



Full wwPDB EM Model Validation Report ⓘ

May 25, 2020 – 11:52 AM EDT

PDB ID : 6V1X
EMDB ID : EMD-21018
Title : Cryo-EM Structure of the Hyperpolarization-Activated Potassium Channel
KAT1: Tetramer
Authors : Clark, M.D.; Contreras, G.F.; Shen, R.; Perozo, E.
Deposited on : 2019-11-21
Resolution : 3.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
buster-report : 1.1.7 (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.10.1

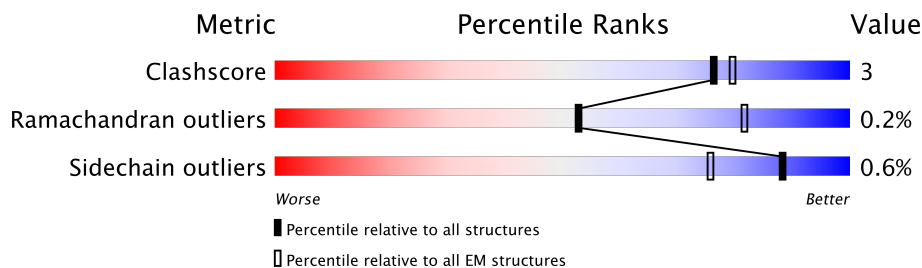
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

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 on 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	512	79% 8% 13%
1	B	512	79% 8% 13%
1	C	512	79% 8% 13%
1	D	512	79% 8% 13%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13996 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 Potassium channel KAT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	446	Total	C	N	O	S	0	0
			3436	2273	569	578	16		
1	B	446	Total	C	N	O	S	0	0
			3436	2273	569	578	16		
1	C	446	Total	C	N	O	S	0	0
			3436	2273	569	578	16		
1	D	446	Total	C	N	O	S	0	0
			3436	2273	569	578	16		

There are 40 discrepancies between the modelled and reference sequences:

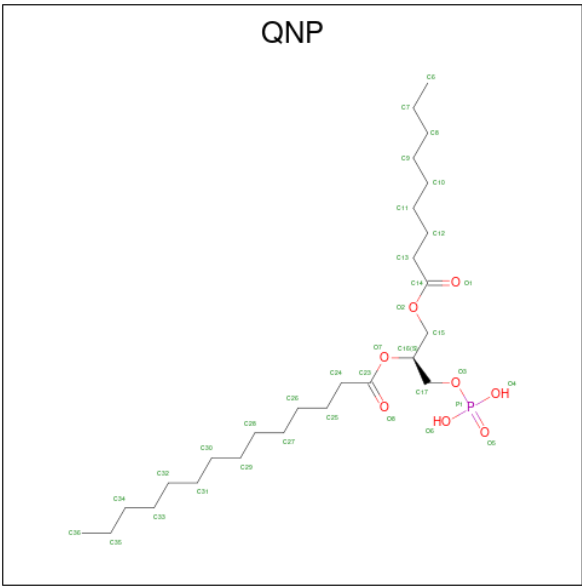
Chain	Residue	Modelled	Actual	Comment	Reference
A	503	SER	-	expression tag	UNP Q39128
A	504	ARG	-	expression tag	UNP Q39128
A	505	GLY	-	expression tag	UNP Q39128
A	506	SER	-	expression tag	UNP Q39128
A	507	LEU	-	expression tag	UNP Q39128
A	508	GLU	-	expression tag	UNP Q39128
A	509	VAL	-	expression tag	UNP Q39128
A	510	LEU	-	expression tag	UNP Q39128
A	511	PHE	-	expression tag	UNP Q39128
A	512	GLN	-	expression tag	UNP Q39128
B	503	SER	-	expression tag	UNP Q39128
B	504	ARG	-	expression tag	UNP Q39128
B	505	GLY	-	expression tag	UNP Q39128
B	506	SER	-	expression tag	UNP Q39128
B	507	LEU	-	expression tag	UNP Q39128
B	508	GLU	-	expression tag	UNP Q39128
B	509	VAL	-	expression tag	UNP Q39128
B	510	LEU	-	expression tag	UNP Q39128
B	511	PHE	-	expression tag	UNP Q39128
B	512	GLN	-	expression tag	UNP Q39128
C	503	SER	-	expression tag	UNP Q39128
C	504	ARG	-	expression tag	UNP Q39128

