:A:128:THR:OG1	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:VAL:HG12	1:A:130:VAL:O	2.17	0.42
1:A:148:ILE:O	1:A:149:LEU:C	2.63	0.42
1:A:201:LEU:O	1:A:202:ASN:C	2.63	0.42
1:A:69:VAL:HA	1:A:70:PRO:HD3	1.78	0.42
1:A:145:MET:CE	1:A:183:SER:HA	2.41	0.42
1:A:46:THR:O	1:A:50:PRO:HD3	2.19	0.42
1:A:28:LEU:O	1:A:31:GLY:N	2.52	0.42
1:A:211:LEU:HD23	1:A:211:LEU:HA	1.84	0.42
3:A:264:2DP:H441	3:A:264:2DP:C50	2.50	0.42
1:A:122:GLY:O	1:A:126:ALA:HB2	2.19	0.42
1:A:138:TRP:CH2	1:A:190:LEU:HD22	2.55	0.42
1:A:126:ALA:C	1:A:134:ARG:NH2	2.78	0.42
1:A:150:TYR:CD2	1:A:154:PHE:CE1	3.07	0.41
1:A:182:TRP:C	1:A:184:ALA:H	2.28	0.41
1:A:95:LEU:HD23	1:A:95:LEU:HA	1.84	0.41
1:A:133:TYR:O	1:A:134:ARG:O	2.38	0.41
1:A:123:LEU:HA	1:A:126:ALA:HB3	2.02	0.41
1:A:152:LEU:HD23	1:A:152:LEU:HA	1.93	0.41
1:A:204:GLU:O	1:A:207:LEU:N	2.54	0.41
1:A:215:ALA:O	1:A:219:PHE:CB	2.60	0.41
1:A:58:LEU:O	1:A:58:LEU:HD12	2.21	0.41
1:A:91:PRO:O	1:A:95:LEU:HG	2.21	0.41
1:A:157:THR:O	1:A:158:SER:O	2.38	0.41
3:A:265:2DP:H561	3:A:265:2DP:H521	1.86	0.41
1:A:149:LEU:O	1:A:152:LEU:HB2	2.21	0.41
1:A:27:PHE:HZ	1:A:221:LEU:HD23	1.85	0.40
1:A:67:THR:CG2	1:A:80:TRP:HD1	2.18	0.40
1:A:134:ARG:NH1	1:A:194:GLU:HB2	2.36	0.40
1:A:155:GLY:C	1:A:157:THR:H	2.28	0.40
3:A:263:2DP:H42	3:A:263:2DP:HM2	2.02	0.40
1:A:56:MET:O	1:A:60:MET:HE3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	220/248 (89%)	150 (68%)	46 (21%)	24 (11%)	0 1

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	134	ARG
1	A	135	PHE
1	A	158	SER
1	A	160	ALA
1	A	168	ALA
1	A	219	PHE
1	A	222	ILE
1	A	43	TYR
1	A	45	ILE
1	A	72	GLY
1	A	99	LEU
1	A	192	GLY
1	A	79	TYR
1	A	156	PHE
1	A	183	SER
1	A	198	ILE
1	A	217	VAL
1	A	25	LEU
1	A	102	ASP
1	A	143	ALA
1	A	214	SER
1	A	220	GLY
1	A	116	GLY
1	A	165	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	179/193 (93%)	116 (65%)	63 (35%)	0 1

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ARG
1	A	17	THR
1	A	19	LEU
1	A	20	MET
1	A	28	LEU
1	A	29	VAL
1	A	30	LYS
1	A	34	VAL
1	A	38	ASP
1	A	40	LYS
1	A	41	LYS
1	A	45	ILE
1	A	55	THR
1	A	58	LEU
1	A	67	THR
1	A	69	VAL
1	A	74	GLU
1	A	82	ARG
1	A	85	ASP
1	A	87	LEU
1	A	92	LEU
1	A	94	LEU
1	A	99	LEU
1	A	107	THR
1	A	108	ILE
1	A	111	LEU
1	A	112	VAL
1	A	119	ILE
1	A	128	THR
1	A	129	LYS
1	A	130	VAL
1	A	132	SER
1	A	136	VAL
1	A	140	ILE
1	A	146	LEU
1	A	148	ILE
1	A	149	LEU
1	A	151	VAL

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Mol	Chain	Res	Type
1	A	159	LYS
1	A	163	MET
1	A	167	VAL
1	A	170	THR
1	A	172	LYS
1	A	174	LEU
1	A	175	ARG
1	A	177	VAL
1	A	178	THR
1	A	187	VAL
1	A	191	ILE
1	A	194	GLU
1	A	198	ILE
1	A	199	VAL
1	A	202	ASN
1	A	203	ILE
1	A	208	PHE
1	A	210	VAL
1	A	216	LYS
1	A	217	VAL
1	A	221	LEU
1	A	223	LEU
1	A	224	LEU
1	A	226	SER
1	A	227	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

9 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	$\# Z > 2$
2	RET	A	249(A)	1	20,20,21	0.94	1 (5%)	27,27,28	1.06	2 (7%)
3	2DP	A	269	-	59,59,59	1.41	10 (16%)	67,74,74	1.08	5 (7%)
3	2DP	A	262	-	59,59,59	1.20	2 (3%)	67,74,74	1.04	4 (5%)
3	2DP	A	268	-	59,59,59	1.36	6 (10%)	67,74,74	1.10	6 (8%)
3	2DP	A	261	-	59,59,59	1.34	7 (11%)	67,74,74	1.09	4 (5%)
3	2DP	A	264	-	59,59,59	1.21	4 (6%)	67,74,74	1.13	8 (11%)
3	2DP	A	263	-	59,59,59	1.24	6 (10%)	67,74,74	1.00	4 (5%)
3	2DP	A	265	-	59,59,59	1.39	8 (13%)	67,74,74	1.08	5 (7%)
3	2DP	A	267	-	59,59,59	1.48	7 (11%)	67,74,74	1.10	7 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	2DP	A	269	-	2/2/12/12	41/70/70/70	-
2	RET	A	249(A)	1	-	0/13/30/31	0/1/1/1
3	2DP	A	262	-	2/2/12/12	38/70/70/70	-
3	2DP	A	268	-	2/2/12/12	42/70/70/70	-
3	2DP	A	261	-	2/2/12/12	39/70/70/70	-
3	2DP	A	264	-	2/2/12/12	45/70/70/70	-
3	2DP	A	263	-	2/2/12/12	43/70/70/70	-
3	2DP	A	265	-	2/2/12/12	33/70/70/70	-
3	2DP	A	267	-	2/2/12/12	41/70/70/70	-

