



## Full wwPDB EM Validation Report ⓘ

Jul 9, 2025 – 12:55 PM JST

PDB ID : 8Y2M / pdb\_00008y2m  
EMDB ID : EMD-38857  
Title : Cryo-EM structure of the FB1-bound Lac1-Lip1 complex  
Authors : Xie, T.; Zhang, Z.; Fang, Q.; Gong, X.  
Deposited on : 2024-01-26  
Resolution : 3.07 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : **FAILED**  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.44

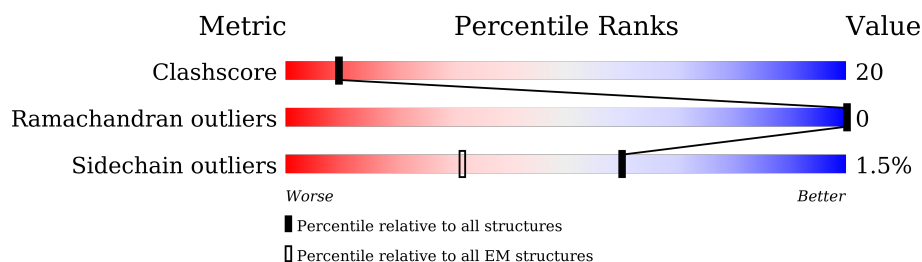
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*


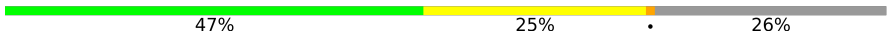


The reported resolution of this entry is 3.07 Å.

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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	428	
1	C	428	
2	B	150	
2	D	150	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7754 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 Ceramide synthase LAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	315	Total	C	N	O	S	0	0
			2636	1783	417	423	13		
1	C	315	Total	C	N	O	S	0	0
			2636	1783	417	423	13		

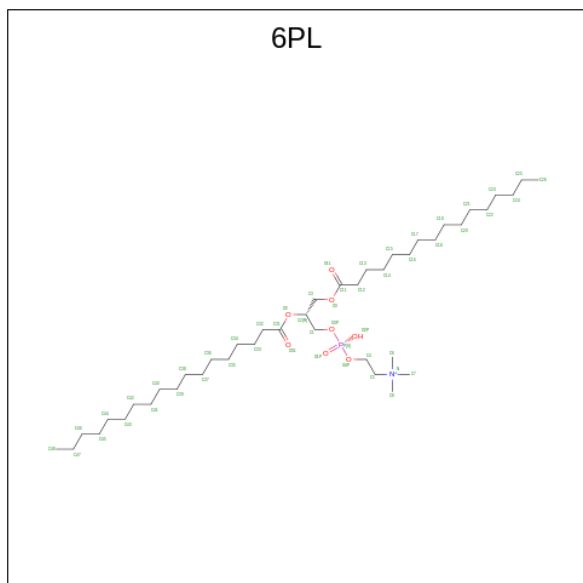
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	419	LEU	-	expression tag	UNP P28496
A	420	GLU	-	expression tag	UNP P28496
A	421	ASP	-	expression tag	UNP P28496
A	422	TYR	-	expression tag	UNP P28496
A	423	LYS	-	expression tag	UNP P28496
A	424	ASP	-	expression tag	UNP P28496
A	425	ASP	-	expression tag	UNP P28496
A	426	ASP	-	expression tag	UNP P28496
A	427	ASP	-	expression tag	UNP P28496
A	428	LYS	-	expression tag	UNP P28496
C	419	LEU	-	expression tag	UNP P28496
C	420	GLU	-	expression tag	UNP P28496
C	421	ASP	-	expression tag	UNP P28496
C	422	TYR	-	expression tag	UNP P28496
C	423	LYS	-	expression tag	UNP P28496
C	424	ASP	-	expression tag	UNP P28496
C	425	ASP	-	expression tag	UNP P28496
C	426	ASP	-	expression tag	UNP P28496
C	427	ASP	-	expression tag	UNP P28496
C	428	LYS	-	expression tag	UNP P28496

- Molecule 2 is a protein called Ceramide synthase subunit LIP1.

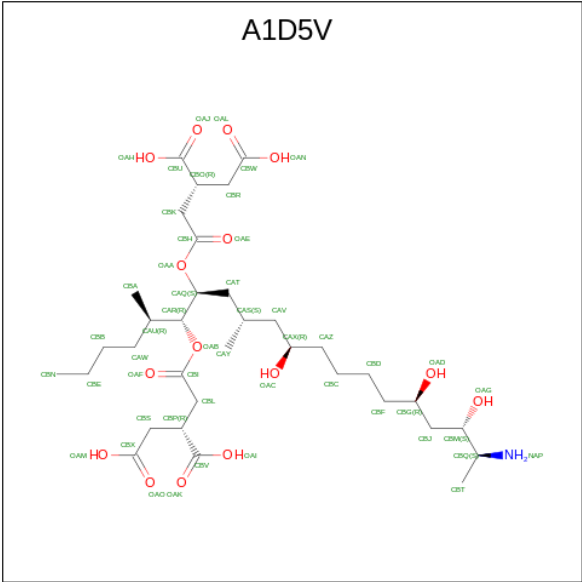
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	133	Total	C	N	O	S	0	0
			1089	703	178	202	6		
2	D	133	Total	C	N	O	S	0	0
			1089	703	178	202	6		

- Molecule 3 is (4S,7R)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSAN-1-AMINIUM 4-OXIDE (CCD ID: 6PL) (formula: C<sub>42</sub>H<sub>85</sub>NO<sub>8</sub>P).



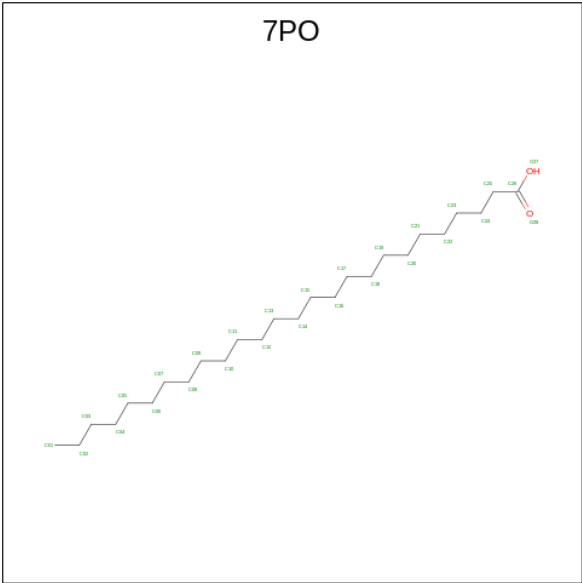
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C			0
			18	18			
3	B	1	Total	C	O	P	0
			40	31	8	1	
3	B	1	Total	C			0
			18	18			
3	C	1	Total	C			0
			18	18			
3	D	1	Total	C	O	P	0
			40	31	8	1	
3	D	1	Total	C			0
			18	18			

- Molecule 4 is (2 {R})-2-[2-[(5 {R},6 {R},7 {S},9 {S},11 {R},16 {R},18 {S},19 {S})-19-azanyl-6-[(3 {R})-3-carboxy-5-oxidanyl-5-oxidanylidene-pentanoyl]oxy-5,9-dimethyl-11,16,18-tris(oxidanyl)icosan-7-yl]oxy-2-oxidanylidene-ethyl]butanedioic acid (CCD ID: A1D5V) (formula: C<sub>34</sub>H<sub>59</sub>NO<sub>15</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			50	34	1	15	
4	C	1	Total	C	N	O	0
			50	34	1	15	

- Molecule 5 is hexacosanoic acid (CCD ID: 7PO) (formula: C<sub>26</sub>H<sub>52</sub>O<sub>2</sub>).

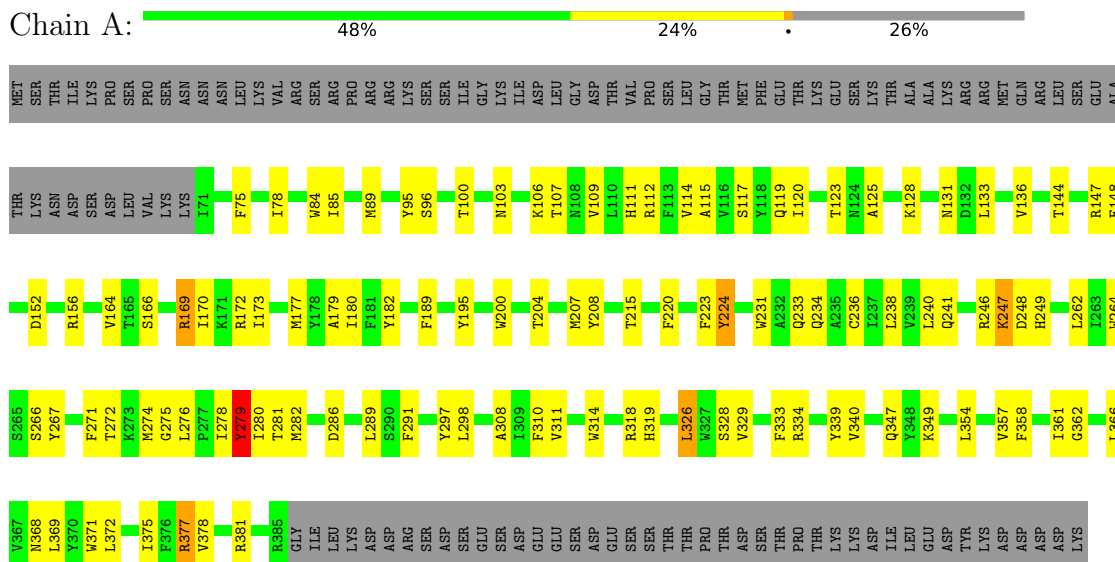


Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	C	0
			26	26	
5	C	1	Total	C	0
			26	26	