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Chain	Residue	Modelled	Actual	Comment	Reference
C	505	GLY	-	expression tag	UNP Q39128
C	506	SER	-	expression tag	UNP Q39128
C	507	LEU	-	expression tag	UNP Q39128
C	508	GLU	-	expression tag	UNP Q39128
C	509	VAL	-	expression tag	UNP Q39128
C	510	LEU	-	expression tag	UNP Q39128
C	511	PHE	-	expression tag	UNP Q39128
C	512	GLN	-	expression tag	UNP Q39128
D	503	SER	-	expression tag	UNP Q39128
D	504	ARG	-	expression tag	UNP Q39128
D	505	GLY	-	expression tag	UNP Q39128
D	506	SER	-	expression tag	UNP Q39128
D	507	LEU	-	expression tag	UNP Q39128
D	508	GLU	-	expression tag	UNP Q39128
D	509	VAL	-	expression tag	UNP Q39128
D	510	LEU	-	expression tag	UNP Q39128
D	511	PHE	-	expression tag	UNP Q39128
D	512	GLN	-	expression tag	UNP Q39128

- Molecule 2 is (2S)-1-(nonanoyloxy)-3-(phosphonoxy)propan-2-yl tetradecanoate (three-letter code: QNP) (formula: C₂₆H₅₁O₈P).



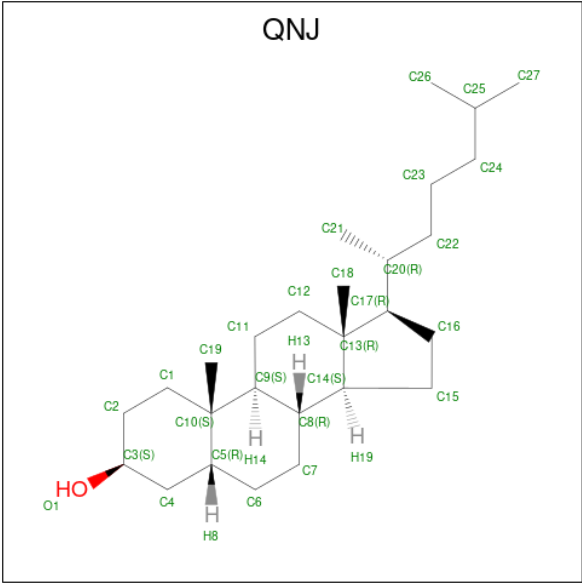
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	O	P	0
			35	26	8	1	
2	B	1	Total	C	O	P	0
			35	26	8	1	

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Mol	Chain	Residues	Atoms				AltConf
2	C	1	Total	C	O	P	0
			35	26	8	1	
2	D	1	Total	C	O	P	0
			35	26	8	1	

- Molecule 3 is (3beta,5beta,14beta,17alpha)-cholestan-3-ol (three-letter code: QNJ) (formula: $C_{27}H_{48}O$).




