Full wwPDB EM Validation Report ⓘ

Apr 28, 2024 – 12:14 AM JST

PDB ID	:	8K66
EMDB ID	:	EMD-36918
Title	:	Cryo-EM structure of Oryza sativa HKT2;1 at 2.5 angstrom
Authors	:	Wang, X.; Shen, X.; Qu, Y.; Wang, C.; Shen, H.
Deposited on	:	2023-07-25
Resolution	:	2.53 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:

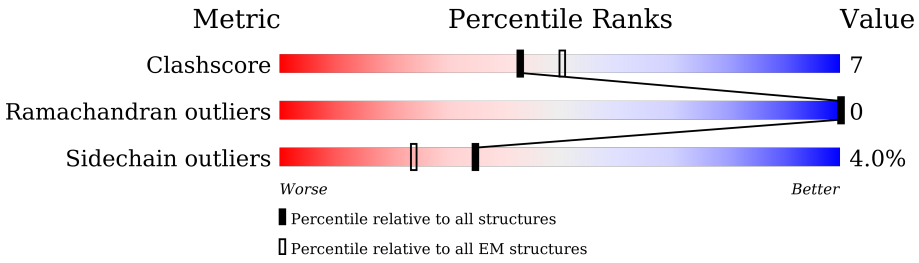
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.53 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	543	67% 13% • 18%
1	B	543	68% 13% • 18%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 7620 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.

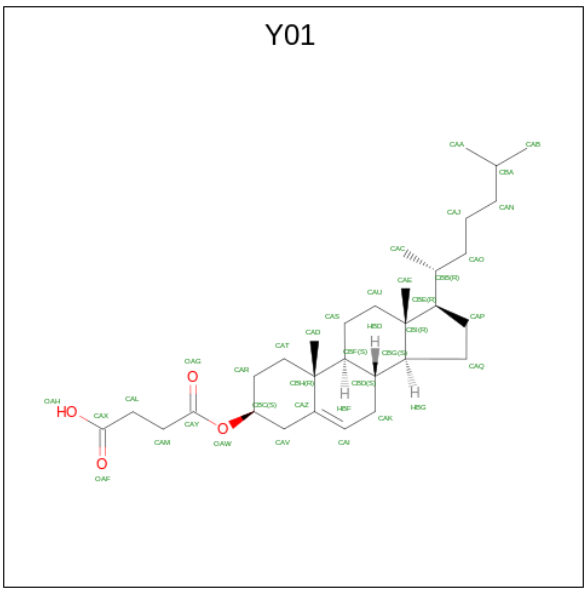
- Molecule 1 is a protein called Cation transporter HKT2;1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	443	Total	C	N	O	S	1	0
			3514	2349	558	590	17		
1	B	443	Total	C	N	O	S	1	0
			3514	2349	558	590	17		

There are 26 discrepancies between the modelled and reference sequences:

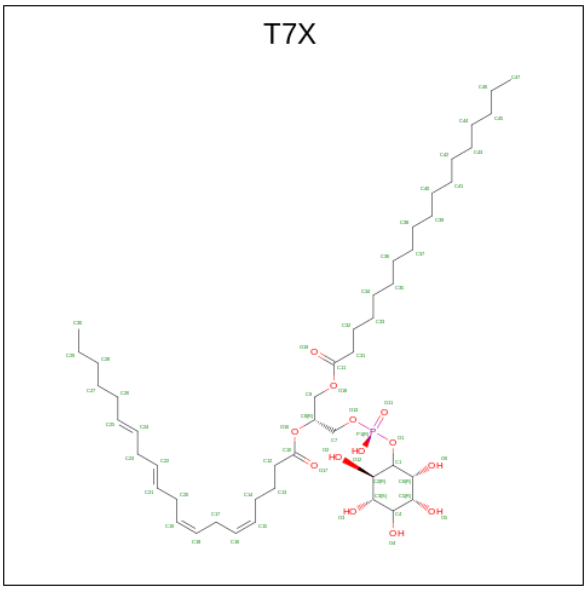
Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	MET	-	initiating methionine	UNP Q0D9S3
A	-11	ALA	-	expression tag	UNP Q0D9S3
A	-10	ASP	-	expression tag	UNP Q0D9S3
A	-9	TYR	-	expression tag	UNP Q0D9S3
A	-8	LYS	-	expression tag	UNP Q0D9S3
A	-7	ASP	-	expression tag	UNP Q0D9S3
A	-6	ASP	-	expression tag	UNP Q0D9S3
A	-5	ASP	-	expression tag	UNP Q0D9S3
A	-4	ASP	-	expression tag	UNP Q0D9S3
A	-3	LYS	-	expression tag	UNP Q0D9S3
A	-2	GLY	-	expression tag	UNP Q0D9S3
A	-1	GLY	-	expression tag	UNP Q0D9S3
A	0	ARG	-	expression tag	UNP Q0D9S3
B	-12	MET	-	initiating methionine	UNP Q0D9S3
B	-11	ALA	-	expression tag	UNP Q0D9S3
B	-10	ASP	-	expression tag	UNP Q0D9S3
B	-9	TYR	-	expression tag	UNP Q0D9S3
B	-8	LYS	-	expression tag	UNP Q0D9S3
B	-7	ASP	-	expression tag	UNP Q0D9S3
B	-6	ASP	-	expression tag	UNP Q0D9S3
B	-5	ASP	-	expression tag	UNP Q0D9S3
B	-4	ASP	-	expression tag	UNP Q0D9S3
B	-3	LYS	-	expression tag	UNP Q0D9S3
B	-2	GLY	-	expression tag	UNP Q0D9S3
B	-1	GLY	-	expression tag	UNP Q0D9S3
B	0	ARG	-	expression tag	UNP Q0D9S3

- Molecule 2 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: $C_{31}H_{50}O_4$).



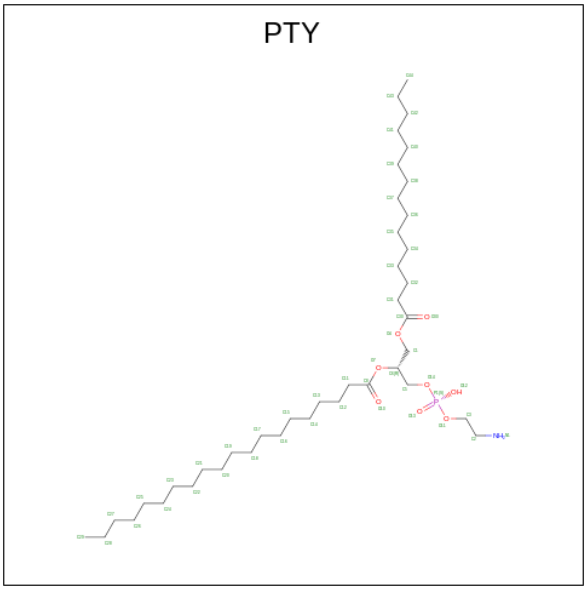
Mol	Chain	Residues	Atoms	AltConf
2	A	1	Total C O 35 31 4	0
2	A	1	Total C O 35 31 4	0
2	B	1	Total C O 35 31 4	0
2	B	1	Total C O 35 31 4	0

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



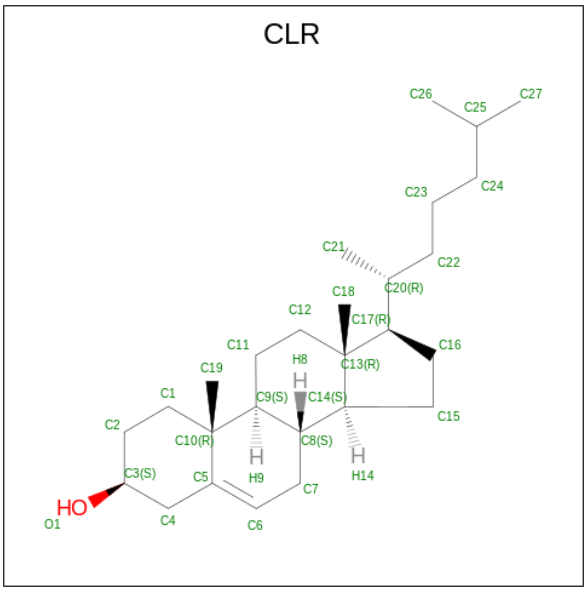
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	O	P	0
			46	32	13	1	
3	B	1	Total	C	O	P	0
			46	32	13	1	

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



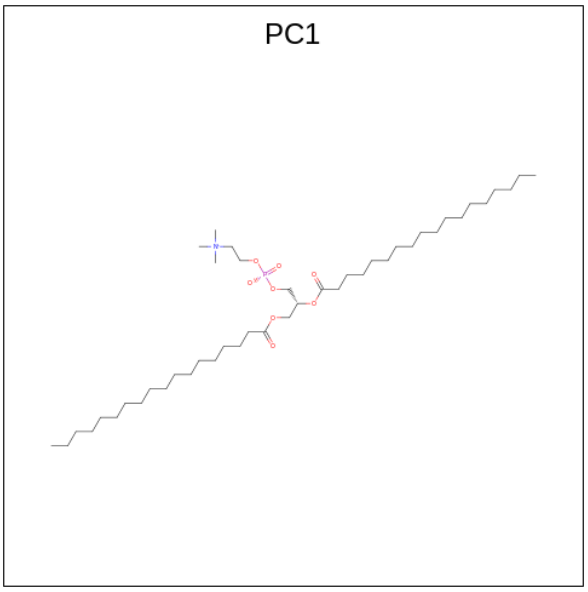
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			34	24	1	8	1	
4	B	1	Total	C	N	O	P	0
			34	24	1	8	1	

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



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

- 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
6	A	1	Total	C	N	O	P	0
			51	41	1	8	1	

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

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

Mol	Chain	Residues	Atoms		AltConf
7	A	2	Total	Na	0
			2	2	
7	B	2	Total	Na	0
			2	2	

- Molecule 8 is water.