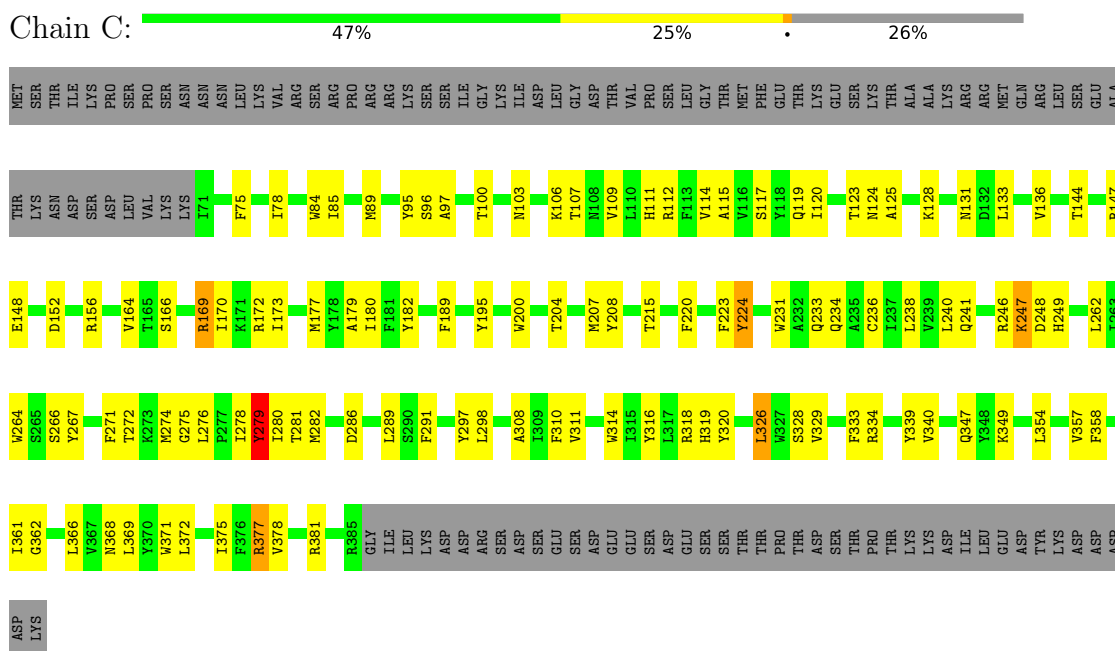
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

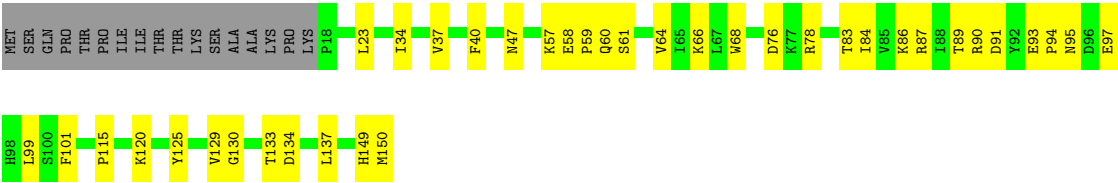
#### • Molecule 1: Ceramide synthase LAC1



#### • Molecule 1: Ceramide synthase LAC1



● Molecule 2: Ceramide synthase subunit LIP1



● Molecule 2: Ceramide synthase subunit LIP1



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	507891	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 7PO, A1D5V, 6PL

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	0.28	0/2726	0.69	6/3710 (0.2%)
1	C	0.28	0/2726	0.69	6/3710 (0.2%)
2	B	0.27	0/1122	0.61	1/1523 (0.1%)
2	D	0.27	0/1122	0.62	1/1523 (0.1%)
All	All	0.28	0/7696	0.67	14/10466 (0.1%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	278	ILE	CA-C-N	-8.48	106.25	120.68
1	C	278	ILE	C-N-CA	-8.48	106.25	120.68
1	A	278	ILE	CA-C-N	-8.46	106.29	120.68
1	A	278	ILE	C-N-CA	-8.46	106.29	120.68
1	A	279	TYR	N-CA-CB	6.69	120.61	110.30
1	C	279	TYR	N-CA-CB	6.65	120.54	110.30
1	C	278	ILE	O-C-N	-6.52	115.11	121.83
1	A	278	ILE	O-C-N	-6.49	115.15	121.83
1	A	279	TYR	CA-C-N	-6.48	110.31	121.97
1	A	279	TYR	C-N-CA	-6.48	110.31	121.97
1	C	279	TYR	CA-C-N	-6.48	110.31	121.97
1	C	279	TYR	C-N-CA	-6.48	110.31	121.97
2	D	59	PRO	CA-N-CD	-5.50	104.30	112.00
2	B	59	PRO	CA-N-CD	-5.47	104.34	112.00

There are no chirality outliers.

There are no planarity outliers.

## 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	2636	0	2623	120	0
1	C	2636	0	2623	123	0
2	B	1089	0	1045	39	0
2	D	1089	0	1045	38	0
3	A	18	0	35	1	0
3	B	58	0	91	5	0
3	C	18	0	35	1	0
3	D	58	0	91	5	0
4	A	50	0	0	10	0
4	C	50	0	0	10	0
5	A	26	0	0	13	0
5	C	26	0	0	13	0
All	All	7754	0	7588	302	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 20.

