



Full wwPDB EM Validation Report ⓘ

Apr 10, 2024 – 02:09 PM JST

PDB ID : 8K69
EMDB ID : EMD-36919
Title : Cryo-EM structure of *Oryza sativa* HKT2;2/1 at 2.3 angstrom
Authors : Wang, X.; Shen, X.; Qu, Y.; Wang, C.; Shen, H.
Deposited on : 2023-07-25
Resolution : 2.33 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 : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

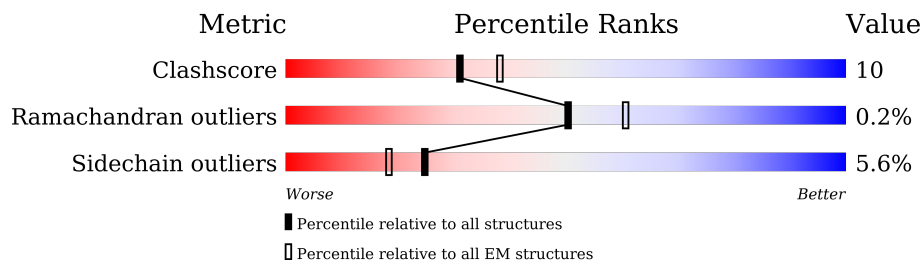
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.33 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	543	
1	B	543	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 7744 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 Cation transporter HKT2;2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	458	3577	2384	568	607	18	1	0
1	B	458	3577	2384	568	607	18	1	0

There are 44 discrepancies between the modelled and reference sequences:

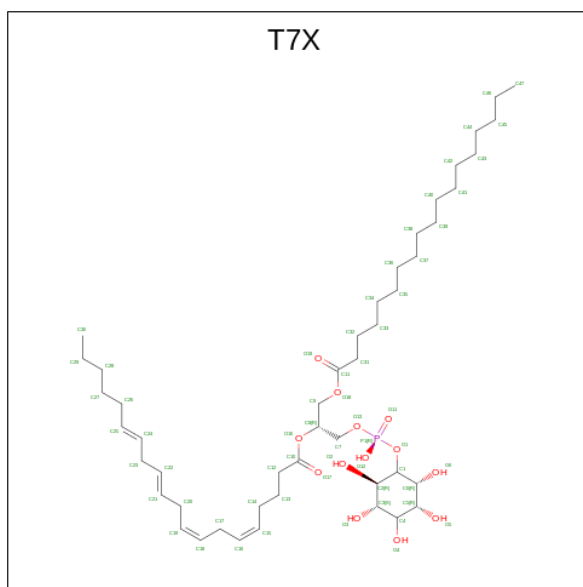
Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	MET	-	initiating methionine	UNP Q93XI5
A	-11	ALA	-	expression tag	UNP Q93XI5
A	-10	ASP	-	expression tag	UNP Q93XI5
A	-9	TYR	-	expression tag	UNP Q93XI5
A	-8	LYS	-	expression tag	UNP Q93XI5
A	-7	ASP	-	expression tag	UNP Q93XI5
A	-6	ASP	-	expression tag	UNP Q93XI5
A	-5	ASP	-	expression tag	UNP Q93XI5
A	-4	ASP	-	expression tag	UNP Q93XI5
A	-3	LYS	-	expression tag	UNP Q93XI5
A	-2	GLY	-	expression tag	UNP Q93XI5
A	-1	GLY	-	expression tag	UNP Q93XI5
A	0	ARG	-	expression tag	UNP Q93XI5
A	167	VAL	ALA	conflict	UNP Q93XI5
A	337	ALA	SER	conflict	UNP Q93XI5
A	420	GLN	ARG	conflict	UNP Q93XI5
A	430	ILE	ASN	conflict	UNP Q93XI5
A	431	SER	ALA	conflict	UNP Q93XI5
A	438	PHE	LEU	conflict	UNP Q93XI5
A	461	ILE	VAL	conflict	UNP Q93XI5
A	471	SER	THR	conflict	UNP Q93XI5
A	509	PHE	SER	conflict	UNP Q93XI5
B	-12	MET	-	initiating methionine	UNP Q93XI5
B	-11	ALA	-	expression tag	UNP Q93XI5
B	-10	ASP	-	expression tag	UNP Q93XI5
B	-9	TYR	-	expression tag	UNP Q93XI5

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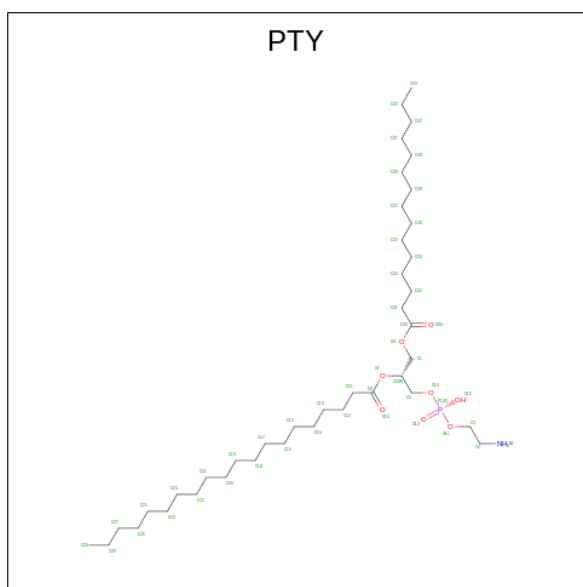
Mol	Chain	Residues	Atoms			AltConf
2	B	1	Total	C	O	0
			35	31	4	
2	B	1	Total	C	O	0
			35	31	4	

- Molecule 3 is Phosphatidylinositol (three-letter code: T7X) (formula: $C_{47}H_{83}O_{13}P$).



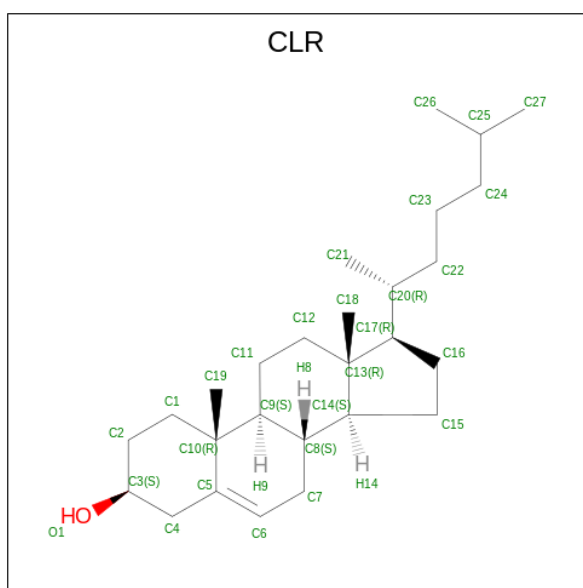
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	O	P	0
			46	32	13	1	
3	B	1	Total	C	O	P	0
			46	32	13	1	

- Molecule 4 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: $C_{40}H_{80}NO_8P$).



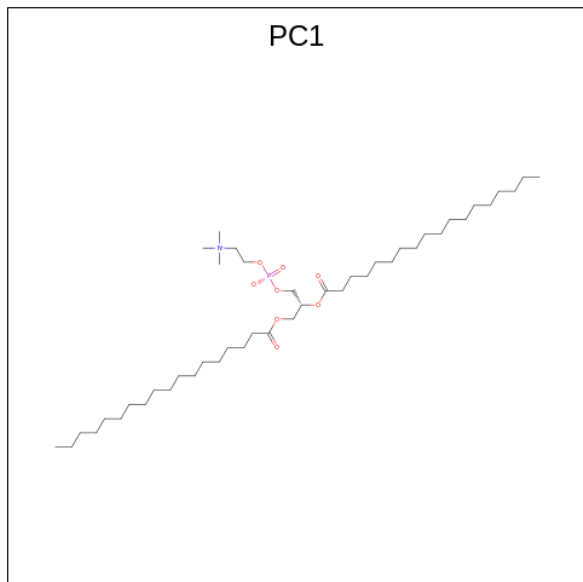
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
4	A	1	34	24	1	8	1	0
4	B	1	34	24	1	8	1	0

- Molecule 5 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
5	A	1	28	27	1	0
5	B	1	28	27	1	0

- Molecule 6 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
6	A	1	51	41	1	8	1	0
6	B	1	51	41	1	8	1	0