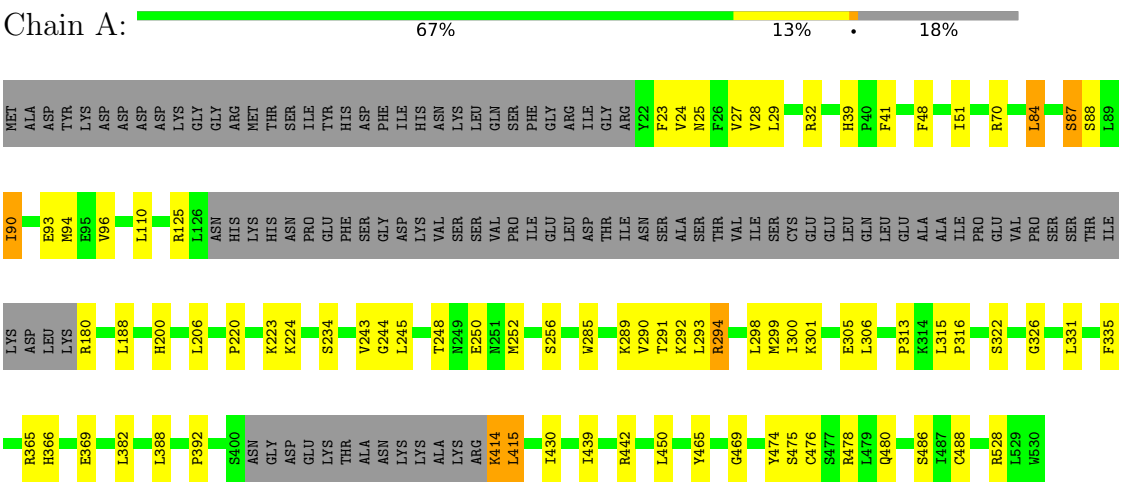
Mol	Chain	Residues	Atoms		AltConf
8	A	65	Total	O	0
			65	65	
8	B	65	Total	O	0
			65	65	

3 Residue-property plots (i)

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.

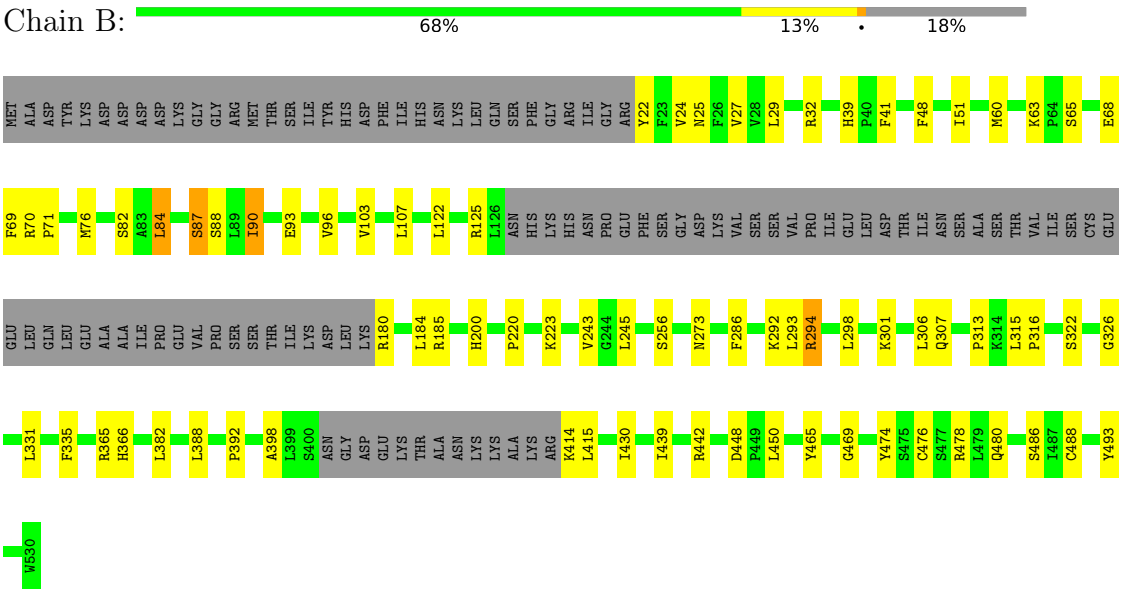
• Molecule 1: Cation transporter HKT2;1

Chain A:



• Molecule 1: Cation transporter HKT2;1

Chain B:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	501277	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 ($e^-/Å^2$)	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

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.30	0/3605	0.43	0/4893
1	B	0.29	0/3605	0.42	0/4893
All	All	0.30	0/7210	0.43	0/9786

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

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	3514	0	3674	52	0
1	B	3514	0	3674	48	0
2	A	70	0	98	4	0
2	B	70	0	98	3	0
3	A	46	0	0	1	0
3	B	46	0	0	0	0
4	A	34	0	41	1	0
4	B	34	0	41	1	0
5	A	28	0	46	3	0
5	B	28	0	46	1	0
6	A	51	0	76	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	51	0	76	2	0
7	A	2	0	0	0	0
7	B	2	0	0	0	0
8	A	65	0	0	10	0
8	B	65	0	0	9	0
All	All	7620	0	7870	109	0