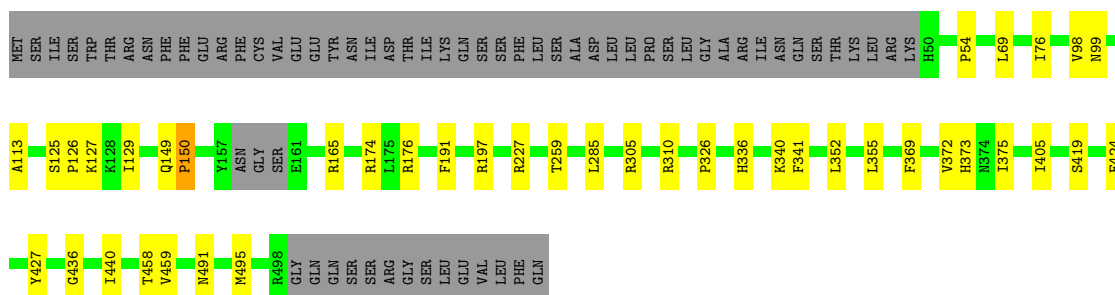
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	O		0
			28	27	1		
3	B	1	Total	C	O		0
			28	27	1		
3	C	1	Total	C	O		0
			28	27	1		
3	D	1	Total	C	O		0
			28	27	1		

3 Residue-property plots


These plots are drawn for all protein, RNA and DNA 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.

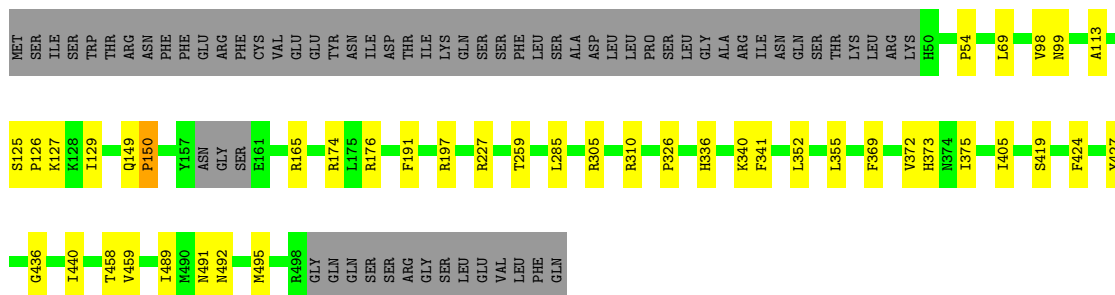
- Molecule 1: Potassium channel KAT1

Chain A: 




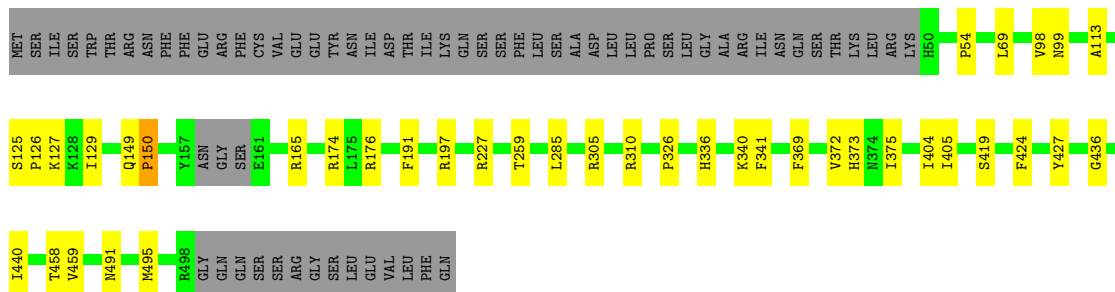
- Molecule 1: Potassium channel KAT1

Chain B: 



- Molecule 1: Potassium channel KAT1

Chain C: 



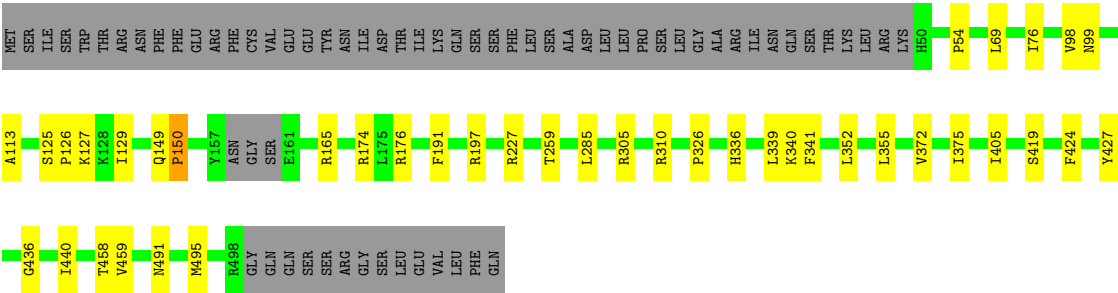
● Molecule 1: Potassium channel KAT1

Chain D:

79%

8%

13%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	91689	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)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k 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: QNP, QNJ

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	0.50	1/3537 (0.0%)	0.62	0/4837
1	B	0.50	1/3537 (0.0%)	0.62	0/4837
1	C	0.50	1/3537 (0.0%)	0.62	0/4837
1	D	0.50	1/3537 (0.0%)	0.62	0/4837
All	All	0.50	4/14148 (0.0%)	0.62	0/19348

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	150	PRO	C-N	7.00	1.50	1.34
1	C	150	PRO	C-N	7.00	1.50	1.34
1	D	150	PRO	C-N	7.00	1.50	1.34
1	B	150	PRO	C-N	6.97	1.50	1.34

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	3436	0	3246	24	0
1	B	3436	0	3246	24	0
1	C	3436	0	3246	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3436	0	3246	25	0
2	A	35	0	0	1	0
2	B	35	0	0	1	0
2	C	35	0	0	1	0
2	D	35	0	0	1	0
3	A	28	0	0	0	0
3	B	28	0	0	0	0
3	C	28	0	0	0	0
3	D	28	0	0	0	0
All	All	13996	0	12984	88	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 3.

All (88) 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:C:424:PHE:CB	1:C:436:GLY:HA3	2.24	0.68
1:B:424:PHE:CB	1:B:436:GLY:HA3	2.24	0.68
1:A:424:PHE:CB	1:A:436:GLY:HA3	2.24	0.67
1:D:424:PHE:CB	1:D:436:GLY:HA3	2.24	0.67
1:A:191:PHE:O	1:B:310:ARG:NH1	2.31	0.64
1:A:419:SER:HA	1:A:440:ILE:HG12	1.89	0.55
1:D:336:HIS:HE1	1:D:340:LYS:HE3	1.72	0.55
1:C:336:HIS:HE1	1:C:340:LYS:HE3	1.72	0.55
1:B:419:SER:HA	1:B:440:ILE:HG12	1.89	0.55
1:A:310:ARG:NH1	1:D:191:PHE:O	2.40	0.55
1:C:191:PHE:O	1:D:310:ARG:NH1	2.40	0.54
1:C:419:SER:HA	1:C:440:ILE:HG12	1.89	0.54
1:A:336:HIS:HE1	1:A:340:LYS:HE3	1.72	0.54
1:B:491:ASN:O	1:B:495:MET:CB	2.56	0.54
1:B:405:ILE:H	1:B:459:VAL:HB	1.73	0.54
1:D:405:ILE:H	1:D:459:VAL:HB	1.73	0.54
1:A:491:ASN:O	1:A:495:MET:CB	2.56	0.53
1:C:405:ILE:H	1:C:459:VAL:HB	1.73	0.53
1:D:491:ASN:O	1:D:495:MET:CB	2.56	0.53
1:B:336:HIS:HE1	1:B:340:LYS:HE3	1.72	0.53
1:A:405:ILE:H	1:A:459:VAL:HB	1.73	0.53
1:B:191:PHE:O	1:C:310:ARG:NH1	2.42	0.53
1:C:491:ASN:O	1:C:495:MET:CB	2.56	0.53
1:D:419:SER:HA	1:D:440:ILE:HG12	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:ASN:OD1	1:A:174:ARG:NH2	2.37	0.53
1:D:99:ASN:OD1	1:D:174:ARG:NH2	2.37	0.52
1:B:99:ASN:OD1	1:B:174:ARG:NH2	2.37	0.51
1:A:336:HIS:CE1	1:A:340:LYS:HE3	2.46	0.50
1:C:336:HIS:CE1	1:C:340:LYS:HE3	2.46	0.50
1:B:336:HIS:CE1	1:B:340:LYS:HE3	2.46	0.50
1:D:336:HIS:CE1	1:D:340:LYS:HE3	2.46	0.50
1:B:69:LEU:HD11	1:B:98:VAL:HG22	1.95	0.49
1:A:69:LEU:HD11	1:A:98:VAL:HG22	1.95	0.49