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	267	2DP	C6-C5	3.71	1.63	1.51
3	A	267	2DP	C4-C5	3.66	1.63	1.51
3	A	263	2DP	C4-C5	3.48	1.62	1.51
3	A	262	2DP	C4-C5	3.43	1.62	1.51
3	A	269	2DP	C4-C5	3.35	1.62	1.51
3	A	261	2DP	C4-C5	3.29	1.62	1.51
3	A	265	2DP	C4-C5	3.10	1.61	1.51
3	A	263	2DP	P1-O6	3.03	1.71	1.59
3	A	261	2DP	P1-O3	3.02	1.71	1.59
3	A	269	2DP	P2-O8	3.00	1.71	1.59
3	A	267	2DP	P2-O8	2.96	1.71	1.59
2	A	249(A)	RET	C14-C13	2.90	1.35	1.33
3	A	267	2DP	P1-O6	2.89	1.70	1.59
3	A	268	2DP	C4-C5	2.87	1.60	1.51
3	A	268	2DP	P2-O8	2.85	1.70	1.59
3	A	264	2DP	C4-C5	2.83	1.60	1.51
3	A	269	2DP	P1-O6	2.78	1.70	1.59
3	A	261	2DP	P1-O6	2.70	1.70	1.59
3	A	265	2DP	C42-C41	2.68	1.60	1.50
3	A	265	2DP	P1-O6	2.59	1.69	1.59
3	A	269	2DP	P1-O3	2.58	1.69	1.59
3	A	265	2DP	P2-O8	2.58	1.69	1.59
3	A	265	2DP	C44-C43	2.56	1.60	1.52
3	A	268	2DP	C42-C41	2.50	1.59	1.50
3	A	268	2DP	P1-O6	2.50	1.69	1.59
3	A	265	2DP	P1-O3	2.46	1.69	1.59
3	A	263	2DP	P1-O3	2.39	1.68	1.59
3	A	261	2DP	P2-O8	2.38	1.68	1.59
3	A	264	2DP	P1-O6	2.37	1.68	1.59
3	A	263	2DP	C6-C5	2.32	1.58	1.51
3	A	269	2DP	C45-C43	2.30	1.63	1.52
3	A	269	2DP	C6-C5	2.30	1.58	1.51
3	A	262	2DP	P2-O8	2.28	1.68	1.59
3	A	269	2DP	C44-C43	2.28	1.60	1.52
3	A	263	2DP	P2-O8	2.25	1.68	1.59
3	A	264	2DP	P2-O8	2.23	1.68	1.59
3	A	265	2DP	O2-C41	2.23	1.49	1.43
3	A	263	2DP	P2-O11	-2.21	1.51	1.58
3	A	269	2DP	C42-C41	2.21	1.58	1.50
3	A	268	2DP	O2-C41	2.19	1.49	1.43
3	A	267	2DP	C44-C43	2.16	1.59	1.52
3	A	267	2DP	P1-O3	2.16	1.67	1.59
3	A	261	2DP	P2-O11	-2.14	1.51	1.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	261	2DP	C42-C41	2.10	1.58	1.50
3	A	267	2DP	O6-C4	2.07	1.52	1.44
3	A	268	2DP	C6-C5	2.07	1.58	1.51
3	A	265	2DP	C46-C47	2.05	1.60	1.52
3	A	264	2DP	C45-C43	2.04	1.62	1.52
3	A	261	2DP	O2-C41	2.04	1.48	1.43
3	A	269	2DP	O6-C4	2.03	1.52	1.44
3	A	269	2DP	C3-C2	2.00	1.57	1.50

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	264	2DP	O2-C41-C42	-3.05	102.37	108.77
3	A	268	2DP	C41-O2-C2	2.90	123.54	115.53
2	A	249(A)	RET	C7-C8-C9	2.87	130.48	126.23
3	A	267	2DP	C21-C22-C23	2.84	125.39	115.97
3	A	261	2DP	C41-O2-C2	2.83	123.36	115.53
3	A	269	2DP	C46-C45-C43	2.78	125.20	115.97
3	A	269	2DP	C19-C18-C17	2.72	120.97	111.27
3	A	265	2DP	C46-C47-C48	2.53	124.38	115.97
3	A	263	2DP	C24-C23-C22	2.51	120.21	111.27
3	A	264	2DP	C19-C18-C20	2.50	120.20	111.27
3	A	264	2DP	C41-O2-C2	2.49	122.40	115.53
3	A	269	2DP	C24-C23-C25	2.48	120.13	111.27
3	A	265	2DP	C24-C23-C22	2.48	120.13	111.27
3	A	267	2DP	C25-C23-C22	2.48	124.62	112.07
3	A	261	2DP	C24-C23-C25	2.47	120.06	111.27
3	A	267	2DP	C16-C17-C18	2.44	124.06	115.97
3	A	267	2DP	C21-C20-C18	2.40	123.93	115.97
3	A	263	2DP	C19-C18-C20	2.39	119.80	111.27
3	A	261	2DP	C19-C18-C17	2.38	119.77	111.27
3	A	264	2DP	C46-C47-C48	2.37	123.83	115.97
3	A	268	2DP	C24-C23-C22	2.34	119.63	111.27
3	A	265	2DP	C19-C18-C17	2.34	119.60	111.27
3	A	267	2DP	C19-C18-C17	2.32	119.55	111.27
3	A	262	2DP	C19-C18-C20	2.31	119.52	111.27
3	A	263	2DP	C24-C23-C25	2.31	119.52	111.27
3	A	268	2DP	C19-C18-C17	2.29	119.43	111.27
3	A	268	2DP	C19-C18-C20	2.27	119.38	111.27
3	A	264	2DP	C46-C45-C43	2.27	123.50	115.97
3	A	262	2DP	C24-C23-C25	2.25	119.29	111.27
3	A	265	2DP	C19-C18-C20	2.23	119.23	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	268	2DP	C46-C47-C48	2.20	123.29	115.97
3	A	261	2DP	C46-C47-C48	2.19	123.25	115.97
3	A	267	2DP	C19-C18-C20	2.17	119.03	111.27
3	A	264	2DP	C24-C23-C25	2.17	119.00	111.27
3	A	264	2DP	C24-C23-C22	2.16	118.99	111.27
3	A	269	2DP	C16-C17-C18	2.16	123.13	115.97
3	A	262	2DP	C19-C18-C17	2.11	118.80	111.27
3	A	264	2DP	C19-C18-C17	2.10	118.77	111.27
2	A	249(A)	RET	C8-C9-C10	-2.09	115.72	119.01
3	A	268	2DP	C21-C22-C23	2.09	122.91	115.97
3	A	262	2DP	C24-C23-C22	2.09	118.71	111.27
3	A	269	2DP	C24-C23-C22	2.08	118.70	111.27
3	A	263	2DP	C19-C18-C17	2.07	118.64	111.27
3	A	267	2DP	C46-C47-C48	2.02	122.68	115.97
3	A	265	2DP	C47-C46-C45	2.02	122.31	113.28

All (16) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	261	2DP	C18
3	A	261	2DP	C23
3	A	262	2DP	C18
3	A	262	2DP	C23
3	A	263	2DP	C18
3	A	263	2DP	C23
3	A	264	2DP	C18
3	A	264	2DP	C23
3	A	265	2DP	C18
3	A	265	2DP	C23
3	A	267	2DP	C18
3	A	267	2DP	C23
3	A	268	2DP	C18
3	A	268	2DP	C23
3	A	269	2DP	C18
3	A	269	2DP	C23

All (322) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	261	2DP	O1-C1-C2-O2
3	A	261	2DP	C5-C4-O6-P1
3	A	261	2DP	C3-O3-P1-O6