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

All (109) 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:478:ARG:NH1	8:A:701:HOH:O	2.00	0.93
1:B:273:ASN:ND2	8:B:802:HOH:O	2.05	0.89
1:A:382:LEU:HD11	8:A:719:HOH:O	1.78	0.83
1:A:245:LEU:O	8:A:702:HOH:O	2.01	0.79
1:A:188:LEU:HD22	1:A:306:LEU:HD23	1.65	0.77
1:B:245:LEU:O	8:B:801:HOH:O	2.05	0.74
1:A:224:LYS:NZ	1:A:250:GLU:OE2	2.21	0.72
1:B:27:VAL:HG23	4:B:705:PTY:H372	1.76	0.68
1:B:474:TYR:O	8:B:803:HOH:O	2.11	0.68
1:A:88:SER:HB2	1:A:243:VAL:O	1.95	0.66
1:A:474:TYR:O	8:A:703:HOH:O	2.13	0.66
1:A:476:CYS:SG	1:A:488[B]:CYS:HB2	2.36	0.65
1:B:476:CYS:SG	1:B:488[B]:CYS:HB2	2.36	0.64
1:A:88:SER:CB	1:A:243:VAL:O	2.46	0.63
1:B:478:ARG:NH2	8:B:811:HOH:O	2.34	0.61
1:A:87:SER:O	1:A:469:GLY:CA	2.49	0.60
1:A:88:SER:O	1:A:88:SER:OG	2.20	0.59
1:B:88:SER:O	1:B:88:SER:OG	2.20	0.57
1:A:476:CYS:O	1:A:480:GLN:HG2	2.06	0.54
1:A:200:HIS:CE1	8:A:730:HOH:O	2.60	0.54
1:A:125:ARG:NH1	1:A:306:LEU:O	2.41	0.54
1:A:285:TRP:CE2	1:A:289:LYS:HD2	2.43	0.54
1:B:476:CYS:O	1:B:480:GLN:HG2	2.07	0.54
1:A:48:PHE:HD1	1:A:84:LEU:HD13	1.73	0.54
1:A:25:ASN:O	1:A:29:LEU:HG	2.08	0.53
1:A:300:ILE:HG13	1:A:301:LYS:H	1.74	0.53
1:B:103:VAL:O	1:B:107:LEU:HG	2.09	0.53
1:A:90:ILE:CG2	8:A:758:HOH:O	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:HIS:CE1	8:B:830:HOH:O	2.62	0.52
1:A:90:ILE:HG22	8:A:758:HOH:O	2.11	0.51
1:A:220:PRO:HA	1:A:223:LYS:HG2	1.93	0.51
1:A:475:SER:HB3	1:A:478:ARG:HD3	1.93	0.51
1:B:87:SER:O	1:B:469:GLY:CA	2.59	0.51
1:B:90:ILE:O	1:B:493:TYR:HB2	2.10	0.51
1:B:322:SER:HA	2:B:702:Y01:HAC2	1.93	0.51
1:A:24:VAL:O	1:A:28:VAL:HG13	2.10	0.50
1:B:48:PHE:HD1	1:B:84:LEU:HD13	1.75	0.50
1:A:322:SER:HA	2:A:601:Y01:HAC2	1.94	0.50
1:A:27:VAL:HG23	4:A:604:PTY:H372	1.92	0.50
1:A:331:LEU:HD22	1:A:388:LEU:HD22	1.94	0.50
1:B:125:ARG:HD3	1:B:185:ARG:HD2	1.93	0.50
1:A:206:LEU:HD12	5:A:605:CLR:H22	1.93	0.50
1:B:365:ARG:HA	1:B:366:HIS:CG	2.48	0.49
1:B:331:LEU:HD22	1:B:388:LEU:HD22	1.94	0.49
1:A:365:ARG:HA	1:A:366:HIS:CG	2.47	0.48
1:B:220:PRO:HA	1:B:223:LYS:HG2	1.95	0.48
6:A:606:PC1:H142	6:A:606:PC1:H111	1.64	0.48
1:A:326:GLY:HA3	6:B:701:PC1:H3A2	1.96	0.48
1:B:25:ASN:O	1:B:29:LEU:HG	2.14	0.48
1:B:63:LYS:HD3	1:B:63:LYS:HA	1.55	0.48
1:A:200:HIS:HE1	8:A:730:HOH:O	1.97	0.47
1:B:365:ARG:NH1	1:B:392:PRO:O	2.48	0.47
1:B:51:ILE:HB	1:B:84:LEU:HD11	1.95	0.47
1:A:294:ARG:O	1:A:298:LEU:HG	2.14	0.47
1:A:88:SER:HB3	1:A:243:VAL:O	2.14	0.47
1:A:248:THR:O	8:A:704:HOH:O	2.21	0.46
1:A:252:MET:HG3	1:A:369:GLU:HB3	1.96	0.46
1:A:365:ARG:NH1	1:A:392:PRO:O	2.48	0.46
1:A:414:LYS:HG2	1:A:415:LEU:H	1.80	0.46
1:A:90:ILE:HD13	1:A:94:MET:SD	2.56	0.45
1:B:184:LEU:HB3	1:B:306:LEU:HD21	1.97	0.45
6:A:606:PC1:H321	6:A:606:PC1:H32	1.75	0.45
1:B:22:TYR:HD1	1:B:24:VAL:H	1.65	0.45
1:B:68:GLU:HA	1:B:70:ARG:NH2	2.32	0.45
1:B:294:ARG:O	1:B:298:LEU:HG	2.15	0.45
6:B:701:PC1:H142	6:B:701:PC1:H111	1.64	0.45
2:B:702:Y01:HAA1	2:B:702:Y01:HAJ2	1.85	0.45
1:A:450:LEU:HB2	8:A:706:HOH:O	2.18	0.44
1:B:125:ARG:NH1	1:B:307:GLN:O	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:ILE:HD11	1:A:465:TYR:CE2	2.52	0.44
1:B:122:LEU:HA	1:B:125:ARG:HD2	2.00	0.44
1:B:430:ILE:HD11	1:B:465:TYR:CE2	2.52	0.44
1:A:93:GLU:O	1:A:96:VAL:HG22	2.17	0.44
1:A:299:MET:HG2	1:A:306:LEU:HD21	1.99	0.44
1:A:315:LEU:HB3	1:A:316:PRO:HD3	2.00	0.44
6:A:606:PC1:H3A2	1:B:326:GLY:HA3	2.00	0.44
1:A:51:ILE:HB	1:A:84:LEU:HD11	1.99	0.43
1:B:315:LEU:HB3	1:B:316:PRO:HD3	2.00	0.43
2:A:601:Y01:HAA1	2:A:601:Y01:HAJ2	1.85	0.43
1:B:88:SER:CB	1:B:243:VAL:O	2.66	0.43
1:B:88:SER:HB2	1:B:243:VAL:O	2.17	0.43
2:A:601:Y01:HAE2	2:A:601:Y01:HBB	1.71	0.43
1:B:450:LEU:HB2	8:B:804:HOH:O	2.18	0.43
1:A:23:PHE:O	1:A:27:VAL:HG12	2.18	0.43
1:B:382:LEU:HD22	8:B:818:HOH:O	2.19	0.43
1:B:293:LEU:HD23	1:B:293:LEU:HA	1.91	0.43
1:B:93:GLU:O	1:B:96:VAL:HG22	2.19	0.42
1:A:313:PRO:HB2	1:A:316:PRO:HD2	2.02	0.42
1:B:313:PRO:HB2	1:B:316:PRO:HD2	2.02	0.42
2:A:601:Y01:HAO2	2:A:601:Y01:HAP1	1.73	0.42
5:A:605:CLR:H213	5:A:605:CLR:H232	1.84	0.42
1:B:122:LEU:HD12	1:B:125:ARG:HH21	1.85	0.41
1:A:285:TRP:CZ2	1:A:289:LYS:HD2	2.54	0.41
1:A:290:VAL:HG23	1:A:291:THR:HG23	2.02	0.41
1:B:39:HIS:HD2	1:B:41:PHE:HB3	1.85	0.41
1:B:69:PHE:CZ	1:B:71:PRO:HB3	2.56	0.41
1:A:293:LEU:HD12	1:A:293:LEU:HA	1.92	0.41
1:B:39:HIS:CD2	1:B:41:PHE:H	2.38	0.41
1:A:244:GLY:HA2	1:A:369:GLU:HG3	2.02	0.41
2:B:702:Y01:HAO2	2:B:702:Y01:HAP1	1.73	0.41
1:A:528:ARG:HD3	1:B:398:ALA:HB3	2.02	0.40
1:B:200:HIS:HE1	8:B:830:HOH:O	1.99	0.40
1:A:439:ILE:O	1:A:442:ARG:NH1	2.45	0.40
1:B:286:PHE:CD2	5:B:706:CLR:H271	2.56	0.40
1:B:448:ASP:OD1	8:B:804:HOH:O	2.22	0.40
1:A:39:HIS:HD2	1:A:41:PHE:HB3	1.86	0.40
1:B:439:ILE:O	1:B:442:ARG:NH1	2.45	0.40
3:A:603:T7X:C19	5:A:605:CLR:H6	2.52	0.40
1:B:60:MET:HG2	1:B:76:MET:HG3	2.03	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	438/543 (81%)	431 (98%)	7 (2%)	0	100	100
1	B	438/543 (81%)	431 (98%)	7 (2%)	0	100	100
All	All	876/1086 (81%)	862 (98%)	14 (2%)	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	391/478 (82%)	375 (96%)	16 (4%)	30	53
1	B	391/478 (82%)	376 (96%)	15 (4%)	33	56
All	All	782/956 (82%)	751 (96%)	31 (4%)	35	54

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ARG
1	A	70	ARG
1	A	84	LEU
1	A	87	SER
1	A	90	ILE
1	A	110	LEU
1	A	180	ARG
1	A	234	SER

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Mol	Chain	Res	Type
1	A	256	SER
1	A	292	LYS
1	A	294	ARG
1	A	305	GLU
1	A	335	PHE
1	A	414	LYS
1	A	415	LEU
1	A	486	SER
1	B	32	ARG
1	B	65	SER
1	B	82	SER
1	B	84	LEU
1	B	87	SER
1	B	90	ILE
1	B	180	ARG
1	B	256	SER
1	B	292	LYS
1	B	294	ARG
1	B	301	LYS
1	B	335	PHE
1	B	414	LYS
1	B	415	LEU
1	B	486	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	39	HIS
1	A	200	HIS
1	A	302	ASN
1	A	421	ASN
1	B	25	ASN
1	B	31	HIS
1	B	39	HIS
1	B	200	HIS
1	B	421	ASN

5.3.3 RNA

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 16 ligands modelled in this entry, 4 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	0.70	0	57,57,57	1.31	7 (12%)
3	T7X	B	704	-	46,46,61	0.97	4 (8%)	56,58,73	1.07	2 (3%)
4	PTY	B	705	-	33,33,49	1.04	4 (12%)	36,38,54	1.12	2 (5%)
2	Y01	A	601	-	38,38,38	0.71	0	57,57,57	1.30	7 (12%)
5	CLR	B	706	-	31,31,31	0.35	0	48,48,48	1.02	4 (8%)
2	Y01	A	602	-	38,38,38	0.76	0	57,57,57	1.24	8 (14%)
5	CLR	A	605	-	31,31,31	0.29	0	48,48,48	0.35	0
4	PTY	A	604	-	33,33,49	1.04	4 (12%)	36,38,54	1.12	2 (5%)
3	T7X	A	603	-	46,46,61	0.97	4 (8%)	56,58,73	1.07	2 (3%)
2	Y01	B	703	-	38,38,38	0.76	0	57,57,57	1.24	7 (12%)
6	PC1	B	701	-	50,50,53	0.97	4 (8%)	56,58,61	1.04	2 (3%)
6	PC1	A	606	-	50,50,53	0.97	4 (8%)	56,58,61	1.04	2 (3%)