All (302) 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:279:TYR:CD2	5:A:503:7PO:C20	2.14	1.30
1:C:279:TYR:CD2	5:C:503:7PO:C20	2.14	1.29
1:A:371:TRP:CZ3	4:A:502:A1D5V:CBF	2.28	1.16
1:C:371:TRP:CZ3	4:C:502:A1D5V:CBF	2.28	1.16
1:C:279:TYR:HD2	5:C:503:7PO:C20	1.52	1.15
1:A:279:TYR:HD2	5:A:503:7PO:C20	1.52	1.14
1:C:326:LEU:HD11	1:C:361:ILE:HG22	1.33	1.11
1:A:326:LEU:HD11	1:A:361:ILE:HG22	1.33	1.07
1:A:279:TYR:CE2	5:A:503:7PO:C20	2.39	1.05
1:C:279:TYR:CE2	5:C:503:7PO:C20	2.39	1.04
1:A:371:TRP:CE3	4:A:502:A1D5V:CBF	2.52	0.93
1:C:371:TRP:CE3	4:C:502:A1D5V:CBF	2.52	0.92
1:C:326:LEU:CD1	1:C:361:ILE:HG22	1.99	0.92
1:A:326:LEU:HD23	1:A:358:PHE:CE1	2.04	0.92
1:A:326:LEU:CD1	1:A:361:ILE:HG22	1.99	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:326:LEU:HD23	1:C:358:PHE:CE1	2.04	0.91
1:A:279:TYR:O	1:A:280:ILE:C	2.15	0.88
1:C:279:TYR:O	1:C:280:ILE:C	2.15	0.83
1:A:166:SER:HB3	1:A:169:ARG:HB2	1.62	0.81
1:A:164:VAL:HG13	1:A:169:ARG:HE	1.46	0.81
1:C:164:VAL:HG13	1:C:169:ARG:HE	1.46	0.80
1:C:166:SER:HB3	1:C:169:ARG:HB2	1.62	0.79
1:C:326:LEU:CD1	1:C:361:ILE:CG2	2.61	0.79
1:A:326:LEU:CD1	1:A:361:ILE:CG2	2.61	0.78
1:C:103:ASN:ND2	1:C:107:THR:O	2.20	0.75
1:C:231:TRP:HZ2	5:C:503:7PO:C26	2.00	0.74
1:A:103:ASN:ND2	1:A:107:THR:O	2.20	0.73
1:A:231:TRP:HZ2	5:A:503:7PO:C26	2.00	0.73
2:B:94:PRO:HG3	2:D:78:ARG:HD3	1.69	0.73
2:B:78:ARG:HD3	2:D:94:PRO:HG3	1.71	0.72
1:A:111:HIS:HA	1:A:114:VAL:HG12	1.73	0.70
1:A:179:ALA:HA	1:A:182:TYR:CE1	2.27	0.69
1:C:179:ALA:HA	1:C:182:TYR:CE1	2.27	0.68
1:C:111:HIS:HA	1:C:114:VAL:HG12	1.73	0.68
1:C:247:LYS:H	1:C:249:HIS:CD2	2.12	0.67
1:C:340:VAL:O	1:C:347:GLN:NE2	2.28	0.67
1:A:340:VAL:O	1:A:347:GLN:NE2	2.28	0.67
1:A:208:TYR:HB3	1:A:349:LYS:HE3	1.77	0.66
1:A:125:ALA:HB1	1:A:215:THR:HB	1.77	0.66
1:A:247:LYS:H	1:A:249:HIS:CD2	2.12	0.66
1:C:208:TYR:HB3	1:C:349:LYS:HE3	1.77	0.66
1:C:125:ALA:HB1	1:C:215:THR:HB	1.77	0.65
2:D:68:TRP:HA	2:D:84:ILE:HD11	1.80	0.64
1:C:172:ARG:HB3	1:C:297:TYR:OH	1.97	0.63
1:A:172:ARG:HB3	1:A:297:TYR:OH	1.97	0.63
1:C:279:TYR:HE2	5:C:503:7PO:C20	2.08	0.63
1:C:282:MET:HG3	5:C:503:7PO:C23	2.28	0.63
2:B:68:TRP:HA	2:B:84:ILE:HD11	1.80	0.63
1:A:282:MET:HG3	5:A:503:7PO:C23	2.28	0.63
1:C:371:TRP:CZ3	4:C:502:A1D5V:CBJ	2.82	0.63
1:A:377:ARG:HG2	1:A:378:VAL:N	2.13	0.62
1:A:371:TRP:CZ3	4:A:502:A1D5V:CBJ	2.82	0.62
1:C:377:ARG:HG2	1:C:378:VAL:N	2.13	0.62
2:B:149:HIS:O	2:D:125:TYR:OH	2.18	0.62
1:A:220:PHE:CE2	1:A:272:THR:HG22	2.34	0.62
1:C:246:ARG:HA	1:C:249:HIS:HD2	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:ARG:HA	1:A:249:HIS:CD2	2.35	0.62
2:B:125:TYR:OH	2:D:149:HIS:O	2.19	0.61
1:C:220:PHE:CE2	1:C:272:THR:HG22	2.34	0.61
1:C:238:LEU:O	1:C:241:GLN:NE2	2.34	0.61
1:A:246:ARG:HA	1:A:249:HIS:HD2	1.65	0.61
1:A:279:TYR:CE2	5:A:503:7PO:C17	2.84	0.61
1:C:247:LYS:H	1:C:249:HIS:HD2	1.49	0.60
1:C:279:TYR:CE2	5:C:503:7PO:C17	2.84	0.60
1:A:247:LYS:H	1:A:249:HIS:HD2	1.49	0.60
1:C:246:ARG:HA	1:C:249:HIS:CD2	2.35	0.60
1:C:326:LEU:HD11	1:C:361:ILE:CG2	2.18	0.60
1:A:279:TYR:HE2	5:A:503:7PO:C20	2.08	0.60
1:A:224:TYR:OH	1:A:275:GLY:HA3	2.02	0.60
1:A:238:LEU:O	1:A:241:GLN:NE2	2.34	0.60
1:C:224:TYR:OH	1:C:275:GLY:HA3	2.02	0.59
1:A:377:ARG:O	1:A:381:ARG:HG3	2.02	0.59
1:C:377:ARG:O	1:C:381:ARG:HG3	2.02	0.59
1:C:152:ASP:OD2	1:C:156:ARG:NH2	2.36	0.59
1:A:95:TYR:HE1	1:A:114:VAL:HG23	1.68	0.59
1:A:152:ASP:OD2	1:A:156:ARG:NH2	2.36	0.58
1:C:95:TYR:HE1	1:C:114:VAL:HG23	1.68	0.58
2:B:61:SER:HB2	2:B:137:LEU:HD21	1.87	0.57
2:D:61:SER:HB2	2:D:137:LEU:HD21	1.87	0.57
2:D:99:LEU:HD23	2:D:99:LEU:H	1.69	0.57
1:C:371:TRP:HZ3	4:C:502:A1D5V:CBJ	2.18	0.57
2:B:40:PHE:HB2	3:B:201:6PL:H172	1.87	0.56
1:C:319:HIS:NE2	1:C:372:LEU:HD22	2.20	0.56
1:A:84:TRP:HB3	1:A:148:GLU:HB2	1.87	0.56
2:B:99:LEU:H	2:B:99:LEU:HD23	1.68	0.56
1:A:371:TRP:HZ3	4:A:502:A1D5V:CBJ	2.18	0.56
1:C:371:TRP:O	1:C:375:ILE:HG12	2.06	0.56
2:D:40:PHE:HB2	3:D:201:6PL:H172	1.87	0.56
1:A:371:TRP:O	1:A:375:ILE:HG12	2.06	0.56
1:C:371:TRP:CH2	4:C:502:A1D5V:CBF	2.88	0.56
2:B:101:PHE:HB3	2:B:129:VAL:HG23	1.86	0.56
1:C:326:LEU:HD12	1:C:361:ILE:CG2	2.36	0.56
1:C:84:TRP:HB3	1:C:148:GLU:HB2	1.87	0.56
1:C:164:VAL:HG13	1:C:169:ARG:NE	2.18	0.56
1:C:362:GLY:O	1:C:366:LEU:HG	2.06	0.55
1:C:369:LEU:HA	1:C:372:LEU:CD2	2.36	0.55
1:A:319:HIS:NE2	1:A:372:LEU:HD22	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:LEU:HA	1:A:372:LEU:CD2	2.37	0.55
1:A:164:VAL:HG13	1:A:169:ARG:NE	2.18	0.55
2:D:101:PHE:HB3	2:D:129:VAL:HG23	1.87	0.55
1:C:369:LEU:O	1:C:372:LEU:HD23	2.07	0.55
1:A:362:GLY:O	1:A:366:LEU:HG	2.06	0.55
1:A:369:LEU:O	1:A:372:LEU:HD23	2.07	0.55
1:A:166:SER:HB3	1:A:169:ARG:CB	2.36	0.55
1:C:119:GLN:NE2	1:C:123:THR:O	2.40	0.54
1:C:246:ARG:O	1:C:247:LYS:HG2	2.08	0.54
1:C:329:VAL:O	1:C:333:PHE:HB2	2.07	0.54
1:A:375:ILE:HD13	4:A:502:A1D5V:CAV	2.38	0.54
1:A:195:TYR:HA	1:A:200:TRP:CE3	2.44	0.53
2:B:97:GLU:OE2	2:B:133:THR:HG23	2.08	0.53
1:C:375:ILE:HD13	4:C:502:A1D5V:CAV	2.38	0.53
2:D:97:GLU:OE2	2:D:133:THR:HG23	2.08	0.53
1:A:371:TRP:CH2	4:A:502:A1D5V:CBF	2.88	0.53
1:A:326:LEU:HD12	1:A:361:ILE:CG2	2.36	0.53
1:C:195:TYR:HA	1:C:200:TRP:CE3	2.44	0.53
1:C:279:TYR:HE2	5:C:503:7PO:C17	2.22	0.53
1:A:329:VAL:O	1:A:333:PHE:HB2	2.07	0.53
1:A:180:ILE:HD11	1:A:291:PHE:HA	1.91	0.53
1:A:271:PHE:HB3	1:A:274:MET:HE2	1.91	0.53
1:A:170:ILE:O	1:A:173:ILE:HG22	2.09	0.52
1:C:133:LEU:HD11	2:D:34:ILE:HG21	1.91	0.52
2:D:93:GLU:OE2	2:D:95:ASN:ND2	2.26	0.52
2:D:64:VAL:HG12	2:D:130:GLY:HA3	1.92	0.52
1:A:119:GLN:NE2	1:A:123:THR:O	2.40	0.52
1:A:246:ARG:O	1:A:247:LYS:HG2	2.08	0.52
1:C:180:ILE:HD11	1:C:291:PHE:HA	1.91	0.52
1:C:318:ARG:NH2	1:C:368:ASN:OD1	2.41	0.52
1:C:166:SER:HB3	1:C:169:ARG:CB	2.36	0.52
1:A:318:ARG:NH2	1:A:368:ASN:OD1	2.41	0.52
1:A:133:LEU:HD11	2:B:34:ILE:HG21	1.91	0.52
1:C:314:TRP:HE1	1:C:319:HIS:HE1	1.57	0.52
1:A:246:ARG:HG3	1:A:246:ARG:HH11	1.75	0.52
1:A:314:TRP:HE1	1:A:319:HIS:HE1	1.57	0.52
2:B:64:VAL:HG12	2:B:130:GLY:HA3	1.92	0.52
2:B:87:ARG:O	2:B:91:ASP:HB2	2.10	0.51
1:C:271:PHE:HB3	1:C:274:MET:HE2	1.91	0.51
2:D:87:ARG:O	2:D:91:ASP:HB2	2.10	0.51
1:C:173:ILE:HG12	1:C:177:MET:HE2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:LEU:HB3	5:A:503:7PO:C18	2.41	0.51
1:C:170:ILE:O	1:C:173:ILE:HG22	2.10	0.51
1:C:262:LEU:HB3	5:C:503:7PO:C18	2.41	0.51
1:C:246:ARG:HG3	1:C:246:ARG:HH11	1.75	0.51
1:A:133:LEU:HG	3:B:202:6PL:H352	1.93	0.50
1:A:264:TRP:HZ2	2:B:37:VAL:HG11	1.77	0.50
1:C:133:LEU:HG	3:D:202:6PL:H352	1.93	0.50
1:A:173:ILE:HG12	1:A:177:MET:HE2	1.92	0.50
2:B:101:PHE:HE1	2:B:150:MET:HE3	1.77	0.50
1:C:286:ASP:OD1	4:C:502:A1D5V:NAP	2.45	0.50
1:A:279:TYR:HE2	5:A:503:7PO:C17	2.22	0.50
2:B:89:THR:O	2:D:78:ARG:NH2	2.45	0.50
2:D:101:PHE:HE1	2:D:150:MET:HE3	1.76	0.50
1:A:286:ASP:OD1	4:A:502:A1D5V:NAP	2.45	0.49