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
			Total	Na	
7	A	3	3	3	0
7	B	3	3	3	0

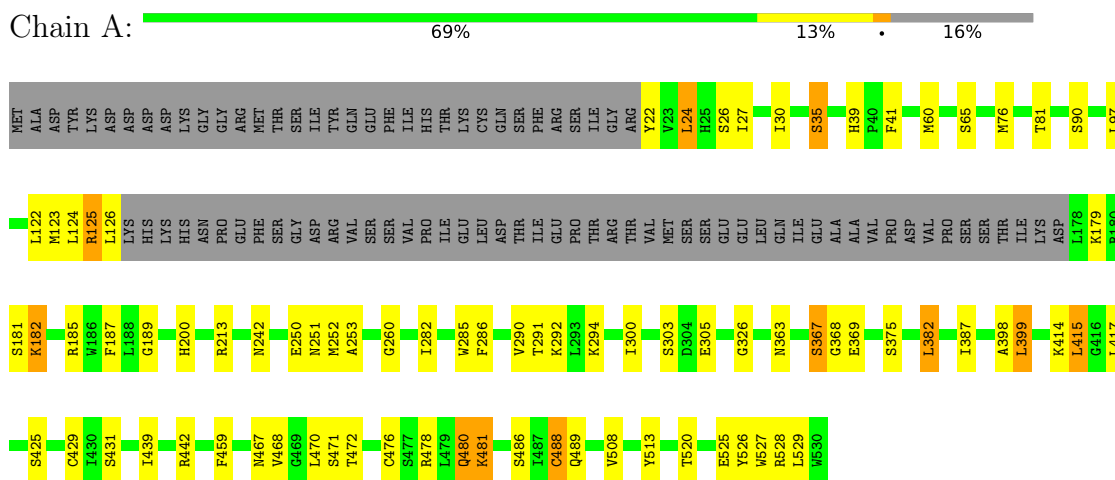
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
8	A	63	63	63	0
8	B	63	63	63	0

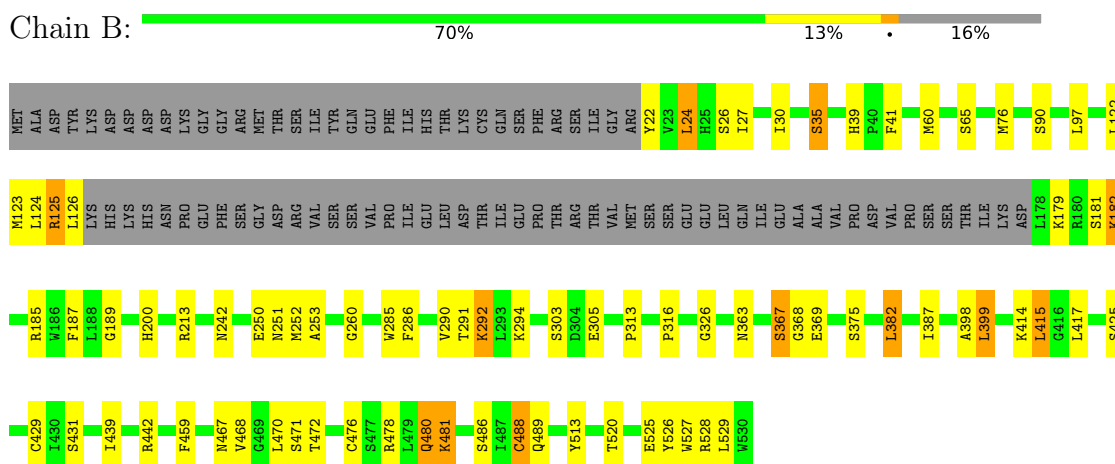
3 Residue-property plots

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: Cation transporter HKT2;2



- Molecule 1: Cation transporter HKT2;2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	639952	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PTY, CLR, NA, T7X, PC1, Y01

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	0.37	0/3667	0.49	0/4978
1	B	0.37	0/3667	0.48	0/4978
All	All	0.37	0/7334	0.49	0/9956