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	-	-	13/19/77/77	0/4/4/4
3	T7X	B	704	-	-	18/41/65/80	0/1/1/1
4	PTY	B	705	-	-	17/37/37/53	-
2	Y01	A	601	-	-	13/19/77/77	0/4/4/4
5	CLR	B	706	-	-	8/10/68/68	0/4/4/4
2	Y01	A	602	-	-	9/19/77/77	0/4/4/4
5	CLR	A	605	-	-	4/10/68/68	0/4/4/4
4	PTY	A	604	-	-	17/37/37/53	-
3	T7X	A	603	-	-	18/41/65/80	0/1/1/1
2	Y01	B	703	-	-	9/19/77/77	0/4/4/4
6	PC1	B	701	-	-	16/54/54/57	-
6	PC1	A	606	-	-	16/54/54/57	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	701	PC1	O21-C2	-2.65	1.40	1.46
3	A	603	T7X	O16-C8	-2.65	1.40	1.46
3	B	704	T7X	O16-C8	-2.64	1.40	1.46
6	A	606	PC1	O21-C2	-2.63	1.40	1.46
4	B	705	PTY	O7-C6	-2.53	1.40	1.46
4	A	604	PTY	O7-C6	-2.50	1.40	1.46
3	B	704	T7X	O18-C11	2.45	1.40	1.33
3	A	603	T7X	O18-C11	2.44	1.40	1.33
4	B	705	PTY	O4-C1	-2.40	1.39	1.45
4	A	604	PTY	O4-C1	-2.36	1.39	1.45
6	B	701	PC1	O31-C31	2.36	1.40	1.33
6	A	606	PC1	O31-C31	2.33	1.40	1.33
4	A	604	PTY	O4-C30	2.22	1.39	1.33
6	B	701	PC1	O31-C3	-2.22	1.40	1.45
4	B	705	PTY	O4-C30	2.21	1.39	1.33
6	A	606	PC1	O31-C3	-2.19	1.40	1.45
3	A	603	T7X	O18-C9	-2.15	1.40	1.45
3	B	704	T7X	O18-C9	-2.11	1.40	1.45
4	B	705	PTY	O7-C8	2.11	1.40	1.34
4	A	604	PTY	O7-C8	2.05	1.40	1.34
6	B	701	PC1	O21-C21	2.03	1.40	1.34
6	A	606	PC1	O21-C21	2.01	1.40	1.34
3	B	704	T7X	O16-C10	2.01	1.40	1.34
3	A	603	T7X	O16-C10	2.01	1.40	1.34

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	702	Y01	CBI-CBE-CBB	-4.49	112.46	119.49
2	A	601	Y01	CBI-CBE-CBB	-4.47	112.49	119.49
4	A	604	PTY	O7-C8-C11	4.07	120.28	111.50
4	B	705	PTY	O7-C8-C11	4.05	120.24	111.50
3	B	704	T7X	O16-C10-C12	3.76	119.61	111.50
3	A	603	T7X	O16-C10-C12	3.74	119.56	111.50
6	B	701	PC1	O21-C21-C22	3.70	119.48	111.50
6	A	606	PC1	O21-C21-C22	3.68	119.44	111.50
2	A	602	Y01	CBI-CBE-CBB	-2.84	115.03	119.49
2	B	703	Y01	CBI-CBE-CBB	-2.83	115.05	119.49
3	A	603	T7X	O18-C11-C31	2.68	120.33	111.91
3	B	704	T7X	O18-C11-C31	2.66	120.27	111.91
6	B	701	PC1	O31-C31-C32	2.63	120.15	111.91
6	A	606	PC1	O31-C31-C32	2.62	120.12	111.91
5	B	706	CLR	C14-C8-C9	-2.59	105.63	109.09
2	A	602	Y01	OAW-CAY-OAG	-2.56	117.51	123.70
2	B	703	Y01	OAW-CAY-OAG	-2.55	117.53	123.70
2	B	702	Y01	CBI-CBG-CBD	-2.50	110.68	114.38
2	B	702	Y01	CAS-CAU-CBI	-2.47	108.55	112.78
2	A	601	Y01	CBI-CBG-CBD	-2.46	110.73	114.38
5	B	706	CLR	C11-C9-C10	2.43	116.28	113.08
2	A	601	Y01	CAS-CAU-CBI	-2.42	108.64	112.78
2	A	601	Y01	OAW-CAY-OAG	-2.41	117.87	123.70
2	B	702	Y01	OAW-CAY-OAG	-2.39	117.92	123.70
2	A	602	Y01	OAW-CAY-CAM	2.31	116.48	111.50
2	A	602	Y01	CAS-CAU-CBI	-2.30	108.84	112.78
4	B	705	PTY	O4-C30-C31	2.29	119.11	111.91
2	B	703	Y01	OAW-CAY-CAM	2.29	116.44	111.50
2	B	703	Y01	CAS-CAU-CBI	-2.29	108.86	112.78
4	A	604	PTY	O4-C30-C31	2.28	119.08	111.91
5	B	706	CLR	C12-C11-C9	2.28	117.07	113.11
2	A	601	Y01	CAJ-CAO-CBB	-2.27	108.51	115.03
2	B	703	Y01	CBI-CBG-CBD	-2.26	111.04	114.38
2	A	602	Y01	CBI-CBG-CBD	-2.25	111.04	114.38
2	B	702	Y01	CAJ-CAO-CBB	-2.25	108.57	115.03
2	B	702	Y01	CBD-CAK-CAI	-2.23	109.53	112.73
2	A	601	Y01	CBD-CAK-CAI	-2.22	109.55	112.73
2	A	602	Y01	CBC-CAV-CAZ	-2.21	108.08	111.52
2	B	703	Y01	CBC-CAV-CAZ	-2.20	108.10	111.52
5	B	706	CLR	C7-C8-C14	2.16	114.03	110.91
2	B	703	Y01	CAR-CBC-CAV	-2.14	107.80	110.99
2	A	601	Y01	OAW-CAY-CAM	2.13	116.09	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	602	Y01	CAR-CBC-CAV	-2.12	107.82	110.99
2	B	702	Y01	OAW-CAY-CAM	2.12	116.07	111.50
2	A	602	Y01	CAC-CBB-CAO	-2.02	107.19	110.36

There are no chirality outliers.

All (158) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	603	T7X	C6-C1-O1-P1
3	A	603	T7X	C7-O13-P1-O11
3	B	704	T7X	C6-C1-O1-P1
3	B	704	T7X	C7-O13-P1-O11
4	A	604	PTY	N1-C2-C3-O11
4	A	604	PTY	C5-O14-P1-O13
4	B	705	PTY	N1-C2-C3-O11
4	B	705	PTY	C5-O14-P1-O13
6	A	606	PC1	O32-C31-O31-C3
6	A	606	PC1	C32-C31-O31-C3
6	B	701	PC1	O32-C31-O31-C3
6	B	701	PC1	C32-C31-O31-C3
3	A	603	T7X	O19-C11-O18-C9
3	B	704	T7X	O19-C11-O18-C9
5	A	605	CLR	C21-C20-C22-C23
3	A	603	T7X	C31-C11-O18-C9
3	B	704	T7X	C31-C11-O18-C9
5	B	706	CLR	C21-C20-C22-C23
2	A	601	Y01	CAO-CBB-CBE-CBI
2	B	702	Y01	CAO-CBB-CBE-CBI
2	A	602	Y01	CAJ-CAO-CBB-CBE
2	B	703	Y01	CAJ-CAO-CBB-CBE
5	A	605	CLR	C17-C20-C22-C23
2	A	601	Y01	CAC-CBB-CBE-CBI
2	B	702	Y01	CAC-CBB-CBE-CBI
2	A	602	Y01	CAX-CAL-CAM-CAY
2	B	703	Y01	CAX-CAL-CAM-CAY
2	A	602	Y01	CAJ-CAO-CBB-CAC
2	B	703	Y01	CAJ-CAO-CBB-CAC
4	A	604	PTY	C8-C11-C12-C13
4	B	705	PTY	C8-C11-C12-C13
2	A	602	Y01	CAO-CAJ-CAN-CBA
2	B	703	Y01	CAO-CAJ-CAN-CBA
5	B	706	CLR	C17-C20-C22-C23