1:A:224:TYR:HE1	1:A:266:SER:HG	1.60	0.49
1:C:264:TRP:HZ2	2:D:37:VAL:HG11	1.77	0.49
1:A:207:MET:CE	1:A:274:MET:HG3	2.43	0.49
1:A:223:PHE:CE2	1:A:279:TYR:CE1	3.01	0.49
2:B:93:GLU:OE2	2:B:95:ASN:ND2	2.26	0.49
1:C:207:MET:CE	1:C:274:MET:HG3	2.43	0.49
1:A:282:MET:CG	5:A:503:7PO:C23	2.91	0.49
1:C:109:VAL:O	1:C:112:ARG:HG2	2.12	0.49
1:C:223:PHE:CE2	1:C:279:TYR:CE1	3.01	0.49
1:A:326:LEU:CD1	1:A:361:ILE:HG21	2.42	0.49
1:C:173:ILE:HD12	1:C:297:TYR:HB3	1.95	0.49
1:C:147:ARG:NH1	1:C:234:GLN:OE1	2.42	0.48
1:A:109:VAL:O	1:A:112:ARG:HG2	2.12	0.48
1:C:109:VAL:HA	1:C:112:ARG:HE	1.78	0.48
1:A:173:ILE:HD12	1:A:297:TYR:HB3	1.95	0.48
2:D:47:ASN:HD21	3:D:201:6PL:H2	1.78	0.48
1:A:109:VAL:HA	1:A:112:ARG:HE	1.78	0.48
1:C:282:MET:CG	5:C:503:7PO:C23	2.91	0.48
2:D:101:PHE:CE1	2:D:150:MET:HE3	2.49	0.48
2:B:47:ASN:HD21	3:B:201:6PL:H2	1.78	0.48
1:A:357:VAL:O	1:A:361:ILE:HG12	2.14	0.48
2:D:86:LYS:O	2:D:90:ARG:HG2	2.14	0.48
2:B:86:LYS:O	2:B:90:ARG:HG2	2.14	0.47
2:B:101:PHE:CE1	2:B:150:MET:HE3	2.49	0.47
1:A:247:LYS:O	1:A:248:ASP:HB3	2.14	0.47
1:C:314:TRP:HH2	1:C:371:TRP:HE3	1.63	0.47
1:C:133:LEU:HD21	2:D:34:ILE:HD13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:MET:HE2	1:C:274:MET:HG3	1.96	0.47
1:C:224:TYR:HE1	1:C:266:SER:HG	1.60	0.47
1:C:279:TYR:O	1:C:281:THR:N	2.48	0.47
1:A:133:LEU:HD21	2:B:34:ILE:HD13	1.97	0.47
1:A:223:PHE:CE2	1:A:279:TYR:HE1	2.32	0.47
1:C:247:LYS:O	1:C:248:ASP:HB3	2.14	0.47
1:C:326:LEU:CD1	1:C:361:ILE:HG21	2.42	0.47
1:C:357:VAL:O	1:C:361:ILE:HG12	2.14	0.47
2:D:134:ASP:O	2:D:134:ASP:OD2	2.33	0.47
1:C:220:PHE:HE1	1:C:276:LEU:HB2	1.80	0.47
1:C:223:PHE:CE2	1:C:279:TYR:HE1	2.32	0.47
1:C:326:LEU:HD12	1:C:361:ILE:HG21	1.97	0.47
1:A:189:PHE:HD2	1:A:223:PHE:HD1	1.64	0.46
1:A:207:MET:HE2	1:A:274:MET:HG3	1.96	0.46
1:A:279:TYR:O	1:A:281:THR:N	2.48	0.46
1:A:106:LYS:HZ2	1:A:117:SER:HB3	1.79	0.46
1:A:334:ARG:HG3	1:A:339:TYR:CZ	2.51	0.46
1:C:103:ASN:ND2	1:C:107:THR:OG1	2.45	0.46
1:C:189:PHE:HD2	1:C:223:PHE:HD1	1.64	0.46
1:C:334:ARG:HG3	1:C:339:TYR:CZ	2.51	0.46
2:B:78:ARG:NH2	2:D:89:THR:O	2.47	0.46
2:B:134:ASP:O	2:B:134:ASP:OD2	2.33	0.46
1:A:147:ARG:NH1	1:A:234:GLN:OE1	2.42	0.46
1:A:220:PHE:HE1	1:A:276:LEU:HB2	1.81	0.46
1:A:314:TRP:HH2	1:A:371:TRP:HE3	1.63	0.46
1:C:106:LYS:HZ2	1:C:117:SER:HB3	1.80	0.46
1:A:326:LEU:HD12	1:A:361:ILE:HG21	1.97	0.46
1:A:173:ILE:HD11	1:A:298:LEU:CD1	2.46	0.45
1:A:289:LEU:HD12	1:A:310:PHE:CZ	2.52	0.45
1:A:289:LEU:HB2	1:A:310:PHE:CE1	2.51	0.45
1:C:223:PHE:HE2	1:C:279:TYR:CE1	2.34	0.45
1:C:204:THR:HB	1:C:328:SER:OG	2.16	0.45
1:A:233:GLN:HA	1:A:236:CYS:SG	2.56	0.45
1:A:329:VAL:O	1:A:333:PHE:CB	2.65	0.45
1:C:289:LEU:HB2	1:C:310:PHE:CE1	2.51	0.45
2:B:94:PRO:HA	2:B:97:GLU:O	2.16	0.45
1:C:289:LEU:HD12	1:C:310:PHE:CZ	2.52	0.45
2:B:150:MET:CG	2:D:78:ARG:HB3	2.46	0.45
1:C:333:PHE:HD2	1:C:354:LEU:HD12	1.82	0.45
1:A:223:PHE:HE2	1:A:279:TYR:CE1	2.34	0.45
2:B:150:MET:SD	2:D:78:ARG:HB3	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:LYS:NZ	1:C:117:SER:HB3	2.32	0.45
1:C:233:GLN:HA	1:C:236:CYS:SG	2.57	0.45
1:A:240:LEU:HD12	2:B:23:LEU:HD13	1.99	0.44
1:A:264:TRP:CZ2	2:B:37:VAL:HG11	2.53	0.44
2:D:94:PRO:HA	2:D:97:GLU:O	2.16	0.44
1:C:329:VAL:O	1:C:333:PHE:CB	2.65	0.44
1:C:173:ILE:HD11	1:C:298:LEU:CD1	2.46	0.44
1:C:279:TYR:HD2	5:C:503:7PO:C21	2.25	0.44
1:A:204:THR:HB	1:A:328:SER:OG	2.16	0.44
1:C:75:PHE:O	1:C:78:ILE:HG22	2.18	0.44
2:D:76:ASP:OD1	2:D:76:ASP:N	2.51	0.44
1:A:333:PHE:HD2	1:A:354:LEU:HD12	1.82	0.44
1:A:224:TYR:HE1	1:A:266:SER:OG	2.00	0.43
1:A:106:LYS:NZ	1:A:117:SER:HB3	2.32	0.43
1:A:144:THR:O	1:A:148:GLU:HG2	2.19	0.43
1:C:231:TRP:CZ2	5:C:503:7PO:C26	2.90	0.43
1:C:264:TRP:CZ2	2:D:37:VAL:HG11	2.52	0.43
2:B:60:GLN:HB2	2:B:64:VAL:HG23	2.01	0.43
1:C:144:THR:O	1:C:148:GLU:HG2	2.19	0.43
1:C:371:TRP:CZ3	4:C:502:A1D5V:CBG	3.01	0.43
1:A:75:PHE:O	1:A:78:ILE:HG22	2.18	0.43
2:B:89:THR:HB	2:D:82:LYS:HE3	2.01	0.43
2:B:78:ARG:HB3	2:D:150:MET:SD	2.59	0.43
1:A:282:MET:CB	5:A:503:7PO:C23	2.97	0.43
1:C:115:ALA:HA	3:C:501:6PL:H331	2.01	0.43
1:C:282:MET:CB	5:C:503:7PO:C23	2.97	0.43
1:A:289:LEU:HD11	4:A:502:A1D5V:CAZ	2.49	0.42
1:A:308:ALA:O	1:A:311:VAL:HG12	2.19	0.42
1:A:371:TRP:CZ3	4:A:502:A1D5V:CBG	3.01	0.42
1:C:240:LEU:HD12	2:D:23:LEU:HD13	2.00	0.42
1:C:289:LEU:HD11	4:C:502:A1D5V:CAZ	2.49	0.42
1:C:369:LEU:HA	1:C:372:LEU:HD23	2.01	0.42
1:C:224:TYR:HE1	1:C:266:SER:OG	2.00	0.42
1:A:103:ASN:ND2	1:A:107:THR:OG1	2.45	0.42
1:A:115:ALA:HA	3:A:501:6PL:H331	2.01	0.42
1:A:369:LEU:HA	1:A:372:LEU:HD23	2.01	0.42
1:C:308:ALA:O	1:C:311:VAL:HG12	2.19	0.42
1:A:173:ILE:HD11	1:A:298:LEU:HD12	2.02	0.42
1:A:279:TYR:HD2	5:A:503:7PO:C21	2.25	0.42
1:C:112:ARG:HD3	1:C:131:ASN:OD1	2.20	0.42
2:D:60:GLN:HB2	2:D:64:VAL:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:ILE:HD11	1:C:298:LEU:HD12	2.01	0.42
2:B:78:ARG:HB3	2:D:150:MET:CG	2.50	0.42
2:D:58:GLU:HB3	2:D:66:LYS:HB3	2.02	0.41
1:A:112:ARG:HD3	1:A:131:ASN:OD1	2.20	0.41
2:B:83:THR:HA	2:B:86:LYS:HG2	2.02	0.41
2:D:115:PRO:HD2	2:D:120:LYS:HA	2.02	0.41
1:A:333:PHE:CD2	1:A:354:LEU:HD12	2.55	0.41
1:C:85:ILE:O	1:C:89:MET:HG2	2.21	0.41
1:A:220:PHE:CD1	1:A:276:LEU:HD13	2.56	0.41
2:B:115:PRO:HD2	2:B:120:LYS:HA	2.03	0.41
1:A:96:SER:O	1:A:100:THR:HG23	2.20	0.41
2:B:57:LYS:NZ	2:B:91:ASP:OD2	2.30	0.41
2:B:58:GLU:HB3	2:B:66:LYS:HB3	2.02	0.41
1:C:247:LYS:O	1:C:248:ASP:CB	2.69	0.41
1:A:128:LYS:NZ	1:A:267:TYR:O	2.46	0.41
1:A:189:PHE:CD2	1:A:223:PHE:HD1	2.39	0.41
2:D:83:THR:HA	2:D:86:LYS:HG2	2.02	0.41
4:A:502:A1D5V:OAG	4:A:502:A1D5V:OAD	2.39	0.41
1:C:96:SER:O	1:C:100:THR:HG23	2.20	0.41
1:C:97:ALA:O	1:C:100:THR:OG1	2.38	0.41
1:C:120:ILE:O	1:C:123:THR:HG22	2.20	0.41
1:C:128:LYS:NZ	1:C:267:TYR:O	2.46	0.41
1:C:136:VAL:HG11	3:D:202:6PL:H421	2.03	0.41
1:C:189:PHE:CD2	1:C:223:PHE:HD1	2.39	0.41
3:D:201:6PL:H371	3:D:201:6PL:H402	1.88	0.41
1:A:136:VAL:HG11	3:B:202:6PL:H421	2.03	0.41
2:B:83:THR:HA	2:B:86:LYS:HE2	2.03	0.41
1:C:333:PHE:CD2	1:C:354:LEU:HD12	2.55	0.40
1:A:231:TRP:CZ2	5:A:503:7PO:C26	2.90	0.40
2:B:78:ARG:CD	2:D:94:PRO:HG3	2.46	0.40
1:A:85:ILE:O	1:A:89:MET:HG2	2.20	0.40
2:B:76:ASP:N	2:B:76:ASP:OD1	2.51	0.40
1:C:220:PHE:CD1	1:C:276:LEU:HD13	2.56	0.40
1:A:120:ILE:O	1:A:123:THR:HG22	2.20	0.40
1:A:220:PHE:CE1	1:A:276:LEU:HD13	2.57	0.40
1:A:247:LYS:O	1:A:248:ASP:CB	2.69	0.40
4:C:502:A1D5V:OAG	4:C:502:A1D5V:OAD	2.39	0.40
2:D:83:THR:HA	2:D:86:LYS:HE2	2.03	0.40
3:B:201:6PL:H371	3:B:201:6PL:H402	1.88	0.40
1:C:123:THR:OG1	1:C:124:ASN:N	2.55	0.40
1:C:316:TYR:O	1:C:320:TYR:HB3	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	313/428 (73%)	286 (91%)	27 (9%)	0	100	100
1	C	313/428 (73%)	286 (91%)	27 (9%)	0	100	100
2	B	131/150 (87%)	119 (91%)	12 (9%)	0	100	100
2	D	131/150 (87%)	119 (91%)	12 (9%)	0	100	100
All	All	888/1156 (77%)	810 (91%)	78 (9%)	0	100	100