1:C:69:LEU:HD11	1:C:98:VAL:HG22	1.95	0.48
1:D:69:LEU:HD11	1:D:98:VAL:HG22	1.95	0.48
1:C:99:ASN:OD1	1:C:174:ARG:NH2	2.37	0.46
1:B:149:GLN:HE21	1:B:165:ARG:HA	1.81	0.46
1:C:149:GLN:HE21	1:C:165:ARG:HA	1.81	0.46
1:A:259:THR:HG22	1:D:285:LEU:HD22	1.98	0.46
1:C:285:LEU:HD22	1:D:259:THR:HG22	1.98	0.46
1:D:149:GLN:HE21	1:D:165:ARG:HA	1.81	0.45
1:A:285:LEU:HD22	1:B:259:THR:HG22	1.98	0.45
1:A:149:GLN:HE21	1:A:165:ARG:HA	1.81	0.45
1:B:427:TYR:CB	1:B:458:THR:OG1	2.65	0.44
1:C:427:TYR:CB	1:C:458:THR:OG1	2.65	0.44
1:D:126:PRO:HA	1:D:129:ILE:HD12	1.99	0.44
1:D:427:TYR:CB	1:D:458:THR:OG1	2.65	0.44
1:A:126:PRO:HA	1:A:129:ILE:HD12	1.99	0.44
1:C:126:PRO:HA	1:C:129:ILE:HD12	1.99	0.44
1:A:427:TYR:CB	1:A:458:THR:OG1	2.65	0.44
1:B:372:VAL:HA	1:B:375:ILE:HD11	2.00	0.44
1:C:372:VAL:HA	1:C:375:ILE:HD11	2.00	0.43
1:B:126:PRO:HA	1:B:129:ILE:HD12	1.99	0.43
1:C:197:ARG:NH1	2:C:602:QNP:O4	2.51	0.43
1:B:197:ARG:NH1	2:B:601:QNP:O4	2.52	0.43
1:D:197:ARG:NH1	2:D:602:QNP:O4	2.51	0.43
1:A:54:PRO:HD3	1:A:113:ALA:HB3	2.01	0.43
1:A:125:SER:O	1:A:127:LYS:N	2.52	0.43
1:B:125:SER:O	1:B:127:LYS:N	2.52	0.43
1:D:372:VAL:HA	1:D:375:ILE:HD11	2.00	0.43
1:C:54:PRO:HD3	1:C:113:ALA:HB3	2.01	0.43
1:B:54:PRO:HD3	1:B:113:ALA:HB3	2.01	0.42
1:A:197:ARG:NH1	2:A:601:QNP:O4	2.51	0.42
1:C:149:GLN:N	1:C:150:PRO:CD	2.82	0.42
1:B:285:LEU:HD22	1:C:259:THR:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:VAL:HA	1:A:375:ILE:HD11	2.00	0.42
1:C:125:SER:O	1:C:127:LYS:N	2.52	0.42
1:D:54:PRO:HD3	1:D:113:ALA:HB3	2.01	0.42
1:D:125:SER:O	1:D:127:LYS:N	2.52	0.42
1:A:149:GLN:N	1:A:150:PRO:CD	2.82	0.42
1:B:149:GLN:N	1:B:150:PRO:CD	2.82	0.42
1:A:305:ARG:HG2	1:A:341:PHE:HE1	1.85	0.42
1:D:69:LEU:HD12	1:D:69:LEU:HA	1.90	0.42
1:B:305:ARG:HG2	1:B:341:PHE:HE1	1.85	0.42
1:D:149:GLN:N	1:D:150:PRO:CD	2.82	0.41
1:D:305:ARG:HG2	1:D:341:PHE:HE1	1.85	0.41
1:C:369:PHE:O	1:C:373:HIS:HB2	2.21	0.41
1:B:369:PHE:O	1:B:373:HIS:HB2	2.21	0.41
1:C:305:ARG:HG2	1:C:341:PHE:HE1	1.85	0.41
1:B:352:LEU:HD23	1:B:355:LEU:HD12	2.03	0.41
1:D:339:LEU:HA	1:D:339:LEU:HD23	1.89	0.40
1:D:76:ILE:HA	1:D:76:ILE:HD13	1.92	0.40
1:B:489:ILE:HA	1:B:492:ASN:HD22	1.87	0.40
1:C:404:ILE:N	1:C:459:VAL:O	2.45	0.40
1:A:352:LEU:HD23	1:A:355:LEU:HD12	2.03	0.40
1:A:76:ILE:HA	1:A:76:ILE:HD13	1.92	0.40
1:A:369:PHE:O	1:A:373:HIS:HB2	2.21	0.40
1:D:352:LEU:HD23	1:D:355:LEU:HD12	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	442/512 (86%)	399 (90%)	42 (10%)	1 (0%)	49	83
1	B	442/512 (86%)	399 (90%)	42 (10%)	1 (0%)	49	83