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Mol	Chain	Res	Type	Atoms
3	A	603	T7X	C11-C31-C32-C33
3	B	704	T7X	C11-C31-C32-C33
5	A	605	CLR	C20-C22-C23-C24
2	A	602	Y01	CAN-CAJ-CAO-CBB
2	B	703	Y01	CAN-CAJ-CAO-CBB
3	A	603	T7X	C31-C32-C33-C34
3	B	704	T7X	C31-C32-C33-C34
4	A	604	PTY	C5-O14-P1-O11
4	B	705	PTY	C5-O14-P1-O11
4	A	604	PTY	C30-C31-C32-C33
4	B	705	PTY	C30-C31-C32-C33
5	B	706	CLR	C13-C17-C20-C22
4	A	604	PTY	C34-C35-C36-C37
4	B	705	PTY	C34-C35-C36-C37
6	A	606	PC1	C26-C27-C28-C29
6	B	701	PC1	C26-C27-C28-C29
6	B	701	PC1	C23-C24-C25-C26
6	A	606	PC1	C23-C24-C25-C26
6	A	606	PC1	C36-C37-C38-C39
6	B	701	PC1	C36-C37-C38-C39
6	A	606	PC1	C24-C25-C26-C27
6	B	701	PC1	C24-C25-C26-C27
4	A	604	PTY	C15-C16-C17-C18
4	B	705	PTY	C15-C16-C17-C18
6	B	701	PC1	C2C-C2D-C2E-C2F
6	A	606	PC1	C2C-C2D-C2E-C2F
4	A	604	PTY	C32-C33-C34-C35
4	B	705	PTY	C32-C33-C34-C35
3	A	603	T7X	C12-C13-C14-C15
3	B	704	T7X	C12-C13-C14-C15
6	A	606	PC1	C2B-C2C-C2D-C2E
6	B	701	PC1	C2B-C2C-C2D-C2E
2	A	602	Y01	CAM-CAY-OAW-CBC
2	B	703	Y01	CAM-CAY-OAW-CBC
5	B	706	CLR	C13-C17-C20-C21
2	A	601	Y01	CAJ-CAO-CBB-CBE
2	B	702	Y01	CAJ-CAO-CBB-CBE
2	A	602	Y01	OAG-CAY-OAW-CBC
2	B	703	Y01	OAG-CAY-OAW-CBC
6	A	606	PC1	C21-C22-C23-C24
6	B	701	PC1	C21-C22-C23-C24
3	A	603	T7X	O13-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
3	B	704	T7X	O13-C7-C8-C9
3	A	603	T7X	C12-C10-O16-C8
3	B	704	T7X	C12-C10-O16-C8
2	A	601	Y01	CAC-CBB-CBE-CAP
2	B	702	Y01	CAC-CBB-CBE-CAP
3	A	603	T7X	C35-C36-C37-C38
3	B	704	T7X	C35-C36-C37-C38
6	A	606	PC1	C3D-C3E-C3F-C3G
6	B	701	PC1	C3D-C3E-C3F-C3G
5	B	706	CLR	C16-C17-C20-C21
2	A	601	Y01	CAO-CBB-CBE-CAP
2	B	702	Y01	CAO-CBB-CBE-CAP
5	B	706	CLR	C16-C17-C20-C22
5	A	605	CLR	C22-C23-C24-C25
3	A	603	T7X	O17-C10-O16-C8
4	A	604	PTY	C11-C12-C13-C14
4	B	705	PTY	C11-C12-C13-C14
3	A	603	T7X	O13-C7-C8-O16
3	B	704	T7X	O13-C7-C8-O16
6	A	606	PC1	C28-C29-C2A-C2B
6	B	701	PC1	C28-C29-C2A-C2B
3	B	704	T7X	O17-C10-O16-C8
6	A	606	PC1	C37-C38-C39-C3A
6	B	701	PC1	C37-C38-C39-C3A
4	A	604	PTY	C16-C17-C18-C19
4	B	705	PTY	C16-C17-C18-C19
5	B	706	CLR	C23-C24-C25-C27
4	A	604	PTY	O14-C5-C6-O7
4	B	705	PTY	O14-C5-C6-O7
6	A	606	PC1	C39-C3A-C3B-C3C
6	B	701	PC1	C39-C3A-C3B-C3C
4	B	705	PTY	C13-C14-C15-C16
4	A	604	PTY	C13-C14-C15-C16
4	A	604	PTY	C35-C36-C37-C38
4	B	705	PTY	C35-C36-C37-C38
4	A	604	PTY	C31-C32-C33-C34
4	B	705	PTY	C31-C32-C33-C34
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	O14-C5-C6-C1
4	B	705	PTY	O14-C5-C6-C1

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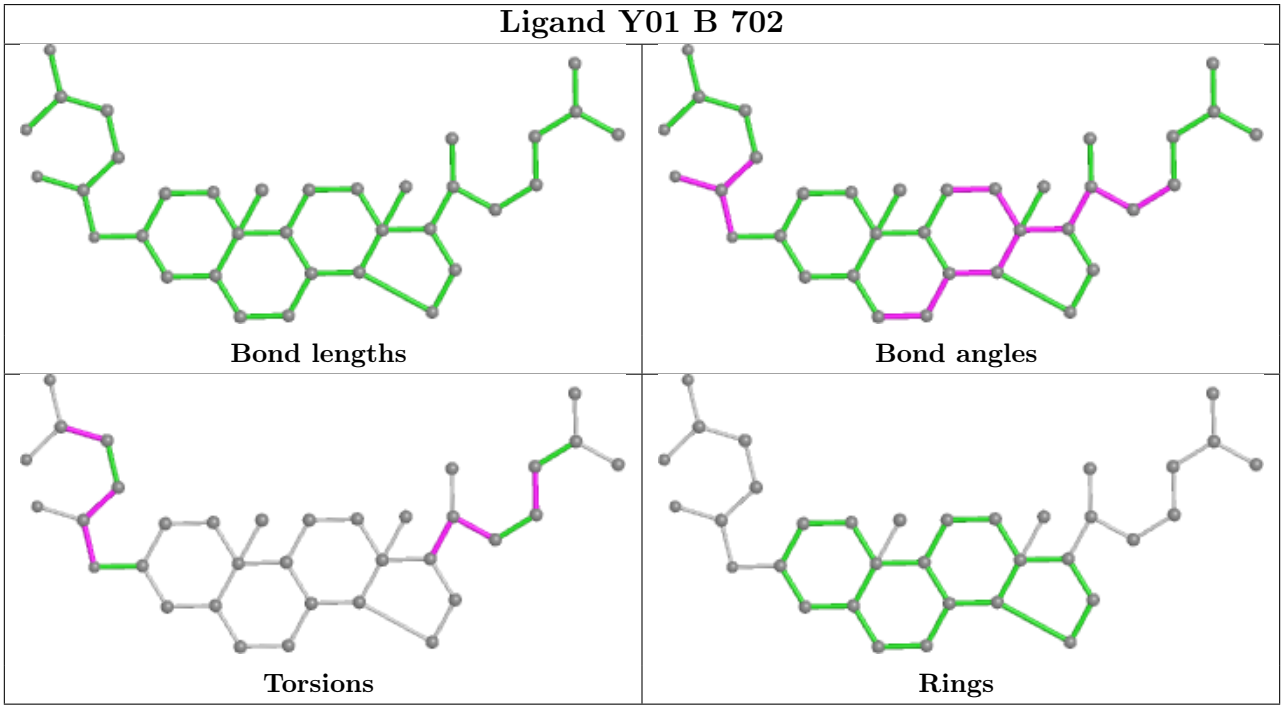
Mol	Chain	Res	Type	Atoms
4	A	604	PTY	C12-C13-C14-C15
4	B	705	PTY	C12-C13-C14-C15
3	A	603	T7X	C33-C34-C35-C36
3	B	704	T7X	C33-C34-C35-C36
2	A	602	Y01	CAM-CAL-CAX-OAH
2	B	703	Y01	CAM-CAL-CAX-OAH
6	A	606	PC1	C22-C23-C24-C25
6	B	701	PC1	C22-C23-C24-C25
2	B	703	Y01	CAM-CAL-CAX-OAF
2	A	602	Y01	CAM-CAL-CAX-OAF
3	A	603	T7X	C7-O13-P1-O1
3	B	704	T7X	C7-O13-P1-O1
2	A	601	Y01	CAO-CAJ-CAN-CBA
2	B	702	Y01	CAO-CAJ-CAN-CBA
3	B	704	T7X	O18-C11-C31-C32
3	A	603	T7X	O18-C11-C31-C32
2	A	601	Y01	CAL-CAM-CAY-OAW
2	B	702	Y01	CAL-CAM-CAY-OAW
4	A	604	PTY	C12-C11-C8-O7
4	B	705	PTY	C12-C11-C8-O7
3	A	603	T7X	C32-C33-C34-C35
3	B	704	T7X	C32-C33-C34-C35
2	A	601	Y01	CAJ-CAO-CBB-CAC
2	B	702	Y01	CAJ-CAO-CBB-CAC
2	B	702	Y01	OAG-CAY-OAW-CBC
2	A	601	Y01	OAG-CAY-OAW-CBC
3	A	603	T7X	O19-C11-C31-C32
2	A	601	Y01	CAM-CAL-CAX-OAF
2	A	601	Y01	CAL-CAM-CAY-OAG
2	B	702	Y01	CAL-CAM-CAY-OAG
3	B	704	T7X	O19-C11-C31-C32
2	B	702	Y01	CAM-CAL-CAX-OAF
6	B	701	PC1	C35-C36-C37-C38
6	A	606	PC1	C35-C36-C37-C38
3	A	603	T7X	O16-C10-C12-C13
3	B	704	T7X	O16-C10-C12-C13
2	A	601	Y01	CAM-CAY-OAW-CBC
2	B	702	Y01	CAM-CAY-OAW-CBC
2	A	601	Y01	CAM-CAL-CAX-OAH
2	B	702	Y01	CAM-CAL-CAX-OAH

There are no ring outliers.