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3577	0	3711	70	0
1	B	3577	0	3711	67	0
2	A	70	0	98	13	0
2	B	70	0	98	13	0
3	A	46	0	0	1	0
3	B	46	0	0	1	0
4	A	34	0	41	1	0
4	B	34	0	41	1	0
5	A	28	0	46	9	0
5	B	28	0	46	5	0
6	A	51	0	76	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	51	0	76	7	0
7	A	3	0	0	0	0
7	B	3	0	0	0	0
8	A	63	0	0	6	0
8	B	63	0	0	6	0
All	All	7744	0	7944	151	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (151) 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:A:605:CLR:H212	5:A:605:CLR:H183	1.38	1.06
5:B:706:CLR:H212	5:B:706:CLR:H183	1.37	1.01
1:A:513:TYR:CE1	2:A:602:Y01:HAA1	1.96	1.00
1:B:513:TYR:CE1	2:B:703:Y01:HAA1	1.96	0.99
2:A:602:Y01:HAJ2	2:A:602:Y01:HAP1	1.55	0.88
1:B:478:ARG:HA	1:B:481:LYS:HE3	1.56	0.88
1:A:478:ARG:HA	1:A:481:LYS:HE3	1.56	0.88
2:B:703:Y01:HAP1	2:B:703:Y01:HAJ2	1.55	0.87
1:A:526:TYR:CE1	1:B:399:LEU:O	2.32	0.83
2:A:602:Y01:HAJ2	2:A:602:Y01:CAP	2.08	0.83
2:B:703:Y01:HAJ2	2:B:703:Y01:CAP	2.08	0.82
1:A:399:LEU:O	1:B:526:TYR:CE1	2.32	0.82
1:A:286:PHE:HB2	5:A:605:CLR:H263	1.66	0.76
1:B:200:HIS:HE1	8:B:833:HOH:O	1.72	0.72
5:B:706:CLR:H212	5:B:706:CLR:C18	2.19	0.72
1:A:200:HIS:HE1	8:A:732:HOH:O	1.72	0.72
1:B:467:ASN:O	8:B:801:HOH:O	2.08	0.72
5:A:605:CLR:H212	5:A:605:CLR:C18	2.20	0.71
1:B:513:TYR:CE1	2:B:703:Y01:CAA	2.73	0.70
1:A:467:ASN:O	8:A:701:HOH:O	2.08	0.70
1:A:200:HIS:CE1	8:A:732:HOH:O	2.45	0.69
1:A:513:TYR:CE1	2:A:602:Y01:CAA	2.73	0.69
1:B:200:HIS:CE1	8:B:833:HOH:O	2.45	0.68
1:A:242:ASN:O	8:A:701:HOH:O	2.14	0.66
1:A:282:ILE:CG2	5:A:605:CLR:H262	2.26	0.65
1:B:242:ASN:O	8:B:801:HOH:O	2.14	0.65
1:B:382:LEU:CD1	1:B:459:PHE:CD2	2.81	0.63
1:A:382:LEU:CD1	1:A:459:PHE:CD2	2.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:GLY:HA3	1:B:468:VAL:O	1.99	0.63
1:B:286:PHE:HB2	5:B:706:CLR:H263	1.80	0.62
1:A:368:GLY:HA3	1:A:468:VAL:O	1.99	0.62
5:A:605:CLR:H183	5:A:605:CLR:C21	2.24	0.61
1:A:480:GLN:NE2	1:A:486:SER:O	2.35	0.60
1:B:480:GLN:NE2	1:B:486:SER:O	2.35	0.60
1:A:417:LEU:HD13	2:A:602:Y01:OAG	2.02	0.60
1:B:417:LEU:HD13	2:B:703:Y01:OAG	2.02	0.60
1:A:425:SER:HB3	6:A:606:PC1:H112	1.84	0.59
1:B:382:LEU:HD11	1:B:459:PHE:CD2	2.38	0.59
1:B:425:SER:HB3	6:B:701:PC1:H112	1.85	0.59
1:A:382:LEU:HD11	1:A:459:PHE:CD2	2.38	0.58
1:A:363:ASN:HA	1:A:367:SER:OG	2.04	0.58
6:A:606:PC1:H391	1:B:326:GLY:HA3	1.86	0.58
5:B:706:CLR:H183	5:B:706:CLR:C21	2.22	0.58
1:B:363:ASN:HA	1:B:367:SER:OG	2.04	0.57
1:A:382:LEU:HD13	1:A:459:PHE:CD2	2.40	0.57
1:B:382:LEU:HD13	1:B:459:PHE:CD2	2.40	0.57
1:A:326:GLY:HA3	6:B:701:PC1:H391	1.86	0.56
1:A:526:TYR:CD1	1:B:399:LEU:O	2.59	0.56
1:A:399:LEU:O	1:B:526:TYR:CD1	2.60	0.54
1:B:125:ARG:HG2	1:B:185:ARG:NH1	2.22	0.54
1:A:125:ARG:HG2	1:A:185:ARG:NH1	2.22	0.54
1:B:513:TYR:CD1	2:B:703:Y01:HAA1	2.42	0.54
1:A:282:ILE:HG22	5:A:605:CLR:H262	1.89	0.53
1:B:529:LEU:HD11	6:B:701:PC1:H2	1.91	0.53
1:A:90:SER:HB3	8:A:751:HOH:O	2.10	0.52
1:B:90:SER:HB3	8:B:851:HOH:O	2.10	0.52
1:B:250:GLU:HB3	1:B:253:ALA:HB3	1.92	0.52
1:A:513:TYR:CD1	2:A:602:Y01:HAA1	2.42	0.51
1:A:529:LEU:HD11	6:A:606:PC1:H2	1.91	0.51
1:B:382:LEU:HD13	1:B:459:PHE:HD2	1.75	0.51
1:A:250:GLU:HB3	1:A:253:ALA:HB3	1.92	0.51
1:A:382:LEU:HD13	1:A:459:PHE:HD2	1.75	0.51
1:B:39:HIS:CD2	1:B:41:PHE:H	2.28	0.51
1:B:527:TRP:CG	6:B:701:PC1:H332	2.46	0.50
1:A:39:HIS:CD2	1:A:41:PHE:H	2.28	0.50
1:A:527:TRP:CG	6:A:606:PC1:H332	2.47	0.50
1:A:125:ARG:HG2	1:A:185:ARG:HH11	1.77	0.50
1:A:286:PHE:CB	5:A:605:CLR:H263	2.37	0.49
1:A:363:ASN:OD1	1:A:369:GLU:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:439:ILE:O	1:B:442:ARG:NH1	2.37	0.49
1:B:122:LEU:HA	1:B:125:ARG:HD3	1.95	0.49
1:B:363:ASN:OD1	1:B:369:GLU:HB2	2.13	0.48
1:A:471:SER:HB3	8:A:758:HOH:O	2.13	0.48
1:B:471:SER:HB3	8:B:858:HOH:O	2.13	0.48
1:B:125:ARG:HG2	1:B:185:ARG:HH11	1.77	0.48
1:A:122:LEU:HA	1:A:125:ARG:HD3	1.95	0.48
5:A:605:CLR:C18	5:A:605:CLR:C21	2.90	0.48
1:B:520:THR:HG22	2:B:703:Y01:HAQ2	1.96	0.48
1:A:439:ILE:O	1:A:442:ARG:NH1	2.37	0.47
6:A:606:PC1:H321	6:A:606:PC1:H32	1.43	0.47
1:A:60:MET:SD	1:A:76:MET:HG3	2.54	0.47
1:A:260:GLY:N	3:A:603:T7X:O11	2.38	0.47
1:A:387:ILE:HD11	1:B:431:SER:HB2	1.97	0.47
2:A:602:Y01:HAP1	2:A:602:Y01:CAJ	2.37	0.47
1:B:65:SER:HB2	1:B:97:LEU:C	2.35	0.47
1:B:35:SER:HB3	1:B:126:LEU:HD12	1.97	0.47
1:A:65:SER:HB2	1:A:97:LEU:C	2.35	0.47
1:A:24:LEU:HD13	1:A:24:LEU:HA	1.76	0.47
1:A:520:THR:HG22	2:A:602:Y01:HAQ2	1.96	0.47
1:A:429:CYS:SG	2:A:602:Y01:HAA3	2.55	0.47
1:A:290:VAL:HG23	1:A:291:THR:HG23	1.96	0.46
1:B:286:PHE:CB	5:B:706:CLR:H263	2.45	0.46
1:B:527:TRP:CE3	6:B:701:PC1:H341	2.51	0.46
1:B:123:MET:HA	1:B:123:MET:HE2	1.97	0.46
1:B:290:VAL:HG23	1:B:291:THR:HG23	1.96	0.46
1:B:429:CYS:SG	2:B:703:Y01:HAA3	2.55	0.46
1:B:60:MET:SD	1:B:76:MET:HG3	2.54	0.46
1:A:35:SER:HB3	1:A:126:LEU:HD12	1.97	0.46
1:A:123:MET:HA	1:A:123:MET:HE2	1.98	0.46
6:B:701:PC1:H32	6:B:701:PC1:H321	1.43	0.46
1:A:431:SER:HB2	1:B:387:ILE:HD11	1.97	0.46
1:B:399:LEU:HA	1:B:399:LEU:HD12	1.59	0.46
1:A:527:TRP:CE3	6:A:606:PC1:H341	2.51	0.45
1:A:417:LEU:HD12	1:A:417:LEU:HA	1.82	0.45
1:B:39:HIS:HD2	1:B:41:PHE:H	1.63	0.45
1:A:476:CYS:SG	1:A:488[B]:CYS:HB2	2.57	0.45
4:B:705:PTY:H142	4:B:705:PTY:H172	1.73	0.45
1:B:294:LYS:HB3	1:B:294:LYS:HE3	1.68	0.45
1:A:382:LEU:CD1	1:A:459:PHE:HD2	2.30	0.44
1:B:375:SER:HB3	1:B:472:THR:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:LYS:HB3	1:A:294:LYS:HE3	1.68	0.44
1:A:375:SER:HB3	1:A:472:THR:O	2.17	0.44
1:B:65:SER:HB2	1:B:97:LEU:O	2.17	0.44
2:A:601:Y01:HAA1	2:A:601:Y01:HAJ2	1.81	0.44
1:B:476:CYS:SG	1:B:488[B]:CYS:HB2	2.57	0.44
1:A:65:SER:HB2	1:A:97:LEU:O	2.17	0.44
1:A:368:GLY:HA2	1:A:470:LEU:HG	2.00	0.44
1:A:39:HIS:HD2	1:A:41:PHE:H	1.63	0.43
1:A:398:ALA:HB3	1:B:528:ARG:HE	1.84	0.43
2:A:602:Y01:HAJ2	2:A:602:Y01:HAP2	1.97	0.43
1:A:213:ARG:HD3	1:A:213:ARG:HA	1.79	0.43
1:A:81:THR:HG21	1:A:508:VAL:HG13	2.00	0.43
1:A:528:ARG:HE	1:B:398:ALA:HB3	1.84	0.43
1:B:213:ARG:HA	1:B:213:ARG:HD3	1.79	0.43
1:B:382:LEU:HD22	1:B:382:LEU:HA	1.79	0.43
2:B:702:Y01:HAC1	2:B:702:Y01:HAU2	2.00	0.43
2:A:601:Y01:HAC1	2:A:601:Y01:HAU2	2.00	0.43
1:B:292:LYS:HB2	1:B:292:LYS:HE2	1.79	0.43
1:A:251:ASN:HD22	1:A:252:MET:H	1.66	0.43
4:A:604:PTY:H142	4:A:604:PTY:H172	1.73	0.43
1:B:285:TRP:CD1	2:B:702:Y01:HAL1	2.54	0.43
1:A:123:MET:HE1	1:A:189:GLY:HA3	2.01	0.42
1:B:24:LEU:HD13	1:B:24:LEU:HA	1.76	0.42
1:B:251:ASN:HD22	1:B:252:MET:H	1.66	0.42
1:B:368:GLY:HA2	1:B:470:LEU:HG	2.00	0.42
1:A:182:LYS:HD3	1:A:185:ARG:HE	1.85	0.42
2:B:703:Y01:HAJ2	2:B:703:Y01:HAP2	1.97	0.42
1:A:27:ILE:HA	1:A:30:ILE:HD12	2.02	0.42
1:B:417:LEU:CD1	2:B:703:Y01:OAG	2.68	0.41
1:A:282:ILE:HG23	5:A:605:CLR:H262	2.01	0.41
1:B:123:MET:HE1	1:B:189:GLY:HA3	2.02	0.41
1:A:285:TRP:CD1	2:A:601:Y01:HAL1	2.54	0.41
1:B:525:GLU:OE1	6:B:701:PC1:H131	2.21	0.41
1:B:182:LYS:HD3	1:B:185:ARG:HE	1.85	0.41
2:B:702:Y01:HAA1	2:B:702:Y01:HAJ2	1.81	0.41
1:B:313:PRO:HB2	1:B:316:PRO:HD2	2.03	0.41
1:A:300:ILE:HD13	1:A:300:ILE:HA	1.88	0.40
1:A:382:LEU:HD22	1:A:382:LEU:HA	1.79	0.40
1:B:27:ILE:HA	1:B:30:ILE:HD12	2.02	0.40
1:A:525:GLU:OE1	6:A:606:PC1:H131	2.22	0.40
1:B:260:GLY:N	3:B:704:T7X:O11	2.38	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	455/543 (84%)	441 (97%)	13 (3%)	1 (0%)	47	55
1	B	455/543 (84%)	441 (97%)	13 (3%)	1 (0%)	47	55
All	All	910/1086 (84%)	882 (97%)	26 (3%)	2 (0%)	50	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	415	LEU
1	B	415	LEU