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	442/512 (86%)	399 (90%)	42 (10%)	1 (0%)	49	83
1	D	442/512 (86%)	399 (90%)	42 (10%)	1 (0%)	49	83
All	All	1768/2048 (86%)	1596 (90%)	168 (10%)	4 (0%)	53	83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	326	PRO
1	B	326	PRO
1	C	326	PRO
1	D	326	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	334/459 (73%)	332 (99%)	2 (1%)	87	95
1	B	334/459 (73%)	332 (99%)	2 (1%)	87	95
1	C	334/459 (73%)	332 (99%)	2 (1%)	87	95
1	D	334/459 (73%)	332 (99%)	2 (1%)	87	95
All	All	1336/1836 (73%)	1328 (99%)	8 (1%)	88	95

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	176	ARG
1	A	227	ARG
1	B	176	ARG
1	B	227	ARG
1	C	176	ARG
1	C	227	ARG
1	D	176	ARG
1	D	227	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	336	HIS
1	A	492	ASN
1	B	336	HIS
1	B	492	ASN
1	C	336	HIS
1	C	492	ASN
1	D	336	HIS
1	D	492	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

8 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	$\# Z > 2$
3	QNJ	B	602	-	31,31,31	1.80	8 (25%)	48,48,48	1.95	12 (25%)
3	QNJ	D	601	-	31,31,31	1.80	8 (25%)	48,48,48	1.95	12 (25%)
2	QNP	A	601	-	34,34,34	1.08	5 (14%)	38,39,39	1.40	5 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	QNP	C	602	-	34,34,34	1.08	5 (14%)	38,39,39	1.40	5 (13%)
2	QNP	D	602	-	34,34,34	1.08	5 (14%)	38,39,39	1.40	5 (13%)
3	QNJ	C	601	-	31,31,31	1.80	8 (25%)	48,48,48	1.95	12 (25%)
3	QNJ	A	602	-	31,31,31	1.80	8 (25%)	48,48,48	1.95	12 (25%)
2	QNP	B	601	-	34,34,34	1.08	5 (14%)	38,39,39	1.40	5 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	QNJ	B	602	-	-	5/10/68/68	0/4/4/4
3	QNJ	D	601	-	-	5/10/68/68	0/4/4/4
2	QNP	A	601	-	-	19/36/36/36	-
2	QNP	C	602	-	-	19/36/36/36	-
2	QNP	D	602	-	-	19/36/36/36	-
3	QNJ	C	601	-	-	5/10/68/68	0/4/4/4
3	QNJ	A	602	-	-	5/10/68/68	0/4/4/4
2	QNP	B	601	-	-	19/36/36/36	-