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Mol	Chain	Res	Type	Atoms
3	A	261	2DP	C6-O8-P2-O9
3	A	261	2DP	C6-O8-P2-O10
3	A	261	2DP	C6-O8-P2-O11
3	A	262	2DP	C5-C4-O6-P1
3	A	262	2DP	C11-C12-C13-C14
3	A	262	2DP	C3-O3-P1-O5
3	A	262	2DP	C3-O3-P1-O6
3	A	262	2DP	CM-O11-P2-O8
3	A	262	2DP	CM-O11-P2-O9
3	A	263	2DP	C2-C3-O3-P1
3	A	263	2DP	O6-C4-C5-C6
3	A	263	2DP	C3-O3-P1-O4
3	A	263	2DP	C3-O3-P1-O5
3	A	263	2DP	C3-O3-P1-O6
3	A	263	2DP	C4-O6-P1-O4
3	A	263	2DP	C4-O6-P1-O5
3	A	264	2DP	C11-C12-C13-C15
3	A	264	2DP	C19-C18-C20-C21
3	A	264	2DP	C3-O3-P1-O4
3	A	264	2DP	C3-O3-P1-O5
3	A	264	2DP	C4-O6-P1-O3
3	A	264	2DP	C4-O6-P1-O4
3	A	264	2DP	C4-O6-P1-O5
3	A	264	2DP	C6-O8-P2-O9
3	A	264	2DP	C6-O8-P2-O11
3	A	265	2DP	C5-C4-O6-P1
3	A	265	2DP	C4-C5-C6-O8
3	A	265	2DP	C41-C42-C43-C44
3	A	265	2DP	C3-O3-P1-O5
3	A	265	2DP	C6-O8-P2-O9
3	A	265	2DP	C6-O8-P2-O11
3	A	267	2DP	O6-C4-C5-C6
3	A	267	2DP	C5-C4-O6-P1
3	A	267	2DP	C41-C42-C43-C44
3	A	267	2DP	C3-O3-P1-O6
3	A	267	2DP	C6-O8-P2-O10
3	A	267	2DP	C6-O8-P2-O11
3	A	267	2DP	CM-O11-P2-O9
3	A	267	2DP	CM-O11-P2-O10
3	A	268	2DP	C2-C3-O3-P1
3	A	268	2DP	O6-C4-C5-C6
3	A	268	2DP	O7-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
3	A	268	2DP	C16-C17-C18-C19
3	A	268	2DP	C3-O3-P1-O6
3	A	268	2DP	C4-O6-P1-O3
3	A	268	2DP	C6-O8-P2-O9
3	A	268	2DP	C6-O8-P2-O10
3	A	268	2DP	C6-O8-P2-O11
3	A	269	2DP	C4-C5-C6-O8
3	A	269	2DP	O7-C5-C6-O8
3	A	269	2DP	C3-O3-P1-O5
3	A	269	2DP	C4-O6-P1-O3
3	A	269	2DP	C4-O6-P1-O5
3	A	269	2DP	C6-O8-P2-O9
3	A	261	2DP	O7-C5-C6-O8
3	A	263	2DP	O6-C4-C5-O7
3	A	265	2DP	O7-C5-C6-O8
3	A	267	2DP	O6-C4-C5-O7
3	A	268	2DP	O6-C4-C5-O7
3	A	263	2DP	C4-C5-C6-O8
3	A	268	2DP	C4-C5-C6-O8
3	A	261	2DP	C16-C17-C18-C19
3	A	261	2DP	C21-C22-C23-C24
3	A	261	2DP	C46-C47-C48-C49
3	A	261	2DP	C54-C53-C55-C56
3	A	262	2DP	C19-C18-C20-C21
3	A	262	2DP	C46-C47-C48-C49
3	A	264	2DP	C44-C43-C45-C46
3	A	264	2DP	C51-C52-C53-C54
3	A	265	2DP	C16-C17-C18-C19
3	A	267	2DP	C16-C17-C18-C19
3	A	267	2DP	C46-C47-C48-C49
3	A	268	2DP	C21-C22-C23-C24
3	A	269	2DP	C44-C43-C45-C46
3	A	269	2DP	C54-C53-C55-C56
3	A	263	2DP	O7-C5-C6-O8
3	A	262	2DP	C55-C56-C57-C58
3	A	263	2DP	C13-C15-C16-C17
3	A	264	2DP	C16-C17-C18-C20
3	A	265	2DP	C52-C53-C55-C56
3	A	265	2DP	C20-C21-C22-C23
3	A	269	2DP	C20-C21-C22-C23
3	A	263	2DP	C15-C16-C17-C18
3	A	264	2DP	C18-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
3	A	265	2DP	C48-C50-C51-C52
3	A	262	2DP	C53-C55-C56-C57
3	A	268	2DP	C25-C26-C27-C28
3	A	261	2DP	C13-C15-C16-C17
3	A	262	2DP	C48-C50-C51-C52
3	A	263	2DP	C18-C20-C21-C22
3	A	263	2DP	C43-C45-C46-C47
3	A	267	2DP	C18-C20-C21-C22
3	A	267	2DP	C43-C45-C46-C47
3	A	262	2DP	O7-C5-C6-O8
3	A	268	2DP	C18-C20-C21-C22
3	A	263	2DP	O1-C11-C12-C13
3	A	265	2DP	O2-C41-C42-C43
3	A	268	2DP	O2-C41-C42-C43
3	A	264	2DP	C23-C25-C26-C27
3	A	265	2DP	C23-C25-C26-C27
3	A	262	2DP	C4-C5-C6-O8
3	A	263	2DP	C48-C50-C51-C52
3	A	267	2DP	C15-C16-C17-C18
3	A	262	2DP	C23-C25-C26-C27
3	A	264	2DP	C53-C55-C56-C57
3	A	261	2DP	C45-C46-C47-C48
3	A	265	2DP	C53-C55-C56-C57
3	A	265	2DP	C55-C56-C57-C58
3	A	261	2DP	C53-C55-C56-C57
3	A	263	2DP	C55-C56-C57-C58
3	A	262	2DP	C26-C27-C28-C29
3	A	269	2DP	C26-C27-C28-C29
3	A	267	2DP	C45-C46-C47-C48
3	A	268	2DP	CM-O11-P2-O9
3	A	267	2DP	C26-C27-C28-C30
3	A	262	2DP	C26-C27-C28-C30
3	A	263	2DP	C26-C27-C28-C29
3	A	264	2DP	C26-C27-C28-C30
3	A	267	2DP	C26-C27-C28-C29
3	A	268	2DP	C26-C27-C28-C30
3	A	268	2DP	C53-C55-C56-C57
3	A	263	2DP	C26-C27-C28-C30
3	A	269	2DP	C43-C45-C46-C47
3	A	269	2DP	C12-C13-C15-C16
3	A	261	2DP	C23-C25-C26-C27
3	A	263	2DP	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	A	267	2DP	C13-C15-C16-C17
3	A	263	2DP	C24-C23-C25-C26
3	A	269	2DP	C53-C55-C56-C57
3	A	264	2DP	C26-C27-C28-C29
3	A	264	2DP	C56-C57-C58-C59
3	A	269	2DP	C48-C50-C51-C52
3	A	268	2DP	C26-C27-C28-C29
3	A	264	2DP	C15-C16-C17-C18
3	A	267	2DP	C1-C2-C3-O3
3	A	261	2DP	C51-C52-C53-C55
3	A	262	2DP	C21-C22-C23-C25
3	A	264	2DP	C21-C22-C23-C25
3	A	267	2DP	C46-C47-C48-C50
3	A	268	2DP	C46-C47-C48-C50
3	A	268	2DP	C51-C52-C53-C55
3	A	261	2DP	C14-C13-C15-C16
3	A	261	2DP	C49-C48-C50-C51
3	A	267	2DP	C21-C22-C23-C24
3	A	268	2DP	C51-C52-C53-C54
3	A	269	2DP	C51-C52-C53-C54
3	A	261	2DP	O1-C1-C2-C3
3	A	262	2DP	O1-C1-C2-C3
3	A	264	2DP	O1-C1-C2-C3
3	A	265	2DP	O1-C1-C2-C3
3	A	269	2DP	O1-C1-C2-C3
3	A	269	2DP	C18-C20-C21-C22
3	A	269	2DP	C55-C56-C57-C58
3	A	269	2DP	C5-C4-O6-P1
3	A	267	2DP	C56-C57-C58-C59
3	A	264	2DP	C50-C51-C52-C53
3	A	268	2DP	C43-C45-C46-C47
3	A	264	2DP	CM-O11-P2-O9
3	A	262	2DP	O2-C2-C3-O3
3	A	261	2DP	O1-C11-C12-C13
3	A	267	2DP	O2-C41-C42-C43
3	A	269	2DP	O1-C11-C12-C13
3	A	262	2DP	C45-C46-C47-C48
3	A	268	2DP	C15-C16-C17-C18
3	A	261	2DP	C24-C23-C25-C26
3	A	262	2DP	C54-C53-C55-C56
3	A	263	2DP	C16-C17-C18-C19
3	A	264	2DP	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
3	A	268	2DP	C48-C50-C51-C52
3	A	263	2DP	C5-C6-O8-P2
3	A	264	2DP	C5-C4-O6-P1
3	A	264	2DP	C5-C6-O8-P2
3	A	267	2DP	C5-C6-O8-P2
3	A	269	2DP	C26-C27-C28-C30
3	A	268	2DP	C20-C21-C22-C23
3	A	262	2DP	C1-C2-C3-O3
3	A	263	2DP	C1-C2-C3-O3
3	A	261	2DP	C12-C13-C15-C16
3	A	261	2DP	C47-C48-C50-C51
3	A	261	2DP	C52-C53-C55-C56
3	A	262	2DP	C47-C48-C50-C51
3	A	263	2DP	C17-C18-C20-C21
3	A	264	2DP	C51-C52-C53-C55
3	A	265	2DP	C17-C18-C20-C21
3	A	269	2DP	C42-C43-C45-C46
3	A	261	2DP	C25-C26-C27-C28
3	A	264	2DP	C56-C57-C58-C60
3	A	264	2DP	O1-C11-C12-C13
3	A	268	2DP	O1-C11-C12-C13
3	A	261	2DP	C18-C20-C21-C22
3	A	267	2DP	C56-C57-C58-C60
3	A	263	2DP	C50-C51-C52-C53
3	A	261	2DP	O2-C2-C3-O3
3	A	263	2DP	O2-C2-C3-O3
3	A	262	2DP	C2-C3-O3-P1
3	A	262	2DP	C25-C26-C27-C28
3	A	263	2DP	C56-C57-C58-C59
3	A	261	2DP	C51-C52-C53-C54
3	A	262	2DP	C49-C48-C50-C51
3	A	267	2DP	C19-C18-C20-C21
3	A	268	2DP	C46-C47-C48-C49
3	A	264	2DP	C42-C41-O2-C2
3	A	265	2DP	C43-C45-C46-C47
3	A	265	2DP	C50-C51-C52-C53
3	A	262	2DP	O2-C41-C42-C43
3	A	265	2DP	O1-C11-C12-C13
3	A	261	2DP	C1-C2-C3-O3
3	A	261	2DP	C17-C18-C20-C21
3	A	262	2DP	C16-C17-C18-C20
3	A	262	2DP	C51-C52-C53-C55