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	393/481 (82%)	370 (94%)	23 (6%)	19	22
1	B	393/481 (82%)	370 (94%)	23 (6%)	19	22
All	All	786/962 (82%)	740 (94%)	46 (6%)	25	22

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	TYR

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Mol	Chain	Res	Type
1	A	24	LEU
1	A	26	SER
1	A	35	SER
1	A	124	LEU
1	A	125	ARG
1	A	179	LYS
1	A	181	SER
1	A	182	LYS
1	A	187	PHE
1	A	292	LYS
1	A	303	SER
1	A	305	GLU
1	A	367	SER
1	A	382	LEU
1	A	399	LEU
1	A	414	LYS
1	A	415	LEU
1	A	480	GLN
1	A	481	LYS
1	A	488[A]	CYS
1	A	488[B]	CYS
1	A	489	GLN
1	B	22	TYR
1	B	24	LEU
1	B	26	SER
1	B	35	SER
1	B	124	LEU
1	B	125	ARG
1	B	179	LYS
1	B	181	SER
1	B	182	LYS
1	B	187	PHE
1	B	292	LYS
1	B	303	SER
1	B	305	GLU
1	B	367	SER
1	B	382	LEU
1	B	399	LEU
1	B	414	LYS
1	B	415	LEU
1	B	480	GLN
1	B	481	LYS

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Mol	Chain	Res	Type
1	B	488[A]	CYS
1	B	488[B]	CYS
1	B	489	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	200	HIS
1	A	251	ASN
1	A	420	GLN
1	A	421	ASN
1	A	483	HIS
1	A	489	GLN
1	B	39	HIS
1	B	200	HIS
1	B	251	ASN
1	B	420	GLN
1	B	421	ASN
1	B	483	HIS
1	B	489	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	Y01	B	702	-	38,38,38	0.80	1 (2%)	57,57,57	1.30	8 (14%)
2	Y01	A	601	-	38,38,38	0.80	1 (2%)	57,57,57	1.29	8 (14%)
3	T7X	A	603	-	46,46,61	0.28	0	56,58,73	0.38	0
2	Y01	B	703	-	38,38,38	0.45	0	57,57,57	0.45	0
5	CLR	A	605	-	31,31,31	0.28	0	48,48,48	0.35	0
4	PTY	A	604	-	33,33,49	0.32	0	36,38,54	0.36	0
3	T7X	B	704	-	46,46,61	0.28	0	56,58,73	0.38	0
2	Y01	A	602	-	38,38,38	0.45	0	57,57,57	0.45	0
6	PC1	B	701	-	50,50,53	0.47	0	56,58,61	0.32	0
5	CLR	B	706	-	31,31,31	0.29	0	48,48,48	0.35	0
4	PTY	B	705	-	33,33,49	0.32	0	36,38,54	0.36	0
6	PC1	A	606	-	50,50,53	0.47	0	56,58,61	0.32	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
2	Y01	B	702	-	-	4/19/77/77	0/4/4/4
2	Y01	A	601	-	-	4/19/77/77	0/4/4/4
3	T7X	A	603	-	-	18/41/65/80	0/1/1/1
2	Y01	B	703	-	-	11/19/77/77	0/4/4/4
5	CLR	A	605	-	-	9/10/68/68	0/4/4/4
4	PTY	A	604	-	-	16/37/37/53	-
3	T7X	B	704	-	-	18/41/65/80	0/1/1/1
2	Y01	A	602	-	-	11/19/77/77	0/4/4/4
6	PC1	B	701	-	-	33/54/54/57	-
5	CLR	B	706	-	-	9/10/68/68	0/4/4/4
4	PTY	B	705	-	-	16/37/37/53	-
6	PC1	A	606	-	-	33/54/54/57	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	Y01	OAW-CBC	-2.27	1.40	1.46
2	B	702	Y01	OAW-CBC	-2.27	1.40	1.46

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	Y01	CBI-CBE-CBB	-3.41	114.15	119.49
2	B	702	Y01	CBI-CBE-CBB	-3.41	114.15	119.49
2	A	601	Y01	CBH-CBF-CBD	-2.85	108.45	112.73
2	B	702	Y01	CBH-CBF-CBD	-2.85	108.45	112.73
2	A	601	Y01	CAJ-CAO-CBB	-2.57	107.65	115.03
2	B	702	Y01	CAJ-CAO-CBB	-2.57	107.65	115.03
2	A	601	Y01	CAS-CAU-CBI	-2.53	108.45	112.78
2	B	702	Y01	CAS-CAU-CBI	-2.53	108.45	112.78
2	A	601	Y01	OAW-CAY-OAG	-2.46	117.75	123.70
2	B	702	Y01	OAW-CAY-OAG	-2.46	117.75	123.70
2	A	601	Y01	CBI-CBG-CBD	-2.26	111.03	114.38
2	B	702	Y01	CBI-CBG-CBD	-2.26	111.03	114.38
2	A	601	Y01	CAS-CBF-CBH	-2.10	110.31	113.08
2	B	702	Y01	CAS-CBF-CBH	-2.10	110.31	113.08
2	A	601	Y01	OAW-CAY-CAM	2.08	115.99	111.50
2	B	702	Y01	OAW-CAY-CAM	2.08	115.99	111.50

There are no chirality outliers.