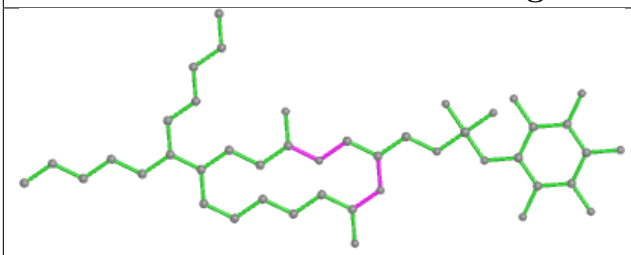
9 monomers are involved in 18 short contacts:

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

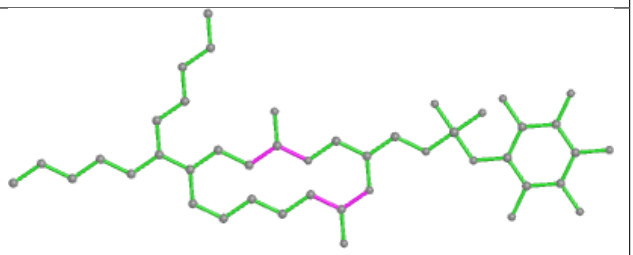
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



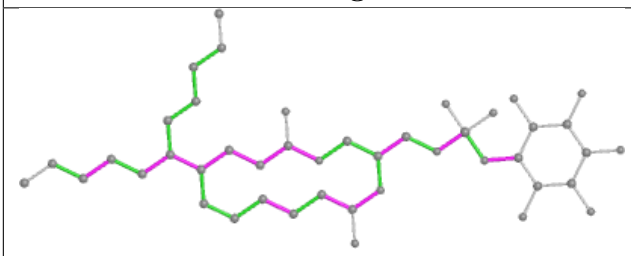
Ligand T7X B 704



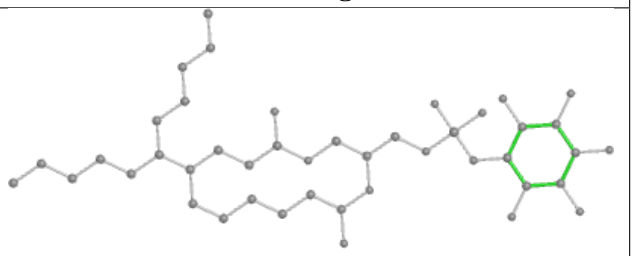
Bond lengths



Bond angles

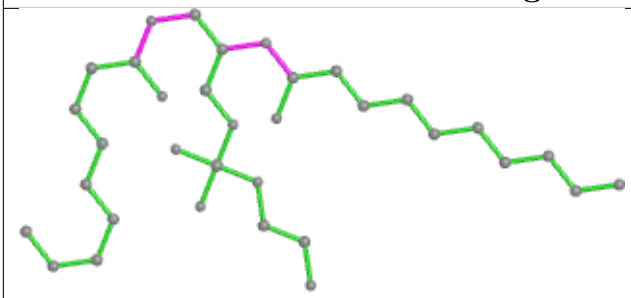


Torsions

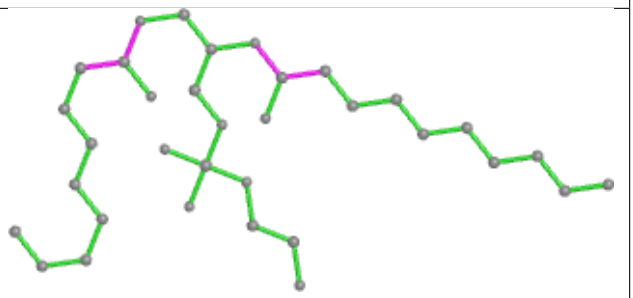


Rings

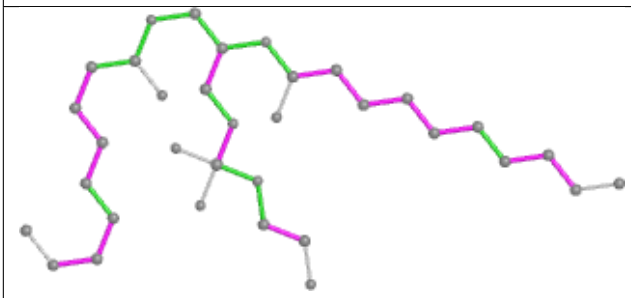
Ligand PTY B 705



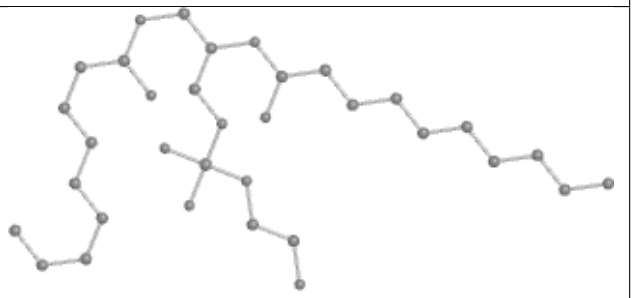
Bond lengths



Bond angles

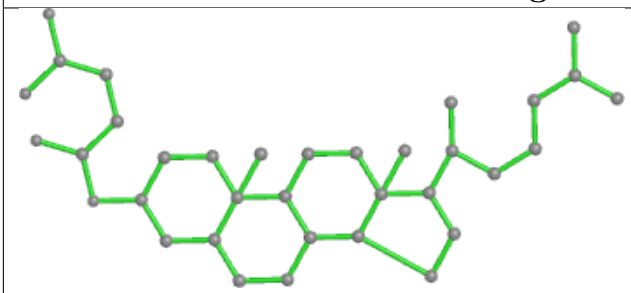


Torsions

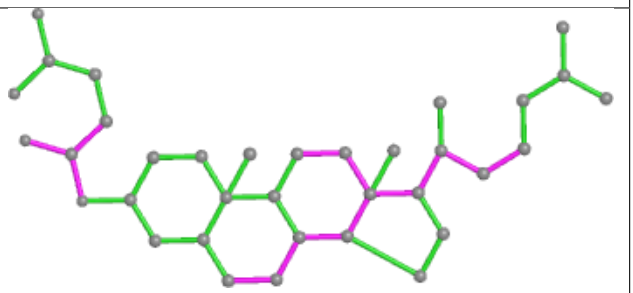


Rings

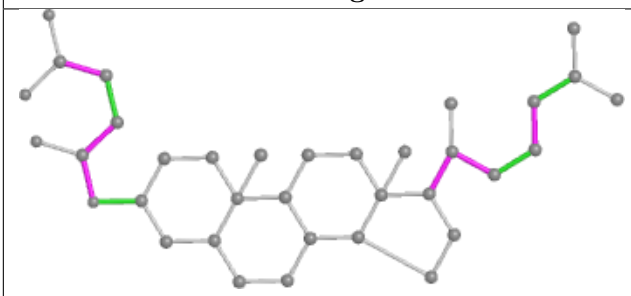
Ligand Y01 A 601



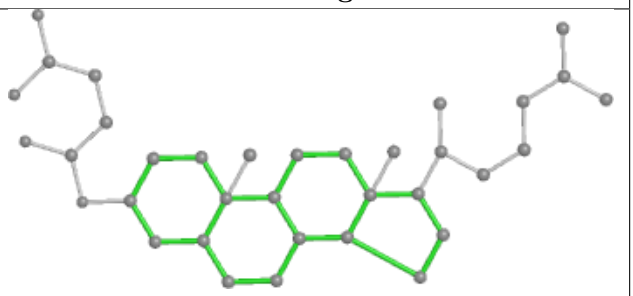
Bond lengths



Bond angles

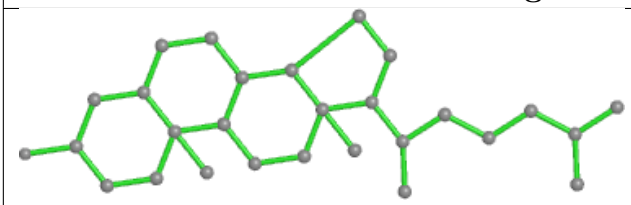


Torsions

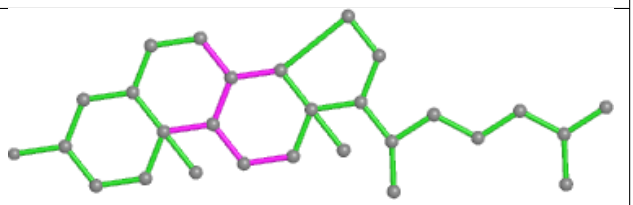


Rings