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Mol	Chain	Res	Type	Atoms
3	A	263	2DP	C21-C22-C23-C25
3	A	264	2DP	C42-C43-C45-C46
3	A	268	2DP	C52-C53-C55-C56
3	A	269	2DP	C16-C17-C18-C20
3	A	269	2DP	C22-C23-C25-C26
3	A	261	2DP	C2-C1-O1-C11
3	A	264	2DP	O2-C2-C3-O3
3	A	267	2DP	O2-C2-C3-O3
3	A	262	2DP	O1-C1-C2-O2
3	A	263	2DP	O1-C1-C2-O2
3	A	264	2DP	O1-C1-C2-O2
3	A	262	2DP	C44-C43-C45-C46
3	A	269	2DP	C13-C15-C16-C17
3	A	264	2DP	C1-C2-C3-O3
3	A	269	2DP	C1-C2-C3-O3
3	A	263	2DP	C12-C13-C15-C16
3	A	267	2DP	C42-C43-C45-C46
3	A	269	2DP	C45-C46-C47-C48
3	A	269	2DP	O2-C2-C3-O3
3	A	262	2DP	C51-C52-C53-C54
3	A	265	2DP	C54-C53-C55-C56
3	A	267	2DP	C24-C23-C25-C26
3	A	268	2DP	C54-C53-C55-C56
3	A	261	2DP	C3-O3-P1-O4
3	A	262	2DP	C11-C12-C13-C15
3	A	263	2DP	C4-O6-P1-O3
3	A	264	2DP	C3-O3-P1-O6
3	A	264	2DP	C6-O8-P2-O10
3	A	265	2DP	C3-O3-P1-O4
3	A	265	2DP	C3-O3-P1-O6
3	A	265	2DP	C6-O8-P2-O10
3	A	267	2DP	C41-C42-C43-C45
3	A	267	2DP	C3-O3-P1-O4
3	A	267	2DP	C6-O8-P2-O9
3	A	268	2DP	C3-O3-P1-O4
3	A	268	2DP	C4-O6-P1-O4
3	A	269	2DP	C3-O3-P1-O4
3	A	269	2DP	C3-O3-P1-O6
3	A	269	2DP	C6-O8-P2-O11
3	A	265	2DP	C2-C3-O3-P1
3	A	267	2DP	C2-C3-O3-P1
3	A	268	2DP	C5-C6-O8-P2