All (182) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	603	T7X	C1-O1-P1-O12
3	A	603	T7X	C7-O13-P1-O12
3	A	603	T7X	C16-C17-C18-C19
3	B	704	T7X	C1-O1-P1-O12
3	B	704	T7X	C7-O13-P1-O12
3	B	704	T7X	C16-C17-C18-C19
4	A	604	PTY	N1-C2-C3-O11
4	B	705	PTY	N1-C2-C3-O11
5	A	605	CLR	C16-C17-C20-C22
5	B	706	CLR	C16-C17-C20-C22
6	A	606	PC1	O13-C11-C12-N
6	A	606	PC1	C32-C31-O31-C3
6	B	701	PC1	O13-C11-C12-N
6	B	701	PC1	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
6	A	606	PC1	O32-C31-O31-C3
6	B	701	PC1	O32-C31-O31-C3
5	A	605	CLR	C16-C17-C20-C21
5	B	706	CLR	C16-C17-C20-C21
5	A	605	CLR	C13-C17-C20-C21
5	B	706	CLR	C13-C17-C20-C21
5	B	706	CLR	C13-C17-C20-C22
5	A	605	CLR	C13-C17-C20-C22
6	A	606	PC1	C2B-C2C-C2D-C2E
6	B	701	PC1	C2B-C2C-C2D-C2E
4	A	604	PTY	C14-C15-C16-C17
4	B	705	PTY	C14-C15-C16-C17
5	B	706	CLR	C17-C20-C22-C23
2	A	602	Y01	CAM-CAY-OAW-CBC
2	B	703	Y01	CAM-CAY-OAW-CBC
3	A	603	T7X	C31-C11-O18-C9
3	B	704	T7X	C31-C11-O18-C9
5	A	605	CLR	C17-C20-C22-C23
5	A	605	CLR	C21-C20-C22-C23
5	B	706	CLR	C21-C20-C22-C23
3	A	603	T7X	O19-C11-O18-C9
3	B	704	T7X	O19-C11-O18-C9
3	A	603	T7X	C10-C12-C13-C14
3	B	704	T7X	C10-C12-C13-C14
4	A	604	PTY	C8-C11-C12-C13
4	B	705	PTY	C8-C11-C12-C13
6	A	606	PC1	C21-C22-C23-C24
6	B	701	PC1	C21-C22-C23-C24
2	A	602	Y01	OAG-CAY-OAW-CBC
2	B	703	Y01	OAG-CAY-OAW-CBC
3	A	603	T7X	C7-O13-P1-O1
3	B	704	T7X	C7-O13-P1-O1
6	A	606	PC1	C1-O11-P-O13
6	B	701	PC1	C1-O11-P-O13
4	B	705	PTY	C31-C30-O4-C1
2	A	602	Y01	CAX-CAL-CAM-CAY
2	B	703	Y01	CAX-CAL-CAM-CAY
6	A	606	PC1	C27-C28-C29-C2A
6	B	701	PC1	C27-C28-C29-C2A
5	B	706	CLR	C23-C24-C25-C26
4	A	604	PTY	C31-C30-O4-C1
3	A	603	T7X	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
3	B	704	T7X	C32-C33-C34-C35
4	A	604	PTY	C15-C16-C17-C18
4	B	705	PTY	C15-C16-C17-C18
6	A	606	PC1	C3B-C3C-C3D-C3E
6	B	701	PC1	C3B-C3C-C3D-C3E
2	A	602	Y01	CAJ-CAN-CBA-CAB
2	B	703	Y01	CAJ-CAN-CBA-CAB
5	A	605	CLR	C23-C24-C25-C26
5	A	605	CLR	C23-C24-C25-C27
4	A	604	PTY	C11-C12-C13-C14
4	B	705	PTY	C11-C12-C13-C14
5	B	706	CLR	C23-C24-C25-C27
3	A	603	T7X	C17-C18-C19-C20
3	B	704	T7X	C17-C18-C19-C20
4	A	604	PTY	C32-C33-C34-C35
4	A	604	PTY	C34-C35-C36-C37
4	B	705	PTY	C32-C33-C34-C35
4	B	705	PTY	C34-C35-C36-C37
4	A	604	PTY	O30-C30-O4-C1
4	B	705	PTY	O30-C30-O4-C1
6	A	606	PC1	C3C-C3D-C3E-C3F
6	B	701	PC1	C3C-C3D-C3E-C3F
6	A	606	PC1	C2A-C2B-C2C-C2D
6	B	701	PC1	C2A-C2B-C2C-C2D
4	A	604	PTY	C31-C32-C33-C34
4	B	705	PTY	C31-C32-C33-C34
6	A	606	PC1	C23-C24-C25-C26
6	B	701	PC1	C23-C24-C25-C26
6	A	606	PC1	C32-C33-C34-C35
6	B	701	PC1	C32-C33-C34-C35
3	A	603	T7X	C14-C15-C16-C17
3	B	704	T7X	C14-C15-C16-C17
6	A	606	PC1	C3A-C3B-C3C-C3D
6	B	701	PC1	C3A-C3B-C3C-C3D
2	A	602	Y01	CAJ-CAN-CBA-CAA
2	B	703	Y01	CAJ-CAN-CBA-CAA
6	A	606	PC1	C36-C37-C38-C39
6	B	701	PC1	C36-C37-C38-C39
3	A	603	T7X	C11-C31-C32-C33
3	B	704	T7X	C11-C31-C32-C33
6	B	701	PC1	C2D-C2E-C2F-C2G
4	A	604	PTY	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
4	B	705	PTY	C12-C13-C14-C15
6	A	606	PC1	C2D-C2E-C2F-C2G
4	A	604	PTY	C35-C36-C37-C38
4	B	705	PTY	C35-C36-C37-C38
4	A	604	PTY	C33-C34-C35-C36
4	B	705	PTY	C33-C34-C35-C36
6	A	606	PC1	C28-C29-C2A-C2B
6	B	701	PC1	C28-C29-C2A-C2B
6	A	606	PC1	C38-C39-C3A-C3B
6	B	701	PC1	C38-C39-C3A-C3B
2	A	602	Y01	CAJ-CAO-CBB-CAC
2	B	703	Y01	CAJ-CAO-CBB-CAC
6	A	606	PC1	C37-C38-C39-C3A
6	B	701	PC1	C37-C38-C39-C3A
3	A	603	T7X	C1-O1-P1-O13
3	B	704	T7X	C1-O1-P1-O13
3	A	603	T7X	C1-O1-P1-O11
3	B	704	T7X	C1-O1-P1-O11
6	A	606	PC1	O11-C1-C2-O21
6	B	701	PC1	O11-C1-C2-O21
6	A	606	PC1	C11-C12-N-C13
6	B	701	PC1	C11-C12-N-C13
5	B	706	CLR	C22-C23-C24-C25
6	A	606	PC1	C25-C26-C27-C28
6	B	701	PC1	C25-C26-C27-C28
6	A	606	PC1	C11-C12-N-C15
6	B	701	PC1	C11-C12-N-C15
3	A	603	T7X	C7-O13-P1-O11
3	B	704	T7X	C7-O13-P1-O11
6	A	606	PC1	C1-O11-P-O14
6	B	701	PC1	C1-O11-P-O14
6	A	606	PC1	O11-C1-C2-C3
6	B	701	PC1	O11-C1-C2-C3
6	A	606	PC1	C29-C2A-C2B-C2C
6	B	701	PC1	C29-C2A-C2B-C2C
6	A	606	PC1	C2E-C2F-C2G-C2H
6	B	701	PC1	C2E-C2F-C2G-C2H
3	A	603	T7X	C35-C36-C37-C38
3	B	704	T7X	C35-C36-C37-C38
6	A	606	PC1	C24-C25-C26-C27
6	B	701	PC1	C24-C25-C26-C27
2	A	601	Y01	OAG-CAY-OAW-CBC