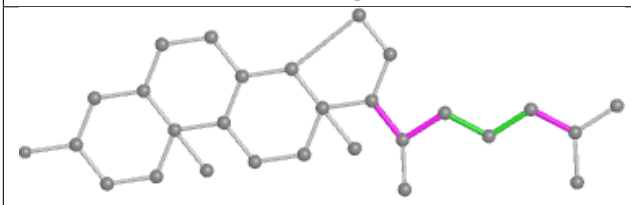
Ligand CLR B 706



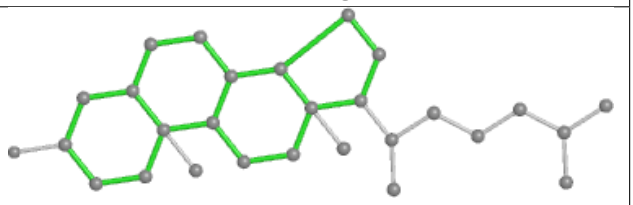
Bond lengths



Bond angles

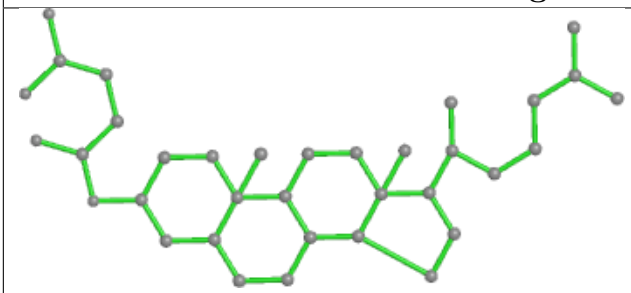


Torsions

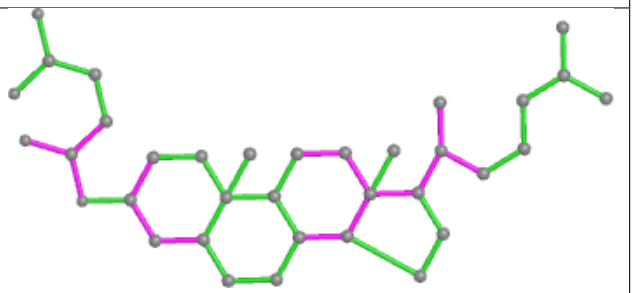


Rings

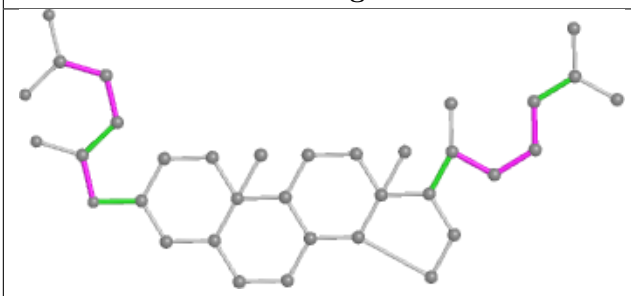
Ligand Y01 A 602



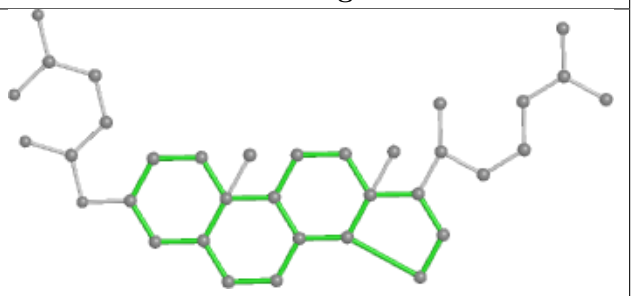
Bond lengths



Bond angles

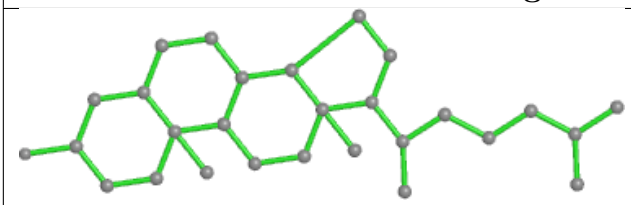


Torsions

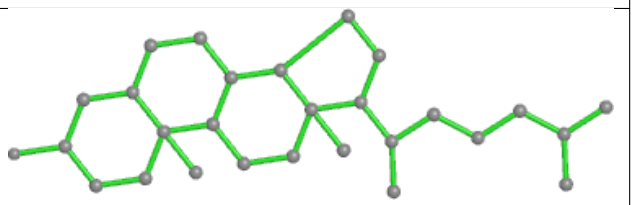


Rings

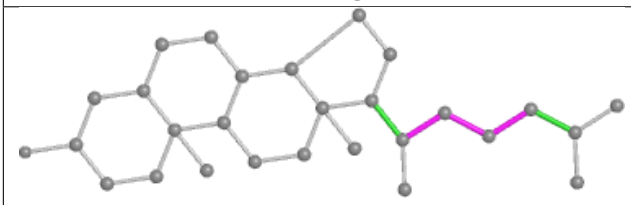
Ligand CLR A 605



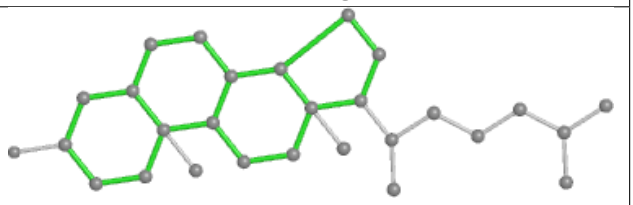
Bond lengths



Bond angles

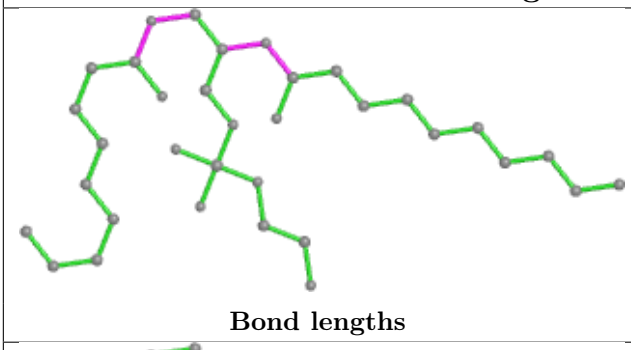


Torsions

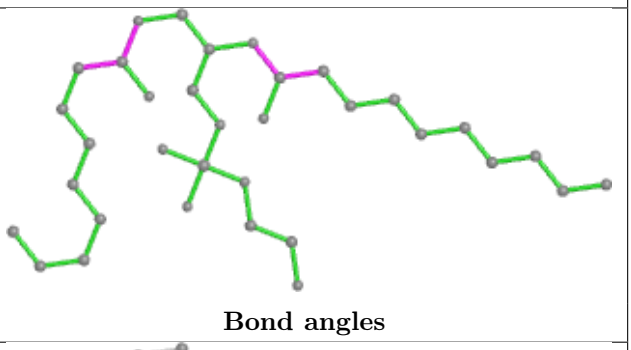


Rings

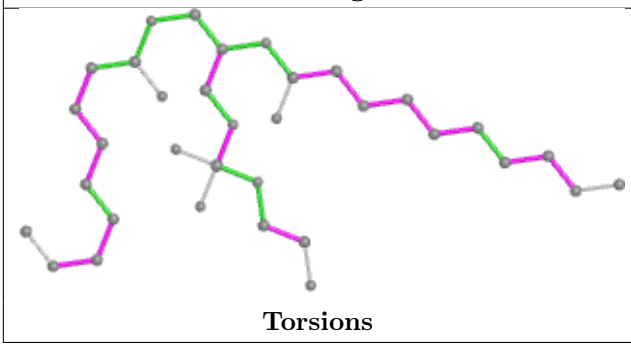
Ligand PTY A 604



Bond lengths



Bond angles



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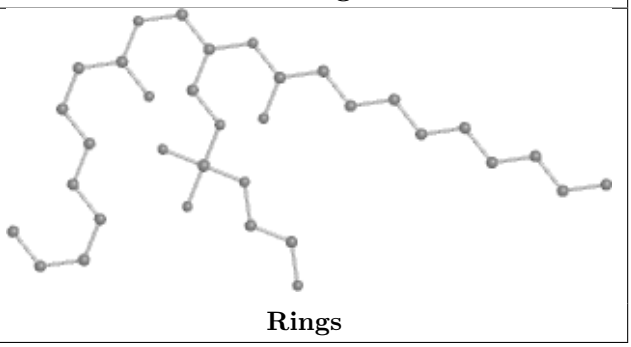
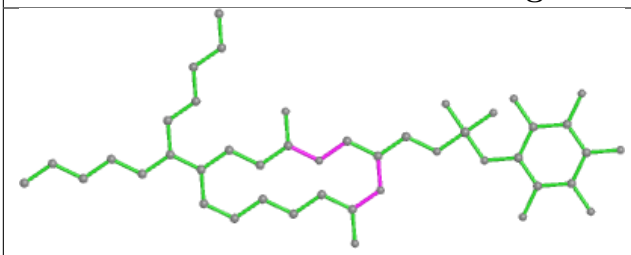
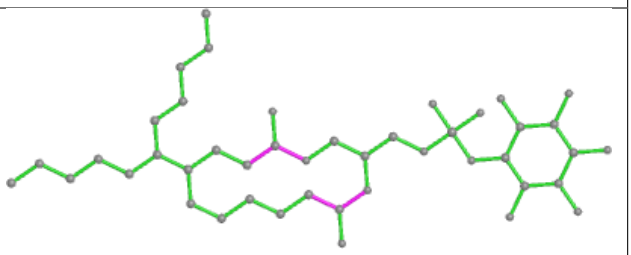