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Mol	Chain	Res	Type	Atoms
3	A	264	2DP	C45-C46-C47-C48
3	A	269	2DP	C56-C57-C58-C60
3	A	263	2DP	C45-C46-C47-C48
3	A	262	2DP	C24-C23-C25-C26
3	A	269	2DP	C16-C17-C18-C19
3	A	264	2DP	C22-C23-C25-C26
3	A	269	2DP	C51-C52-C53-C55
3	A	261	2DP	C4-C5-C6-O8
3	A	264	2DP	C4-C5-C6-O8
3	A	264	2DP	C20-C21-C22-C23
3	A	269	2DP	C2-C3-O3-P1
3	A	269	2DP	O1-C1-C2-O2
3	A	264	2DP	CM-O11-P2-O10
3	A	268	2DP	CM-O11-P2-O10
3	A	263	2DP	O2-C41-C42-C43
3	A	262	2DP	C2-C1-O1-C11
3	A	267	2DP	C2-C1-O1-C11
3	A	261	2DP	C44-C43-C45-C46
3	A	263	2DP	C14-C13-C15-C16
3	A	265	2DP	C51-C52-C53-C54
3	A	263	2DP	C56-C57-C58-C60
3	A	268	2DP	C17-C18-C20-C21
3	A	263	2DP	C23-C25-C26-C27
3	A	269	2DP	C12-C11-O1-C1
3	A	262	2DP	C15-C16-C17-C18
3	A	267	2DP	C54-C53-C55-C56
3	A	269	2DP	C21-C22-C23-C24
3	A	263	2DP	C25-C26-C27-C28
3	A	261	2DP	C22-C23-C25-C26
3	A	261	2DP	C42-C43-C45-C46
3	A	262	2DP	C46-C47-C48-C50
3	A	263	2DP	C51-C52-C53-C55
3	A	264	2DP	C47-C48-C50-C51
3	A	265	2DP	C21-C22-C23-C25
3	A	267	2DP	C17-C18-C20-C21
3	A	269	2DP	C17-C18-C20-C21
3	A	269	2DP	C52-C53-C55-C56
3	A	265	2DP	C26-C27-C28-C29
3	A	267	2DP	O1-C11-C12-C13
3	A	263	2DP	C22-C23-C25-C26
3	A	265	2DP	C14-C13-C15-C16
3	A	268	2DP	C24-C23-C25-C26

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Mol	Chain	Res	Type	Atoms
3	A	268	2DP	C56-C57-C58-C60
3	A	265	2DP	C24-C23-C25-C26
3	A	267	2DP	C44-C43-C45-C46
3	A	262	2DP	C42-C41-O2-C2
3	A	268	2DP	C2-C1-O1-C11
3	A	261	2DP	C46-C47-C48-C50
3	A	263	2DP	C42-C43-C45-C46
3	A	264	2DP	C46-C47-C48-C50
3	A	265	2DP	C12-C13-C15-C16
3	A	265	2DP	C51-C52-C53-C55
3	A	267	2DP	C52-C53-C55-C56
3	A	268	2DP	C12-C13-C15-C16
3	A	267	2DP	C53-C55-C56-C57
3	A	264	2DP	C49-C48-C50-C51
3	A	268	2DP	C5-C4-O6-P1
3	A	261	2DP	O2-C41-C42-C43
3	A	269	2DP	C56-C57-C58-C59
3	A	267	2DP	C48-C50-C51-C52
3	A	268	2DP	C21-C22-C23-C25
3	A	268	2DP	C56-C57-C58-C59
3	A	261	2DP	C48-C50-C51-C52
3	A	263	2DP	C51-C52-C53-C54
3	A	263	2DP	C42-C41-O2-C2
3	A	265	2DP	O1-C1-C2-O2
3	A	264	2DP	C1-C2-O2-C41

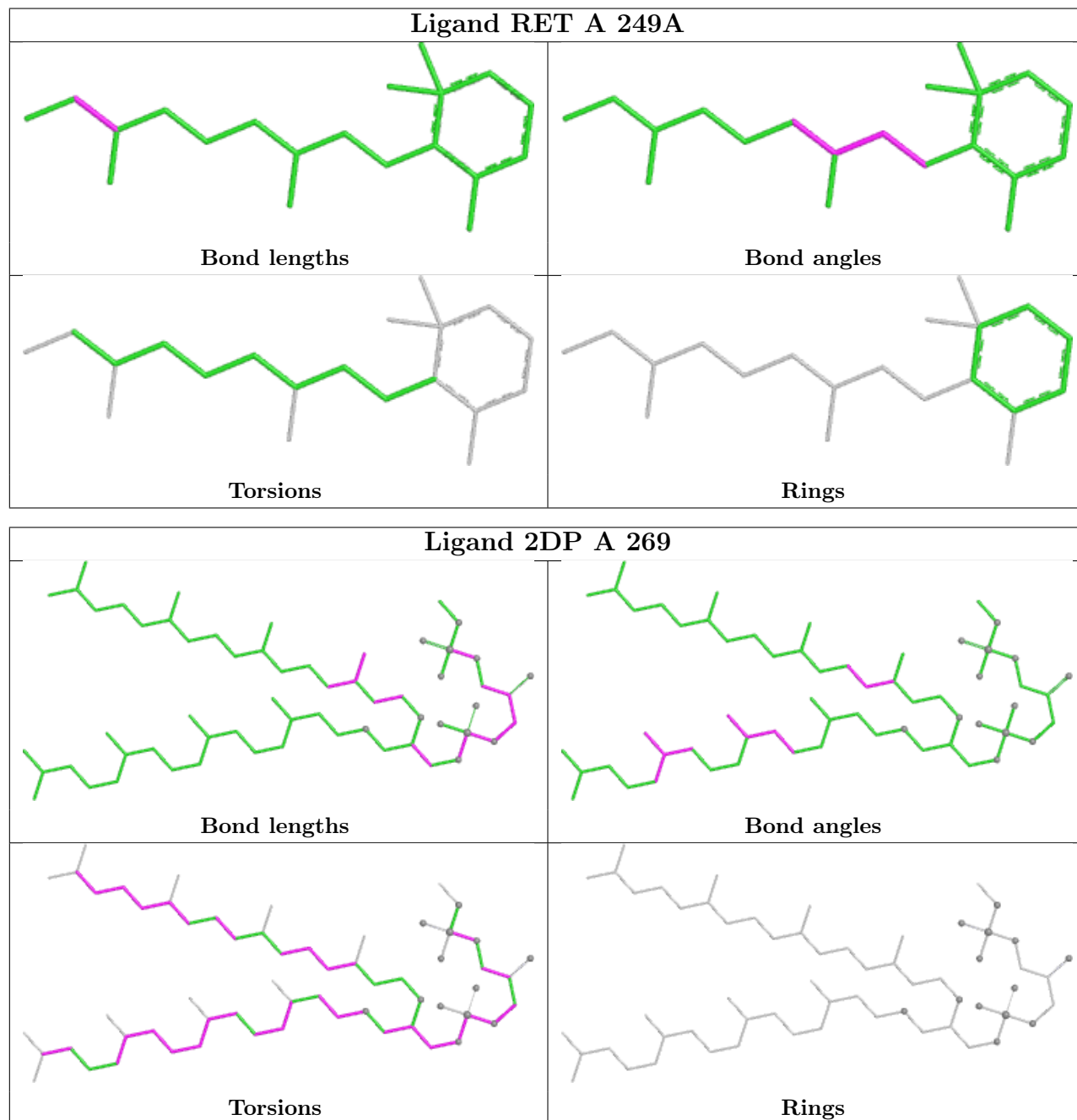
There are no ring outliers.