There are no Ramachandran outliers to report.

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	279/391 (71%)	273 (98%)	6 (2%)	47	68
1	C	279/391 (71%)	273 (98%)	6 (2%)	47	68
2	B	120/135 (89%)	120 (100%)	0	100	100
2	D	120/135 (89%)	120 (100%)	0	100	100
All	All	798/1052 (76%)	786 (98%)	12 (2%)	60	78

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	169	ARG
1	A	224	TYR
1	A	247	LYS
1	A	279	TYR
1	A	326	LEU
1	A	377	ARG
1	C	169	ARG
1	C	224	TYR
1	C	247	LYS
1	C	279	TYR
1	C	326	LEU
1	C	377	ARG

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

Mol	Chain	Res	Type
1	A	249	HIS
1	A	332	GLN
1	C	249	HIS
1	C	332	GLN
1	C	342	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

10 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
4	A1D5V	C	502	-	49,49,49	2.09	10 (20%)	60,64,64	2.36	19 (31%)
3	6PL	D	201	-	39,39,51	1.38	5 (12%)	43,44,59	1.15	2 (4%)
3	6PL	B	202	-	17,17,51	0.63	0	16,16,59	0.93	0
3	6PL	D	202	-	17,17,51	0.63	0	16,16,59	0.93	0
4	A1D5V	A	502	-	49,49,49	2.09	11 (22%)	60,64,64	2.37	19 (31%)
5	7PO	A	503	-	25,25,27	0.46	0	24,24,27	1.52	3 (12%)
3	6PL	C	501	-	17,17,51	0.66	0	16,16,59	0.85	0
3	6PL	B	201	-	39,39,51	1.37	5 (12%)	43,44,59	1.16	2 (4%)
5	7PO	C	503	-	25,25,27	0.47	0	24,24,27	1.52	3 (12%)
3	6PL	A	501	-	17,17,51	0.66	0	16,16,59	0.85	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	A1D5V	C	502	-	-	37/67/67/67	-
3	6PL	D	201	-	-	17/41/41/55	-
3	6PL	B	202	-	-	6/15/15/55	-
3	6PL	D	202	-	-	6/15/15/55	-
4	A1D5V	A	502	-	-	37/67/67/67	-
5	7PO	A	503	-	-	10/23/23/25	-
3	6PL	C	501	-	-	7/15/15/55	-
3	6PL	B	201	-	-	17/41/41/55	-
5	7PO	C	503	-	-	10/23/23/25	-
3	6PL	A	501	-	-	7/15/15/55	-

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	502	A1D5V	CBM-CBQ	10.71	1.63	1.53
4	C	502	A1D5V	CBM-CBQ	10.70	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	201	6PL	O3-C11	3.90	1.44	1.33
3	B	201	6PL	O3-C11	3.88	1.44	1.33
4	A	502	A1D5V	CBJ-CBM	3.17	1.60	1.53
4	C	502	A1D5V	CBJ-CBM	3.17	1.60	1.53
3	D	201	6PL	P-O4P	3.07	1.66	1.54
3	B	201	6PL	O2-C31	3.06	1.42	1.34
3	D	201	6PL	O2-C31	3.05	1.42	1.34
3	B	201	6PL	P-O4P	3.04	1.66	1.54
3	B	201	6PL	O2-C2	-2.95	1.39	1.46
3	D	201	6PL	O2-C2	-2.93	1.39	1.46
4	A	502	A1D5V	CBD-CBC	2.70	1.66	1.51
4	C	502	A1D5V	CBD-CBC	2.68	1.66	1.51
3	D	201	6PL	P-O3P	2.59	1.68	1.60
4	C	502	A1D5V	CAR-CAQ	2.59	1.56	1.52
4	A	502	A1D5V	CAR-CAQ	2.56	1.56	1.52
3	B	201	6PL	P-O3P	2.55	1.68	1.60
4	C	502	A1D5V	CAV-CAX	2.39	1.58	1.52
4	A	502	A1D5V	CAV-CAX	2.35	1.58	1.52
4	A	502	A1D5V	OAC-CAX	-2.35	1.36	1.43
4	C	502	A1D5V	CBD-CBF	2.34	1.62	1.52
4	C	502	A1D5V	OAC-CAX	-2.31	1.36	1.43
4	A	502	A1D5V	CBD-CBF	2.31	1.62	1.52
4	C	502	A1D5V	CBL-CBP	-2.28	1.48	1.53
4	A	502	A1D5V	CBL-CBP	-2.23	1.48	1.53
4	C	502	A1D5V	OAI-CBV	-2.23	1.23	1.30
4	A	502	A1D5V	OAI-CBV	-2.22	1.23	1.30
4	A	502	A1D5V	CAT-CAQ	2.15	1.56	1.52
4	C	502	A1D5V	CAT-CAQ	2.15	1.56	1.52
4	A	502	A1D5V	OAHCUBU	-2.01	1.24	1.30