Rings

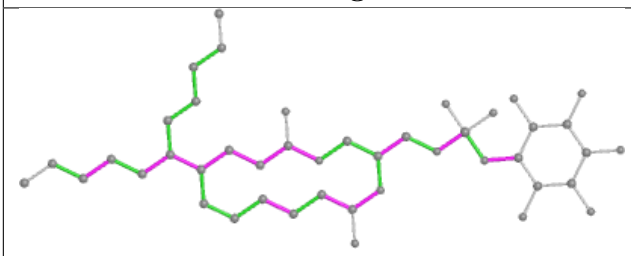
Ligand T7X A 603



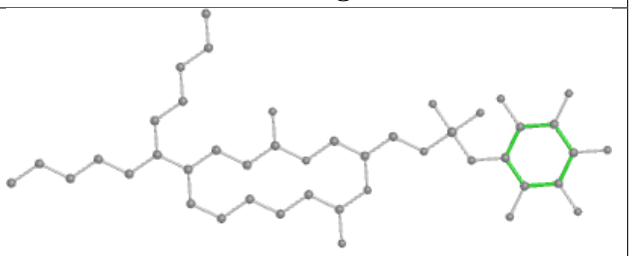
Bond lengths



Bond angles

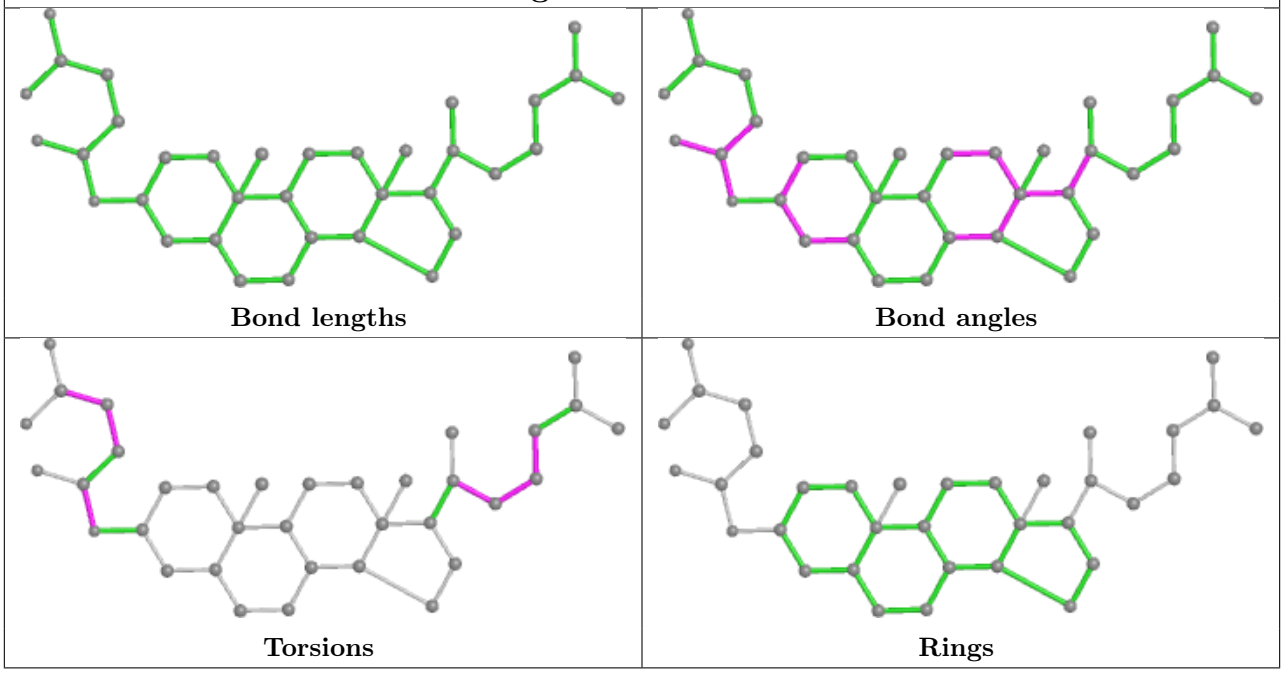


Torsions

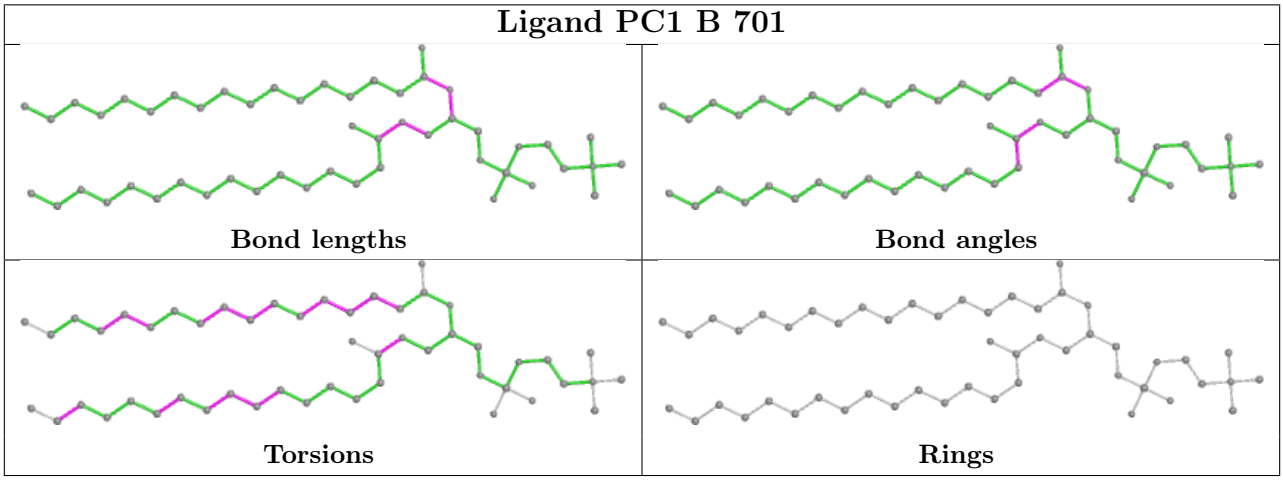


Rings

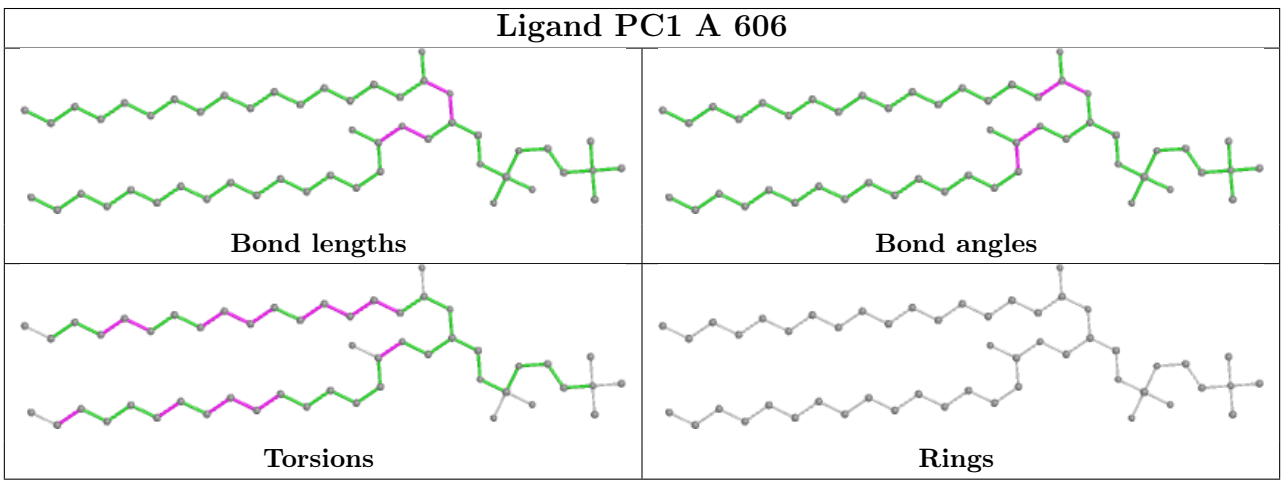
Ligand Y01 B 703



Ligand PC1 B 701



Ligand PC1 A 606



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.