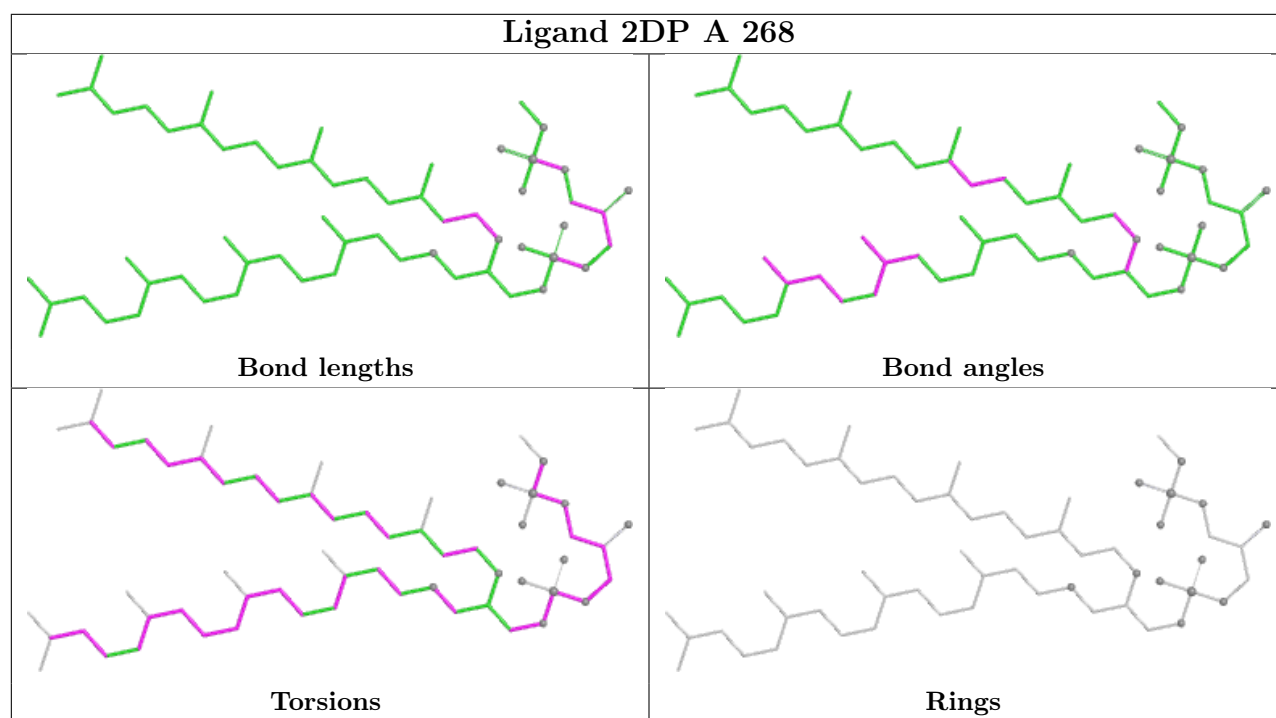
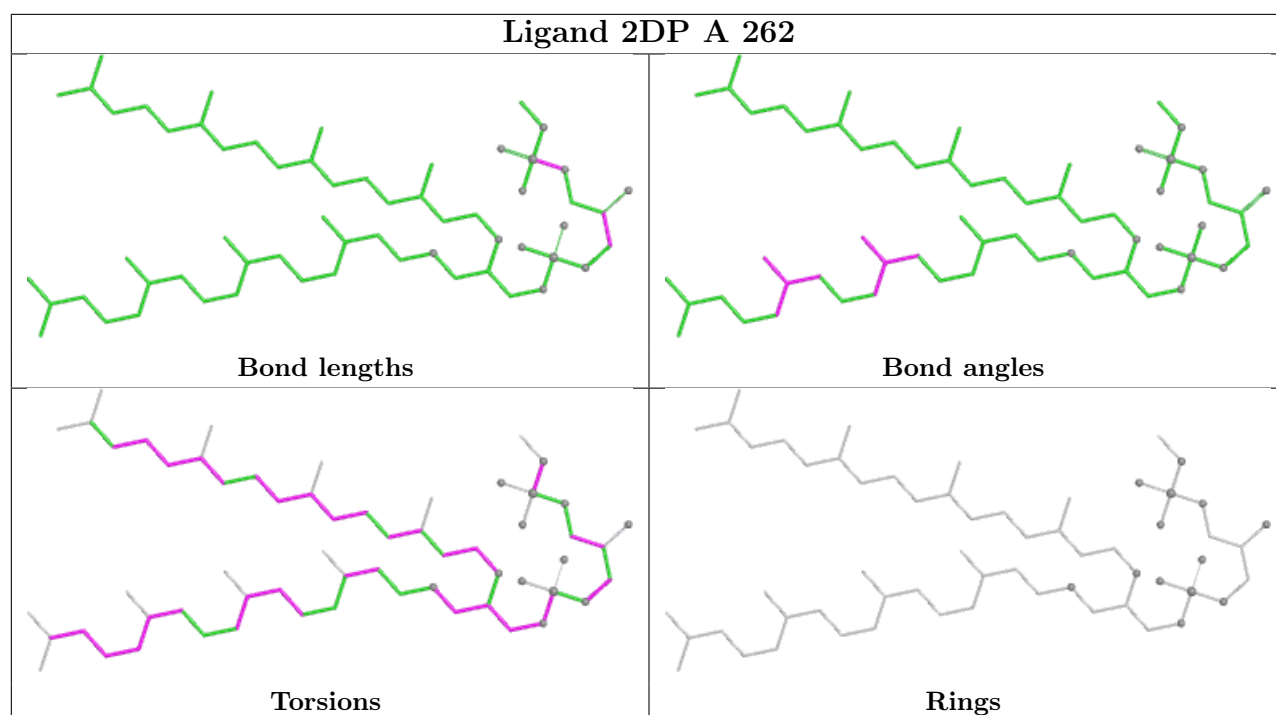
9 monomers are involved in 46 short contacts:

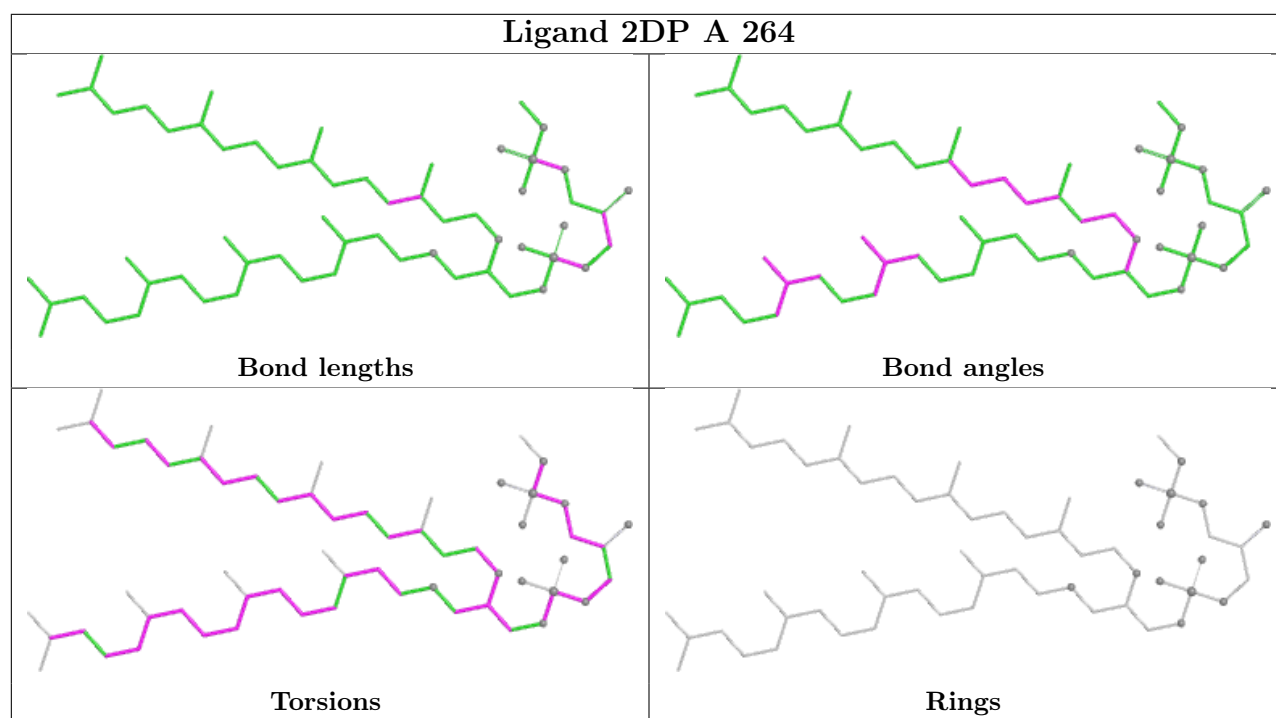
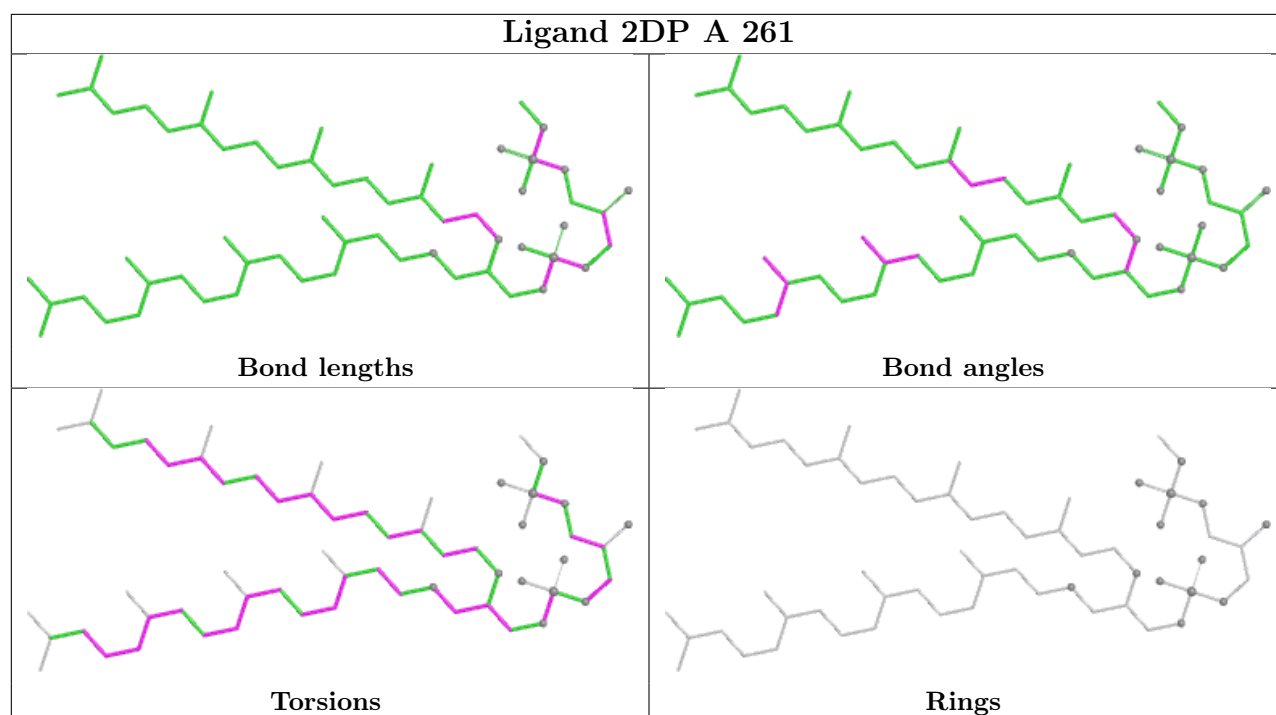
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	249(A)	RET	6	0
3	A	269	2DP	6	0
3	A	262	2DP	10	0
3	A	268	2DP	6	0
3	A	261	2DP	4	0
3	A	264	2DP	5	0
3	A	263	2DP	7	0
3	A	265	2DP	2	0
3	A	267	2DP	8	0