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	502	A1D5V	OAK-CBV-CBP	-7.72	104.04	122.93
4	A	502	A1D5V	OAK-CBV-CBP	-7.70	104.08	122.93
4	A	502	A1D5V	OAC-CAX-CAZ	-6.83	89.68	109.21
4	C	502	A1D5V	OAC-CAX-CAZ	-6.81	89.73	109.21
4	A	502	A1D5V	OAA-CBH-CBK	5.16	120.94	111.46
4	C	502	A1D5V	OAA-CBH-CBK	5.13	120.89	111.46
4	C	502	A1D5V	CAS-CAV-CAX	-4.51	107.83	115.59
4	A	502	A1D5V	CAS-CAV-CAX	-4.49	107.87	115.59
5	A	503	7PO	C19-C20-C21	-4.28	92.71	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	503	7PO	C19-C20-C21	-4.28	92.71	114.42
4	C	502	A1D5V	CBC-CBD-CBF	4.09	128.11	113.62
4	A	502	A1D5V	CBC-CBD-CBF	4.09	128.08	113.62
4	C	502	A1D5V	CAQ-OAA-CBH	4.06	125.73	117.83
4	A	502	A1D5V	CAQ-OAA-CBH	4.06	125.72	117.83
5	A	503	7PO	C18-C17-C16	-3.86	94.84	114.42
5	C	503	7PO	C18-C17-C16	-3.85	94.87	114.42
3	B	201	6PL	O2-C31-C32	3.74	119.57	111.50
3	D	201	6PL	O2-C31-C32	3.73	119.53	111.50
4	A	502	A1D5V	OAF-CBI-CBL	-3.62	116.74	124.73
4	C	502	A1D5V	OAF-CBI-CBL	-3.60	116.77	124.73
4	C	502	A1D5V	CAV-CAX-CAZ	3.32	119.65	112.51
4	A	502	A1D5V	CAV-CAX-CAZ	3.32	119.63	112.51
4	A	502	A1D5V	OAB-CBI-CBL	3.30	117.53	111.46
4	C	502	A1D5V	OAB-CBI-CBL	3.28	117.49	111.46
4	C	502	A1D5V	OAA-CAQ-CAT	3.11	112.87	107.10
4	A	502	A1D5V	OAA-CAQ-CAT	3.09	112.82	107.10
4	A	502	A1D5V	CBD-CBC-CAZ	-3.09	102.69	113.62
4	C	502	A1D5V	CBD-CBC-CAZ	-3.09	102.70	113.62
4	C	502	A1D5V	OAL-CBW-CBR	-2.81	113.79	122.80
4	A	502	A1D5V	OAL-CBW-CBR	-2.81	113.80	122.80
4	A	502	A1D5V	CBB-CAW-CAU	-2.80	106.99	115.03
4	C	502	A1D5V	CBB-CAW-CAU	-2.78	107.05	115.03
3	B	201	6PL	O3-C11-C12	2.71	120.40	111.91
5	A	503	7PO	C17-C16-C15	2.70	128.11	114.42
5	C	503	7PO	C17-C16-C15	2.69	128.10	114.42
4	C	502	A1D5V	OAI-CBV-CBP	2.68	121.22	114.21
3	D	201	6PL	O3-C11-C12	2.68	120.31	111.91
4	A	502	A1D5V	OAI-CBV-CBP	2.67	121.20	114.21
4	C	502	A1D5V	OAG-CBM-CBQ	2.52	113.95	109.44
4	A	502	A1D5V	OAG-CBM-CBQ	2.52	113.94	109.44
4	A	502	A1D5V	CBS-CBP-CBL	-2.36	106.21	111.80
4	C	502	A1D5V	CBS-CBP-CBL	-2.34	106.25	111.80
4	A	502	A1D5V	OAJ-CBU-CBO	-2.32	117.24	122.93
4	C	502	A1D5V	OAJ-CBU-CBO	-2.30	117.30	122.93
4	A	502	A1D5V	OAE-CBH-CBK	-2.26	119.74	124.73
4	C	502	A1D5V	OAE-CBH-CBK	-2.25	119.76	124.73
4	A	502	A1D5V	CAV-CAS-CAT	2.14	119.75	111.03
4	C	502	A1D5V	CAV-CAS-CAT	2.13	119.74	111.03

There are no chirality outliers.

All (154) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	502	A1D5V	CAT-CAQ-CAR-CAU
4	A	502	A1D5V	OAA-CAQ-CAT-CAS
4	A	502	A1D5V	CAQ-CAR-CAU-CBA
4	A	502	A1D5V	CAY-CAS-CAT-CAQ
4	A	502	A1D5V	CAS-CAV-CAX-OAC
4	A	502	A1D5V	CBF-CBG-CBJ-CBM
4	A	502	A1D5V	OAD-CBG-CBJ-CBM
4	A	502	A1D5V	CBL-CBI-OAB-CAR
4	A	502	A1D5V	OAF-CBI-OAB-CAR
4	A	502	A1D5V	CBG-CBJ-CBM-CBQ
4	A	502	A1D5V	CBG-CBJ-CBM-OAG
4	A	502	A1D5V	CBI-CBL-CBP-CBS
4	A	502	A1D5V	CBK-CBO-CBR-CBW
4	A	502	A1D5V	CBU-CBO-CBR-CBW
4	A	502	A1D5V	CBL-CBP-CBS-CBX
4	A	502	A1D5V	CBV-CBP-CBS-CBX
4	C	502	A1D5V	CAT-CAQ-CAR-CAU
4	C	502	A1D5V	OAA-CAQ-CAT-CAS
4	C	502	A1D5V	CAQ-CAR-CAU-CBA
4	C	502	A1D5V	CAY-CAS-CAT-CAQ
4	C	502	A1D5V	CAS-CAV-CAX-OAC
4	C	502	A1D5V	CBF-CBG-CBJ-CBM
4	C	502	A1D5V	OAD-CBG-CBJ-CBM
4	C	502	A1D5V	CBL-CBI-OAB-CAR
4	C	502	A1D5V	OAF-CBI-OAB-CAR
4	C	502	A1D5V	CBG-CBJ-CBM-CBQ
4	C	502	A1D5V	CBG-CBJ-CBM-OAG
4	C	502	A1D5V	CBI-CBL-CBP-CBS
4	C	502	A1D5V	CBK-CBO-CBR-CBW
4	C	502	A1D5V	CBU-CBO-CBR-CBW
4	C	502	A1D5V	CBL-CBP-CBS-CBX
4	C	502	A1D5V	CBV-CBP-CBS-CBX
3	B	201	6PL	O11-C11-O3-C3
3	D	201	6PL	O11-C11-O3-C3
3	B	201	6PL	C12-C11-O3-C3
3	D	201	6PL	C12-C11-O3-C3
5	A	503	7PO	C15-C16-C17-C18
4	A	502	A1D5V	CAR-CAQ-OAA-CBH
4	C	502	A1D5V	CAR-CAQ-OAA-CBH
5	C	503	7PO	C15-C16-C17-C18
4	A	502	A1D5V	CAU-CAW-CBB-CBE
4	C	502	A1D5V	CAU-CAW-CBB-CBE
4	A	502	A1D5V	CBA-CAU-CAW-CBB

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Mol	Chain	Res	Type	Atoms
4	C	502	A1D5V	CBA-CAU-CAW-CBB
5	C	503	7PO	C17-C18-C19-C20
5	A	503	7PO	C17-C18-C19-C20
4	A	502	A1D5V	CAS-CAV-CAX-CAZ
4	C	502	A1D5V	CAS-CAV-CAX-CAZ
3	B	201	6PL	C17-C18-C19-C20
3	D	201	6PL	C17-C18-C19-C20
3	B	201	6PL	C36-C37-C38-C39
3	D	201	6PL	C36-C37-C38-C39
3	D	202	6PL	C42-C43-C44-C45
3	B	202	6PL	C42-C43-C44-C45
3	B	201	6PL	C34-C35-C36-C37
3	B	202	6PL	C37-C38-C39-C40
3	D	201	6PL	C34-C35-C36-C37
3	D	202	6PL	C37-C38-C39-C40
5	A	503	7PO	C13-C14-C15-C16
5	C	503	7PO	C13-C14-C15-C16
3	B	201	6PL	C19-C20-C21-C22
3	D	201	6PL	C19-C20-C21-C22
4	A	502	A1D5V	CAU-CAR-OAB-CBI
4	C	502	A1D5V	CAU-CAR-OAB-CBI
5	A	503	7PO	C02-C03-C04-C05
5	C	503	7PO	C02-C03-C04-C05
5	A	503	7PO	C12-C13-C14-C15
5	C	503	7PO	C12-C13-C14-C15
3	A	501	6PL	C42-C43-C44-C45
3	C	501	6PL	C42-C43-C44-C45
4	A	502	A1D5V	OAA-CAQ-CAR-CAU
4	C	502	A1D5V	OAA-CAQ-CAR-CAU
3	B	201	6PL	C20-C21-C22-C23
3	D	201	6PL	C20-C21-C22-C23
3	B	202	6PL	C41-C42-C43-C44
3	D	202	6PL	C41-C42-C43-C44
3	A	501	6PL	C45-C46-C47-C48
3	C	501	6PL	C45-C46-C47-C48
3	B	201	6PL	C23-C24-C25-C26
3	D	201	6PL	C23-C24-C25-C26
3	B	201	6PL	C21-C22-C23-C24
3	B	201	6PL	C14-C15-C16-C17
3	D	201	6PL	C14-C15-C16-C17
3	D	201	6PL	C21-C22-C23-C24
4	A	502	A1D5V	CAT-CAQ-CAR-OAB