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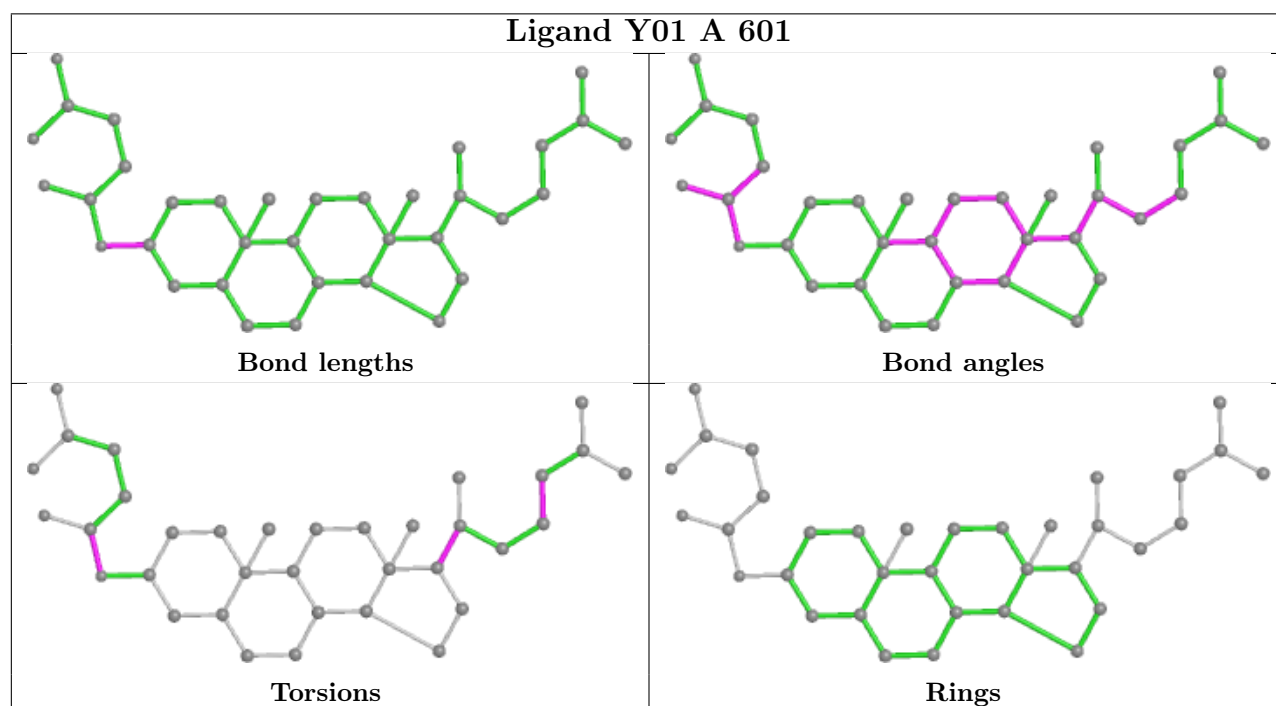
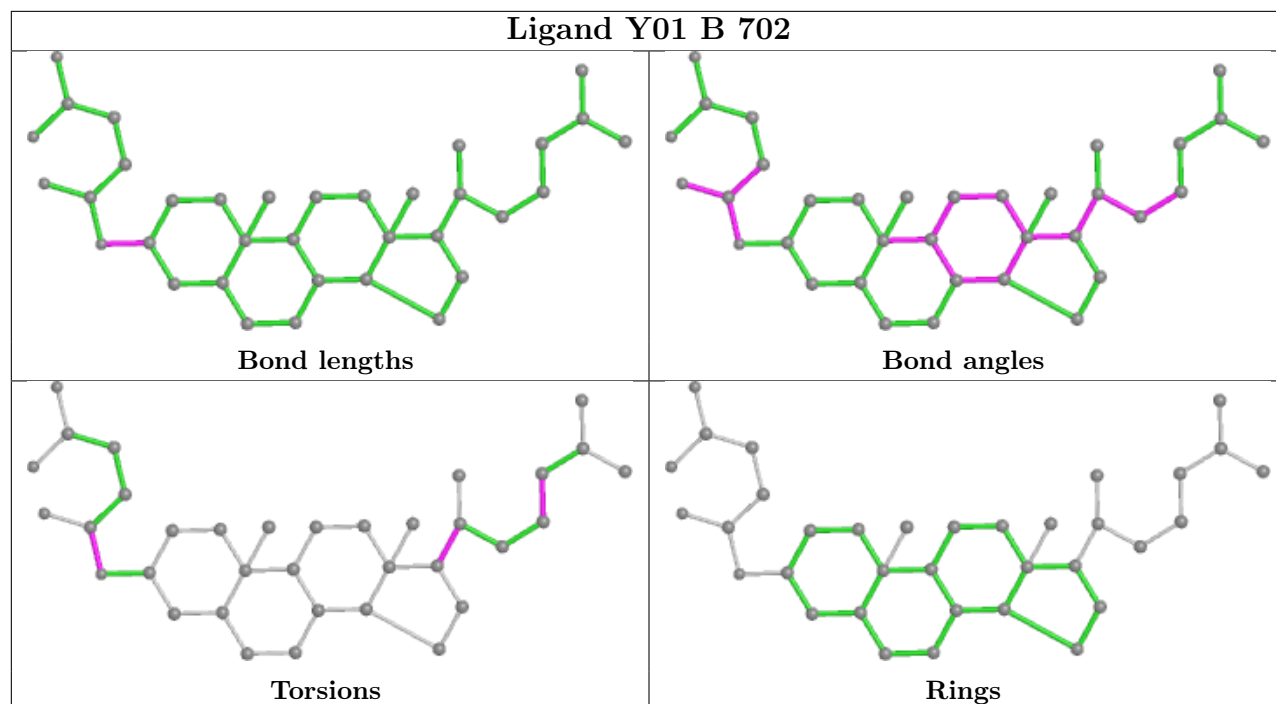
Mol	Chain	Res	Type	Atoms
2	B	702	Y01	OAG-CAY-OAW-CBC
2	A	601	Y01	CAM-CAY-OAW-CBC
2	B	702	Y01	CAM-CAY-OAW-CBC
4	A	604	PTY	C5-O14-P1-O11
4	B	705	PTY	C5-O14-P1-O11
6	A	606	PC1	C35-C36-C37-C38
6	B	701	PC1	C35-C36-C37-C38
6	A	606	PC1	C11-C12-N-C14
6	B	701	PC1	C11-C12-N-C14
6	A	606	PC1	O21-C2-C3-O31
6	B	701	PC1	O21-C2-C3-O31
2	A	602	Y01	CAO-CAJ-CAN-CBA
2	B	703	Y01	CAO-CAJ-CAN-CBA
5	A	605	CLR	C22-C23-C24-C25
2	A	602	Y01	CAM-CAL-CAX-OAH
2	B	703	Y01	CAM-CAL-CAX-OAH
4	A	604	PTY	O14-C5-C6-O7
4	B	705	PTY	O14-C5-C6-O7
3	A	603	T7X	C20-C21-C22-C23
3	B	704	T7X	C20-C21-C22-C23
6	A	606	PC1	C33-C34-C35-C36
6	B	701	PC1	C33-C34-C35-C36
2	A	602	Y01	CAM-CAL-CAX-OAF
2	B	703	Y01	CAM-CAL-CAX-OAF
4	A	604	PTY	C3-O11-P1-O14
4	B	705	PTY	C3-O11-P1-O14
2	A	601	Y01	CAO-CAJ-CAN-CBA
2	B	702	Y01	CAO-CAJ-CAN-CBA
2	A	602	Y01	CAL-CAM-CAY-OAW
2	B	703	Y01	CAL-CAM-CAY-OAW
3	A	603	T7X	O16-C8-C9-O18
3	B	704	T7X	O16-C8-C9-O18
2	A	601	Y01	CAC-CBB-CBE-CBI
2	B	702	Y01	CAC-CBB-CBE-CBI
6	A	606	PC1	C1-C2-C3-O31
6	B	701	PC1	C1-C2-C3-O31
2	A	602	Y01	CAL-CAM-CAY-OAG
2	B	703	Y01	CAL-CAM-CAY-OAG
6	A	606	PC1	C12-C11-O13-P
6	B	701	PC1	C12-C11-O13-P
3	B	704	T7X	C33-C34-C35-C36
3	A	603	T7X	C33-C34-C35-C36

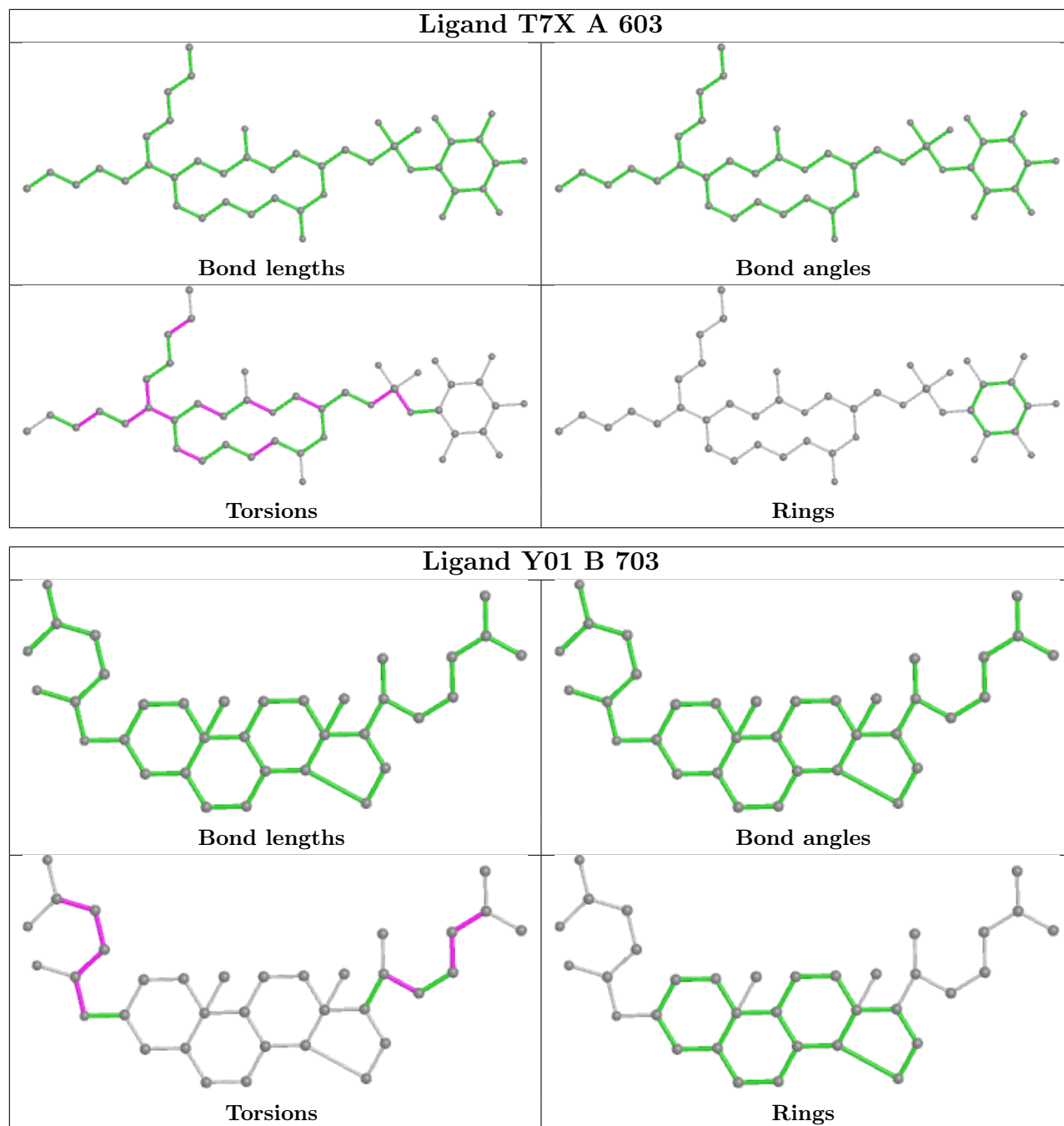
There are no ring outliers.