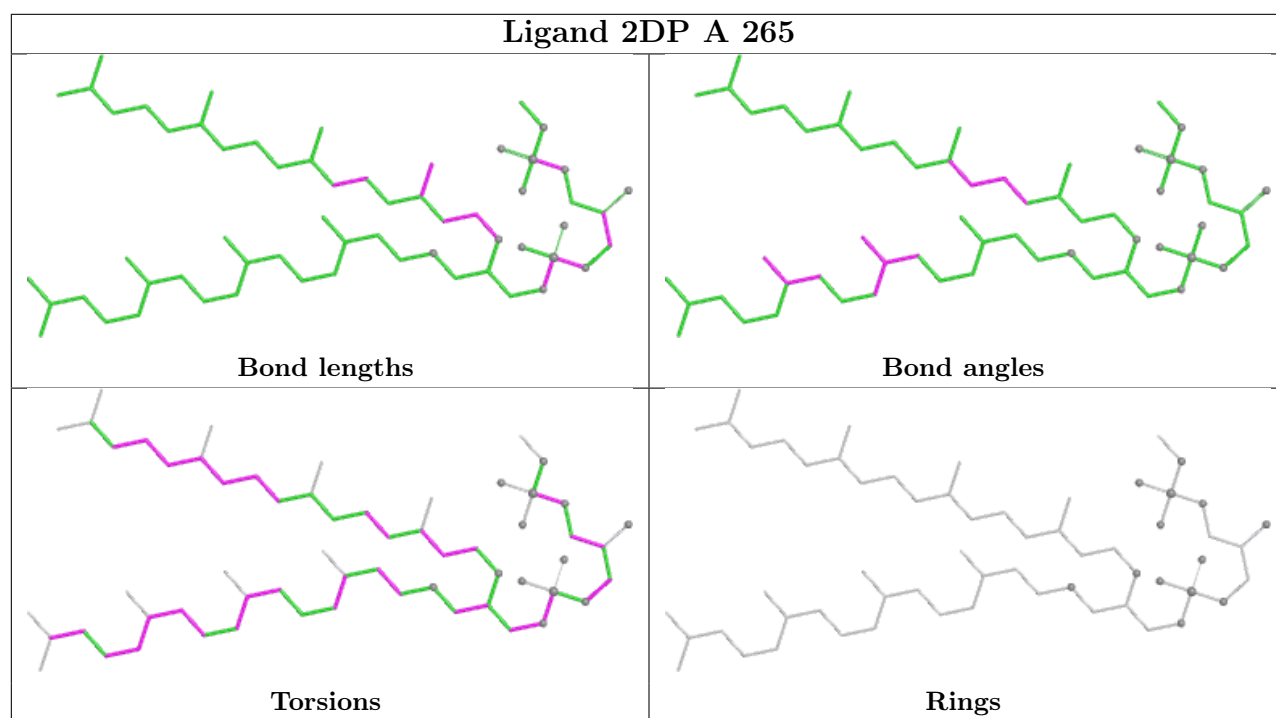
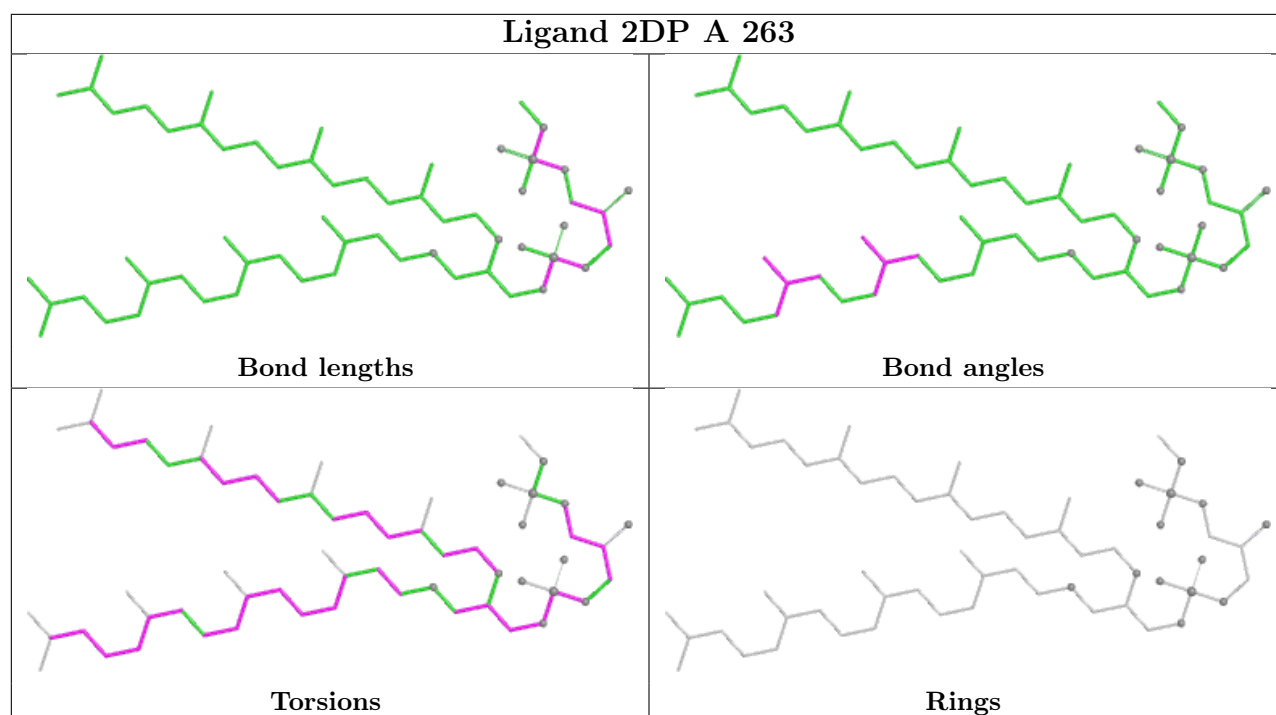
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

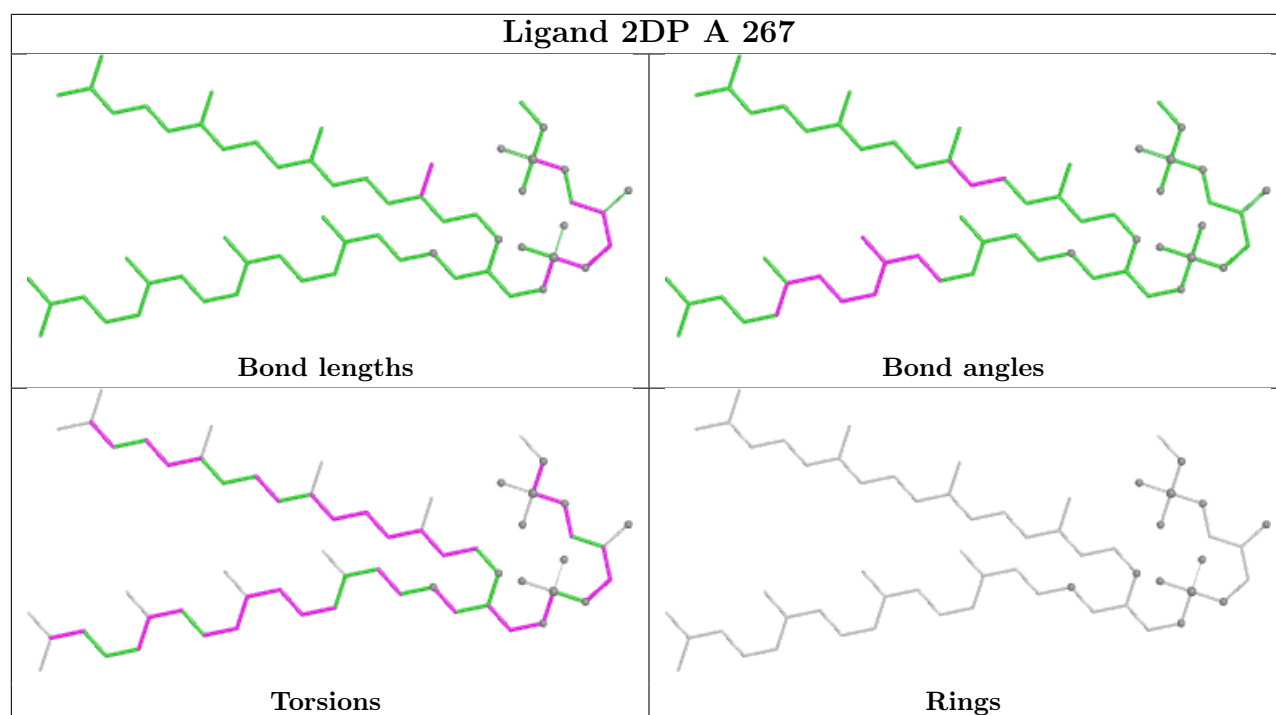
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.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











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.