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Mol	Chain	Res	Type	Atoms
4	C	502	A1D5V	CAT-CAQ-CAR-OAB
3	B	201	6PL	O3P-C1-C2-O2
3	D	201	6PL	O3P-C1-C2-O2
3	B	201	6PL	C39-C40-C41-C42
3	D	201	6PL	C39-C40-C41-C42
3	B	201	6PL	O3P-C1-C2-C3
3	D	201	6PL	O3P-C1-C2-C3
3	C	501	6PL	C41-C42-C43-C44
3	A	501	6PL	C41-C42-C43-C44
4	A	502	A1D5V	OAA-CAQ-CAR-OAB
4	C	502	A1D5V	OAA-CAQ-CAR-OAB
5	C	503	7PO	C21-C22-C23-C24
5	A	503	7PO	C21-C22-C23-C24
4	A	502	A1D5V	CAX-CAZ-CBC-CBD
4	C	502	A1D5V	CAX-CAZ-CBC-CBD
4	A	502	A1D5V	CAT-CAQ-OAA-CBH
4	C	502	A1D5V	CAT-CAQ-OAA-CBH
3	A	501	6PL	C39-C40-C41-C42
3	C	501	6PL	C39-C40-C41-C42
3	B	202	6PL	C43-C44-C45-C46
3	D	202	6PL	C43-C44-C45-C46
5	A	503	7PO	C16-C17-C18-C19
5	C	503	7PO	C16-C17-C18-C19
3	B	202	6PL	C32-C33-C34-C35
3	D	202	6PL	C32-C33-C34-C35
4	A	502	A1D5V	CBI-CBL-CBP-CBV
4	C	502	A1D5V	CBI-CBL-CBP-CBV
5	A	503	7PO	C08-C09-C10-C11
5	C	503	7PO	C08-C09-C10-C11
4	A	502	A1D5V	CAR-CAU-CAW-CBB
4	C	502	A1D5V	CAR-CAU-CAW-CBB
3	B	201	6PL	C1-C2-C3-O3
3	D	201	6PL	C1-C2-C3-O3
3	B	201	6PL	O2-C2-C3-O3
3	D	201	6PL	O2-C2-C3-O3
4	A	502	A1D5V	CAQ-CAR-OAB-CBI
4	C	502	A1D5V	CAQ-CAR-OAB-CBI
4	A	502	A1D5V	CBP-CBS-CBX-OAO
4	C	502	A1D5V	CBP-CBS-CBX-OAO
4	A	502	A1D5V	OAB-CBI-CBL-CBP
4	C	502	A1D5V	OAB-CBI-CBL-CBP
4	C	502	A1D5V	CAW-CBB-CBE-CBN

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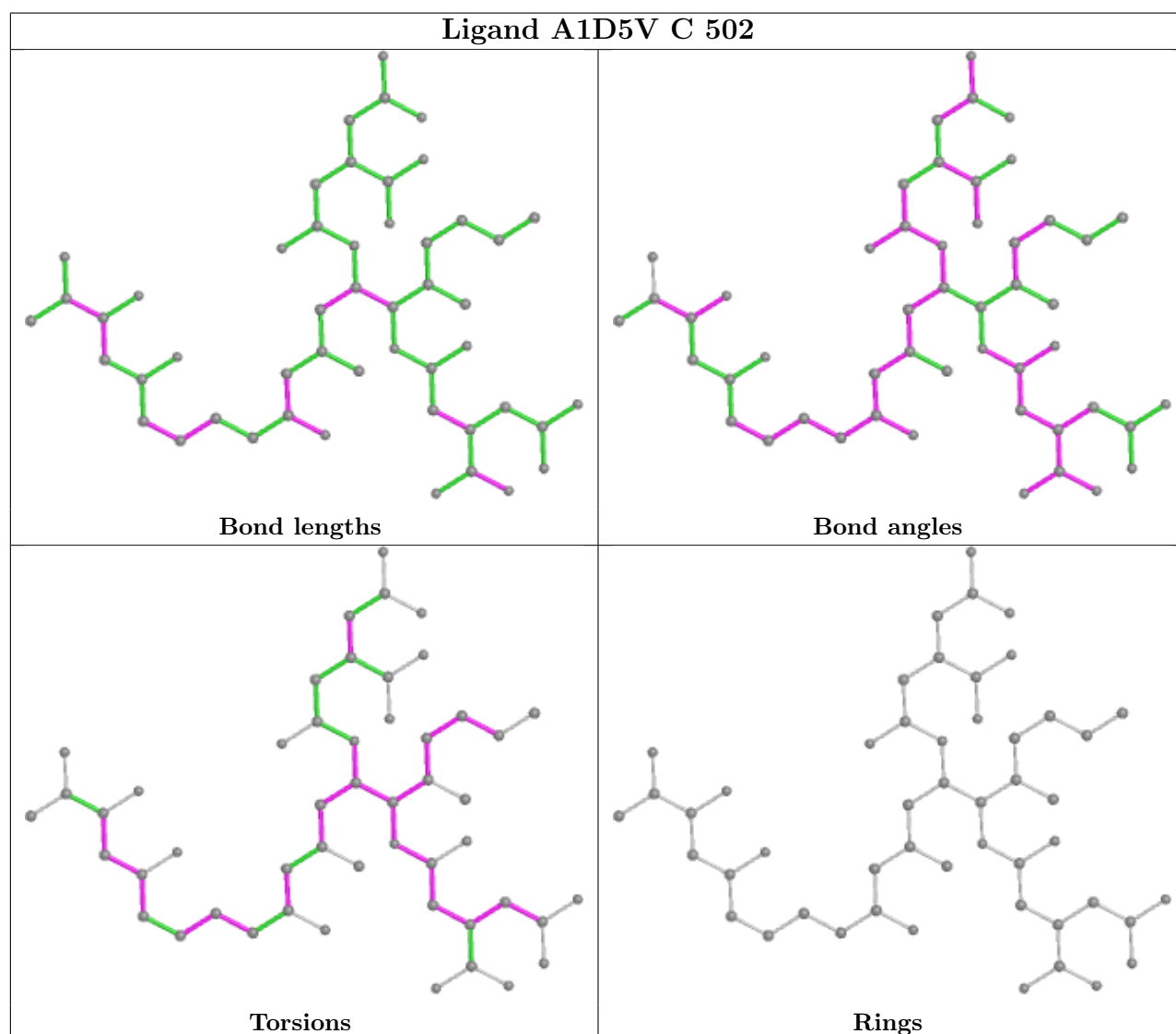
Mol	Chain	Res	Type	Atoms
4	A	502	A1D5V	CAW-CBB-CBE-CBN
3	B	202	6PL	C45-C46-C47-C48
3	D	202	6PL	C45-C46-C47-C48
3	A	501	6PL	C38-C39-C40-C41
3	C	501	6PL	C38-C39-C40-C41
4	A	502	A1D5V	OAF-CBI-CBL-CBP
4	C	502	A1D5V	OAF-CBI-CBL-CBP
5	A	503	7PO	C01-C02-C03-C04
5	C	503	7PO	C01-C02-C03-C04
4	A	502	A1D5V	CBD-CBF-CBG-CBJ
4	C	502	A1D5V	CBD-CBF-CBG-CBJ
3	A	501	6PL	C40-C41-C42-C43
3	C	501	6PL	C40-C41-C42-C43
3	D	201	6PL	C35-C36-C37-C38
5	A	503	7PO	C04-C05-C06-C07
3	B	201	6PL	C35-C36-C37-C38
5	C	503	7PO	C04-C05-C06-C07
4	A	502	A1D5V	CBP-CBS-CBX-OAM
4	C	502	A1D5V	CBP-CBS-CBX-OAM
4	A	502	A1D5V	CAZ-CBC-CBD-CBF
4	C	502	A1D5V	CAZ-CBC-CBD-CBF
3	B	201	6PL	C22-C23-C24-C25
3	D	201	6PL	C22-C23-C24-C25
4	A	502	A1D5V	OAB-CAR-CAU-CAW
4	C	502	A1D5V	OAB-CAR-CAU-CAW
3	A	501	6PL	C36-C37-C38-C39
3	C	501	6PL	C36-C37-C38-C39

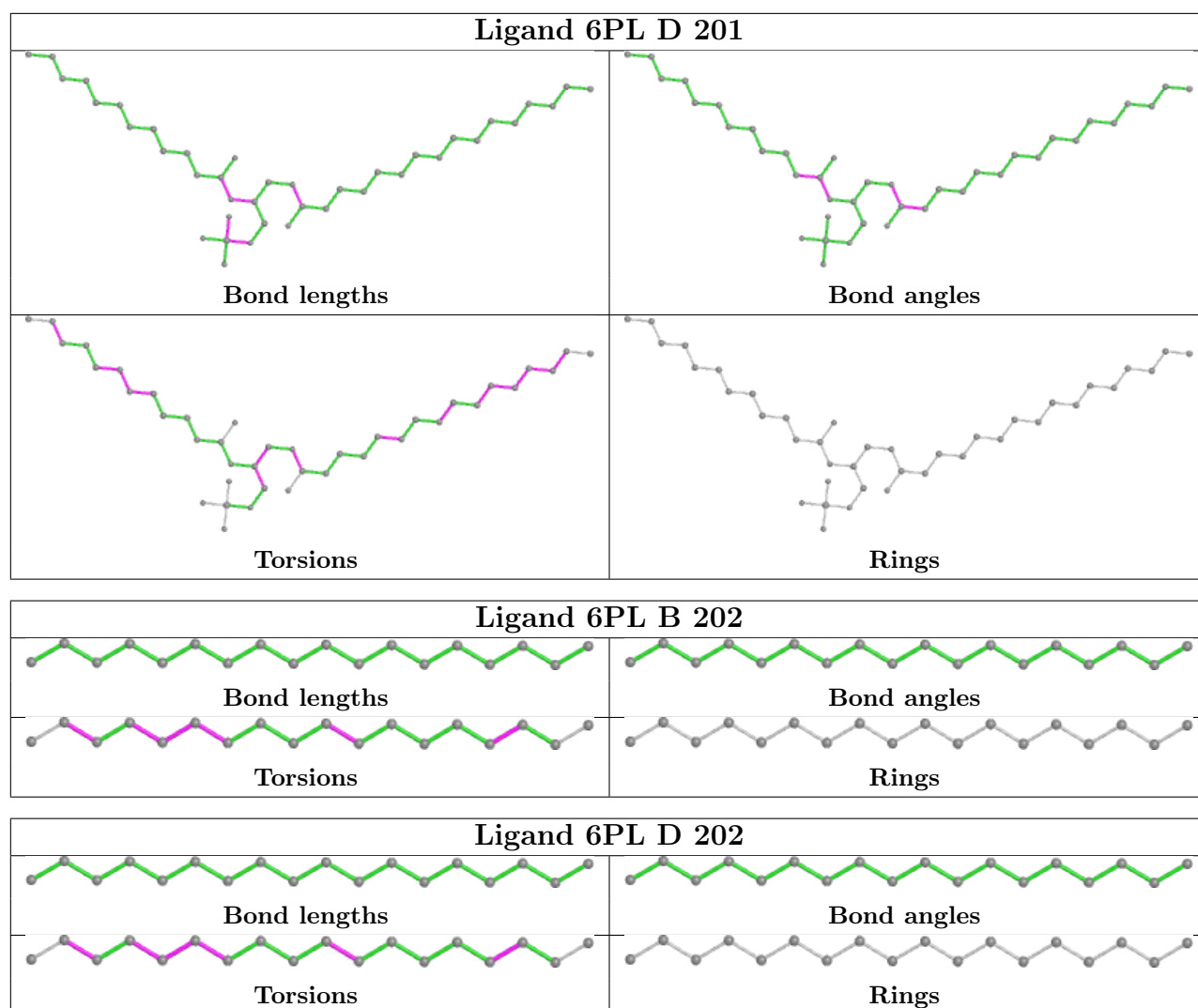
There are no ring outliers.