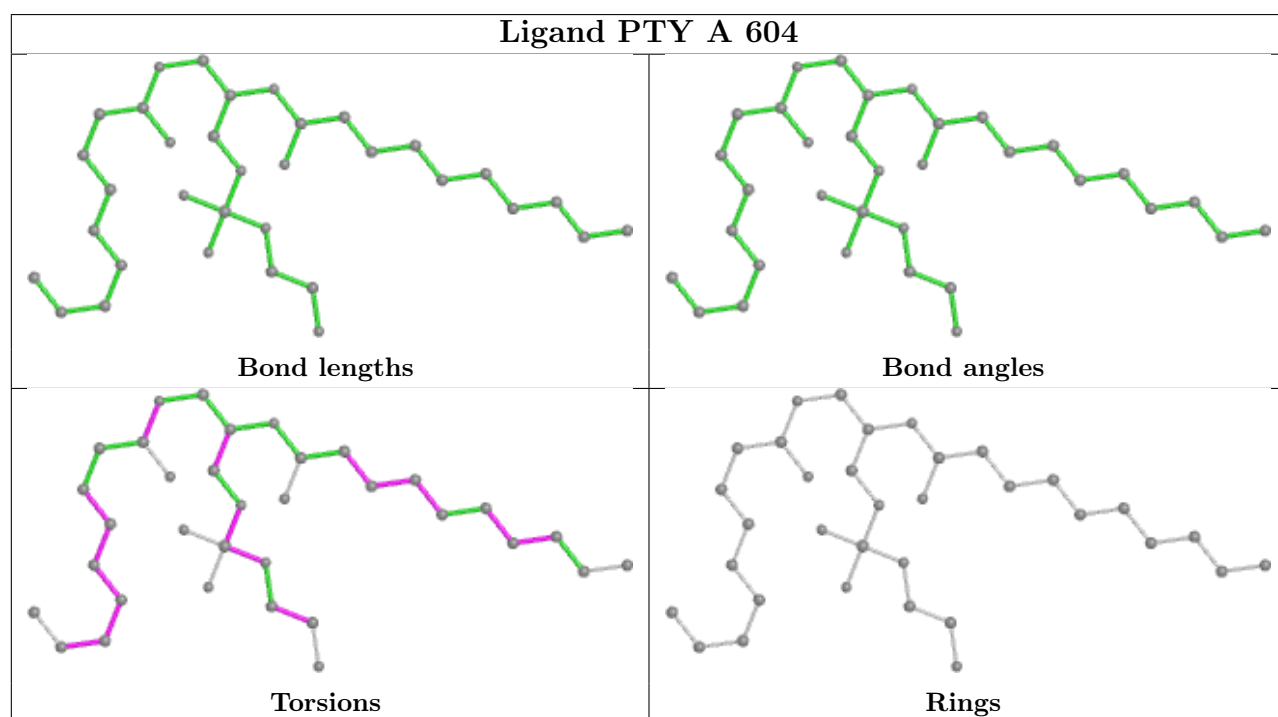
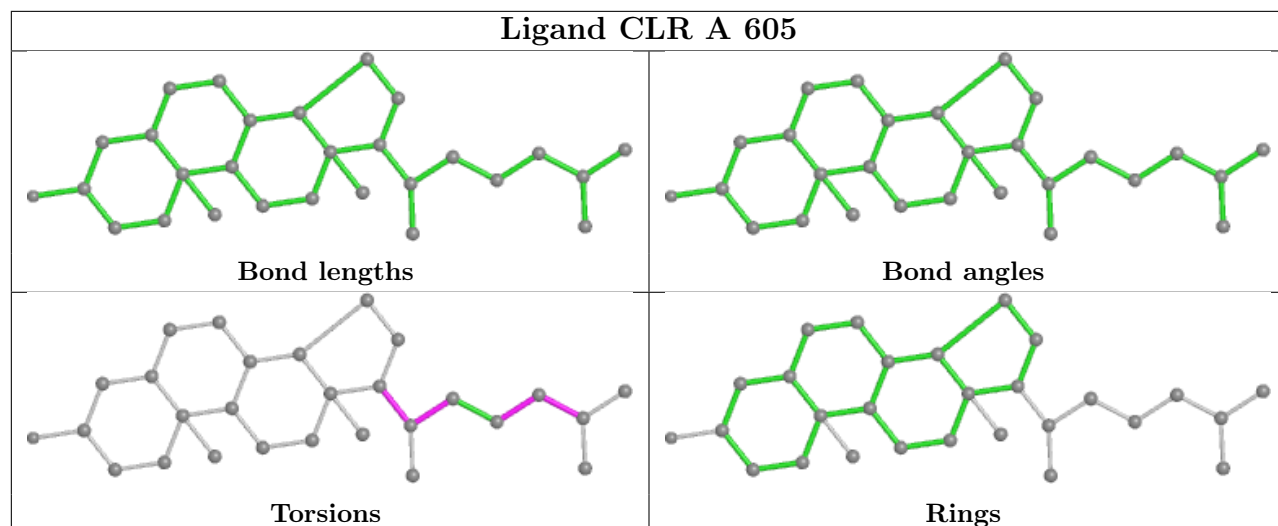
12 monomers are involved in 58 short contacts:

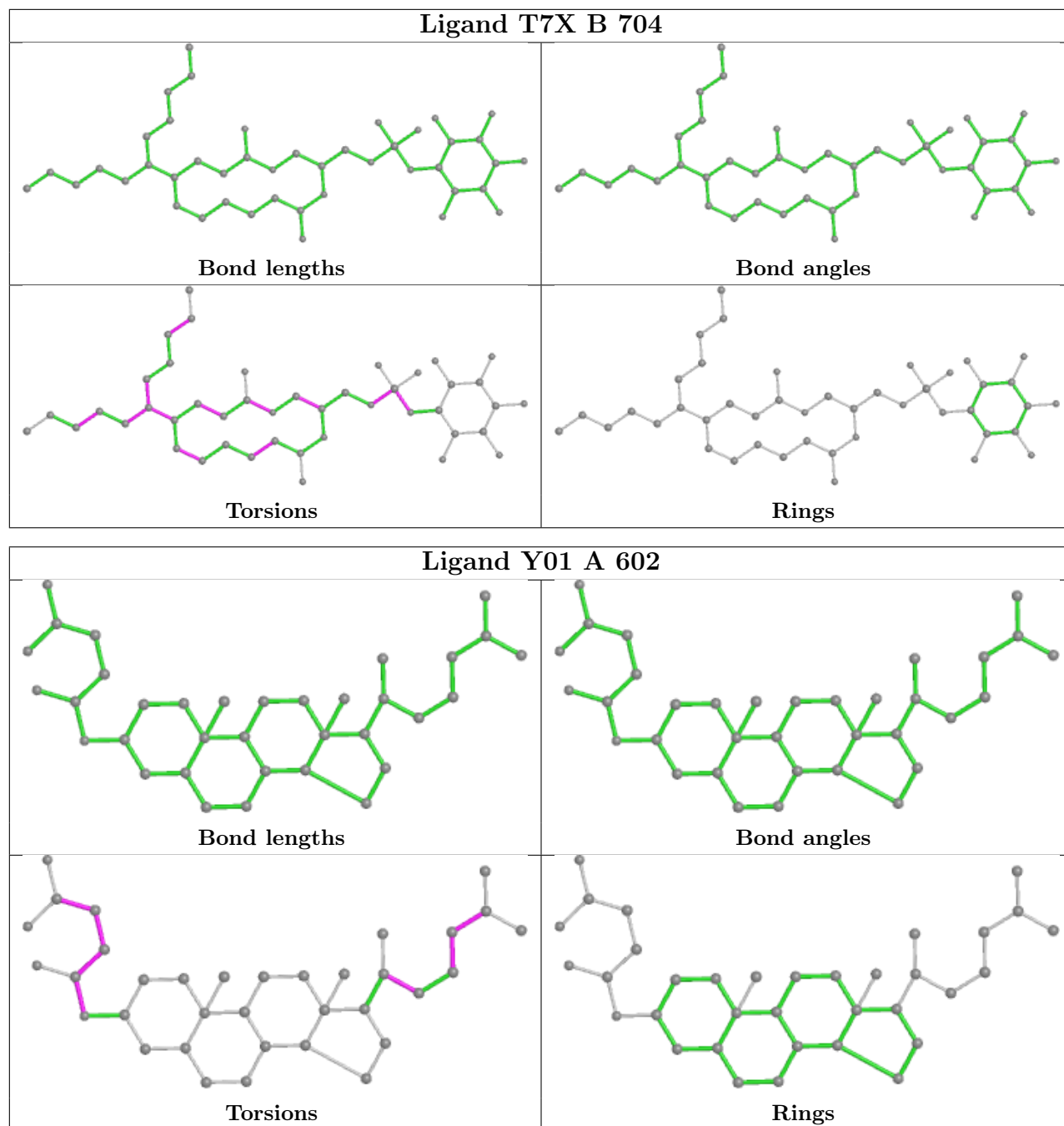
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	702	Y01	3	0
2	A	601	Y01	3	0
3	A	603	T7X	1	0
2	B	703	Y01	10	0
5	A	605	CLR	9	0
4	A	604	PTY	1	0
3	B	704	T7X	1	0
2	A	602	Y01	10	0
6	B	701	PC1	7	0
5	B	706	CLR	5	0
4	B	705	PTY	1	0
6	A	606	PC1	7	0

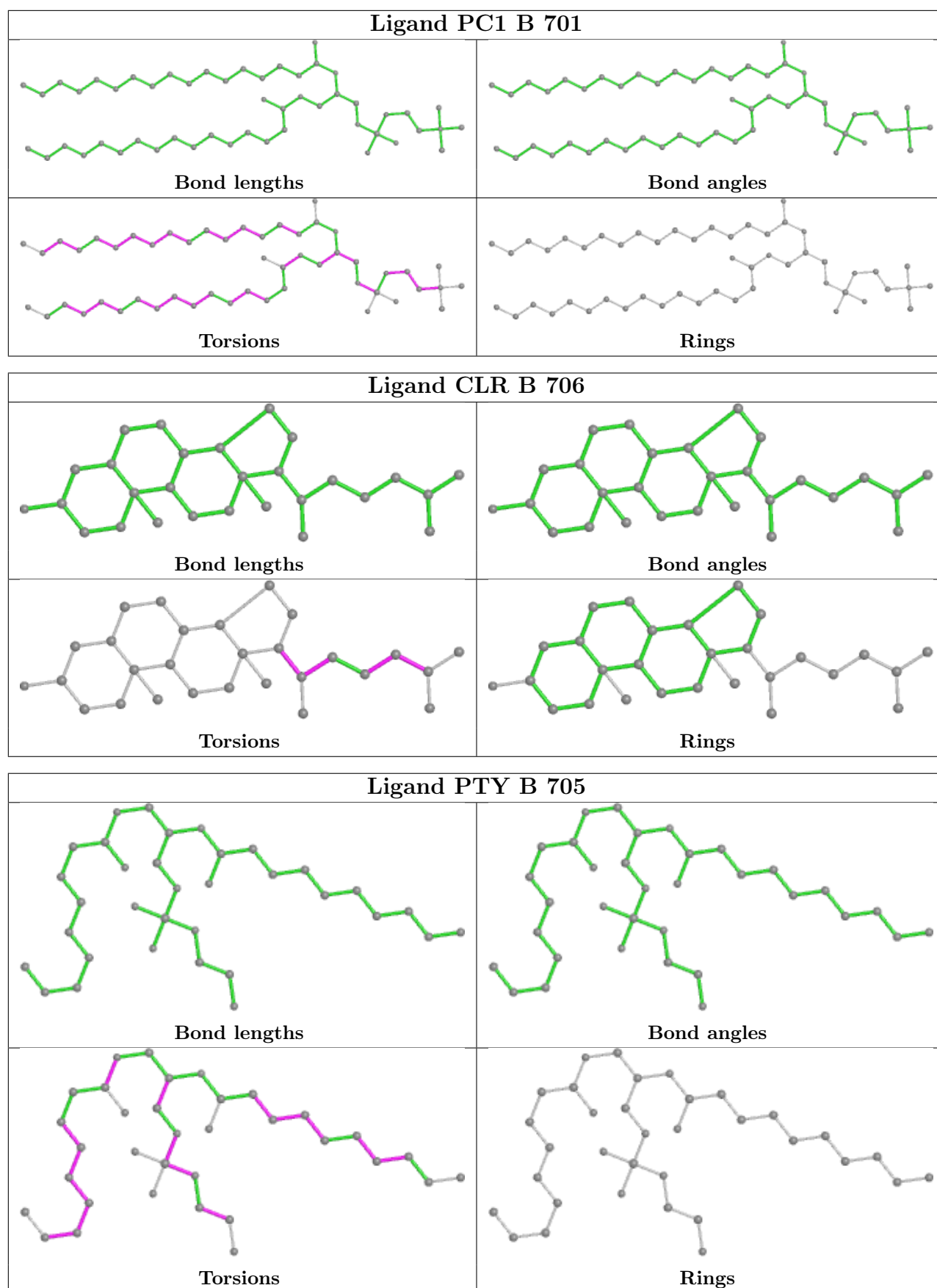
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

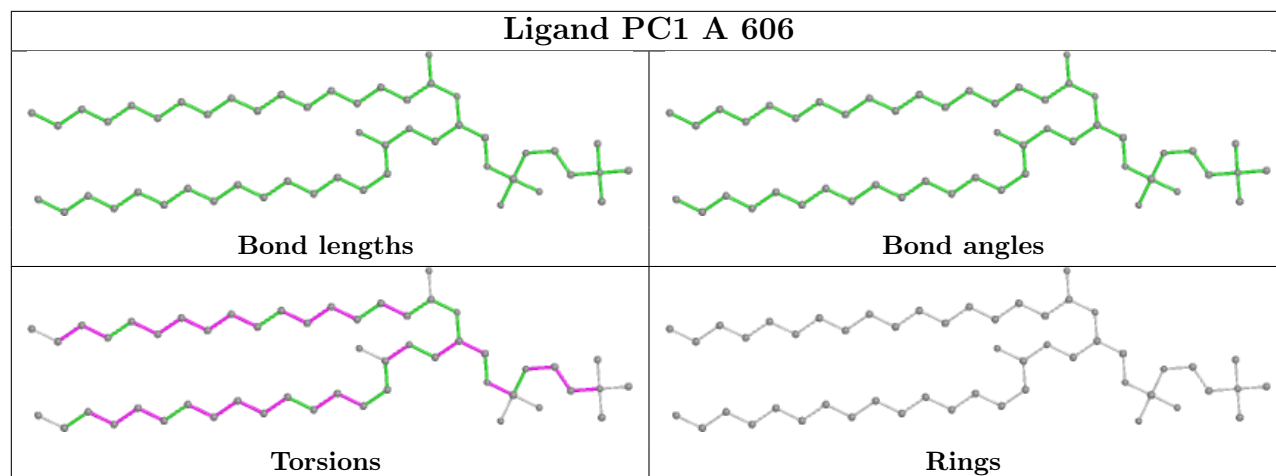












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.