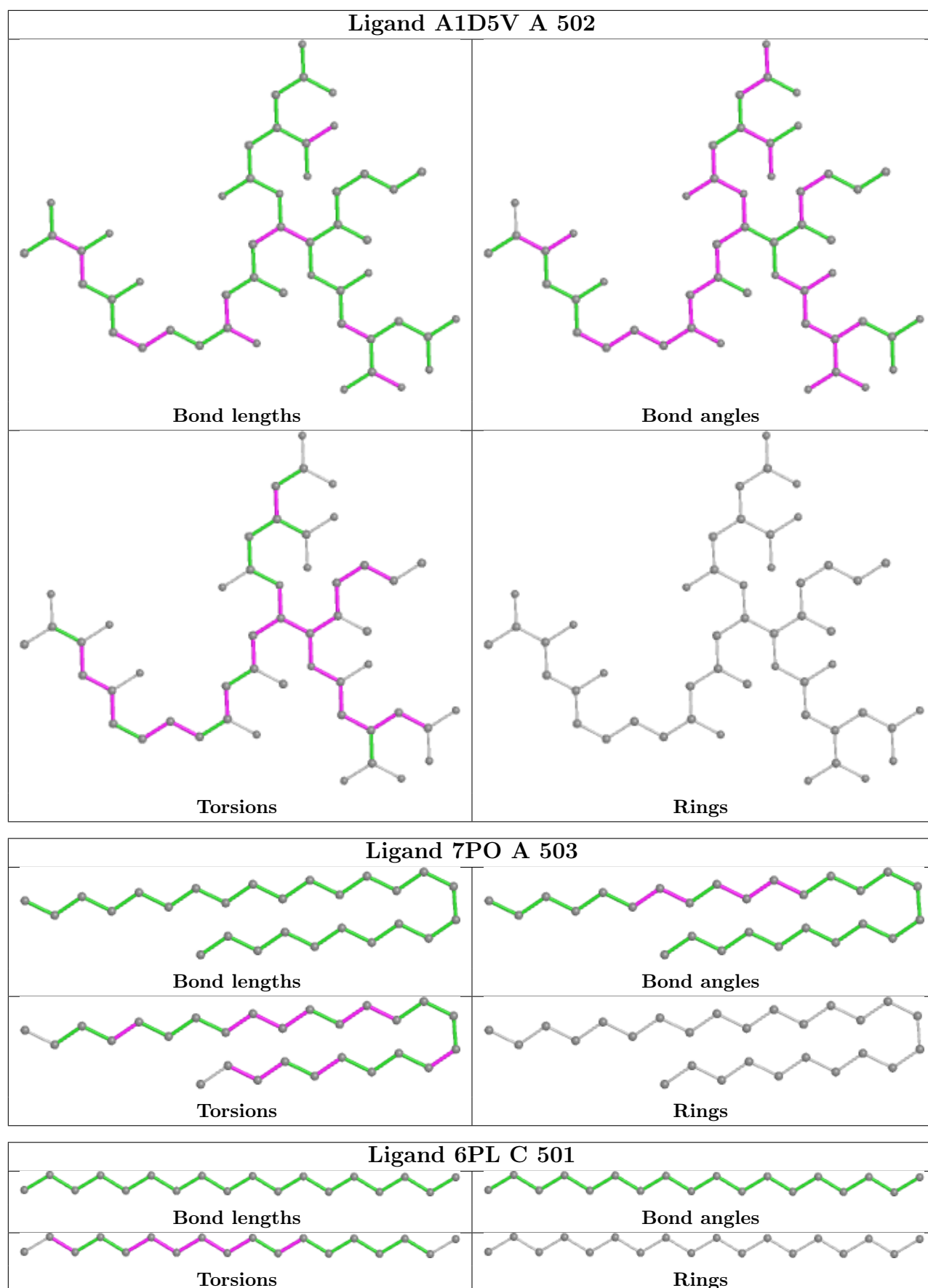
10 monomers are involved in 58 short contacts:

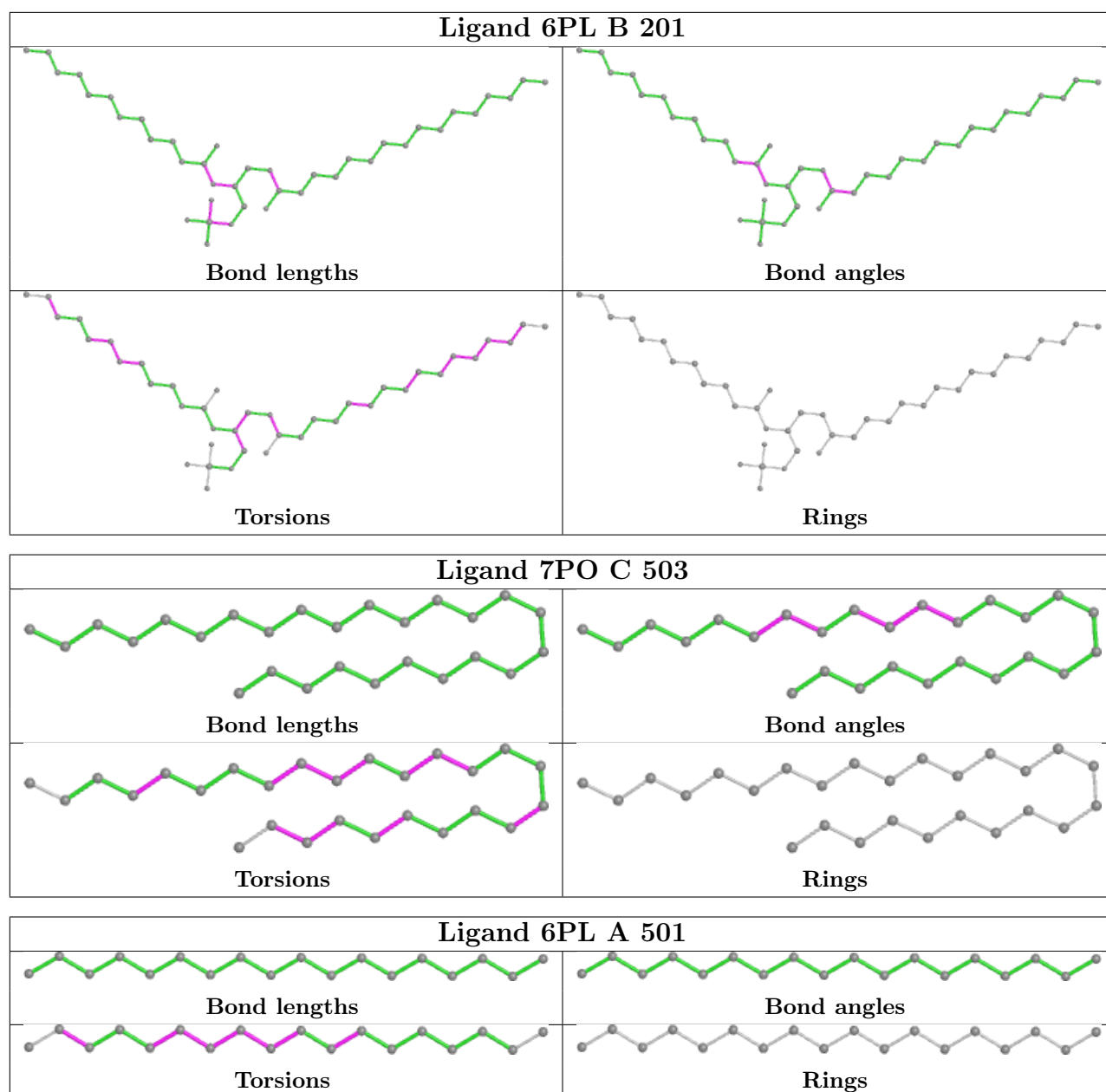
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	502	A1D5V	10	0
3	D	201	6PL	3	0
3	B	202	6PL	2	0
3	D	202	6PL	2	0
4	A	502	A1D5V	10	0
5	A	503	7PO	13	0
3	C	501	6PL	1	0
3	B	201	6PL	3	0
5	C	503	7PO	13	0
3	A	501	6PL	1	0

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









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.