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	QNJ	C19-C10	-4.43	1.46	1.54
3	D	601	QNJ	C19-C10	-4.43	1.46	1.54
3	C	601	QNJ	C19-C10	-4.43	1.46	1.54
3	A	602	QNJ	C19-C10	-4.43	1.46	1.54
3	B	602	QNJ	C12-C11	-3.59	1.45	1.53
3	D	601	QNJ	C12-C11	-3.59	1.45	1.53
3	C	601	QNJ	C12-C11	-3.59	1.45	1.53
3	A	602	QNJ	C12-C11	-3.59	1.45	1.53
3	B	602	QNJ	C20-C17	3.22	1.60	1.54
3	D	601	QNJ	C20-C17	3.22	1.60	1.54
3	C	601	QNJ	C20-C17	3.22	1.60	1.54
3	A	602	QNJ	C20-C17	3.22	1.60	1.54
3	B	602	QNJ	O1-C3	-3.12	1.34	1.43
3	D	601	QNJ	O1-C3	-3.12	1.34	1.43
3	C	601	QNJ	O1-C3	-3.12	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	QNJ	O1-C3	-3.12	1.34	1.43
3	B	602	QNJ	C22-C20	-3.03	1.46	1.54
3	D	601	QNJ	C22-C20	-3.03	1.46	1.54
3	C	601	QNJ	C22-C20	-3.03	1.46	1.54
3	A	602	QNJ	C22-C20	-3.03	1.46	1.54
3	B	602	QNJ	C10-C9	-2.95	1.50	1.56
3	D	601	QNJ	C10-C9	-2.95	1.50	1.56
3	C	601	QNJ	C10-C9	-2.95	1.50	1.56
3	A	602	QNJ	C10-C9	-2.95	1.50	1.56
2	A	601	QNP	O7-C16	-2.71	1.39	1.46
2	C	602	QNP	O7-C16	-2.71	1.39	1.46
2	D	602	QNP	O7-C16	-2.71	1.39	1.46
2	B	601	QNP	O7-C16	-2.70	1.39	1.46
2	A	601	QNP	O2-C14	2.40	1.40	1.33
2	D	602	QNP	O2-C14	2.40	1.40	1.33
2	C	602	QNP	O2-C14	2.39	1.40	1.33
2	B	601	QNP	O2-C14	2.38	1.40	1.33
3	B	602	QNJ	C11-C9	-2.29	1.49	1.53
3	D	601	QNJ	C11-C9	-2.29	1.49	1.53
3	C	601	QNJ	C11-C9	-2.29	1.49	1.53
3	A	602	QNJ	C11-C9	-2.29	1.49	1.53
2	D	602	QNP	O2-C15	-2.26	1.40	1.45
2	C	602	QNP	O2-C15	-2.25	1.40	1.45
2	A	601	QNP	O2-C15	-2.23	1.40	1.45
2	B	601	QNP	O2-C15	-2.22	1.40	1.45
3	B	602	QNJ	C1-C2	-2.17	1.48	1.53
3	D	601	QNJ	C1-C2	-2.17	1.48	1.53
3	C	601	QNJ	C1-C2	-2.17	1.48	1.53
3	A	602	QNJ	C1-C2	-2.17	1.48	1.53
2	D	602	QNP	O7-C23	2.17	1.40	1.34
2	B	601	QNP	O7-C23	2.16	1.40	1.34
2	C	602	QNP	O7-C23	2.15	1.40	1.34
2	A	601	QNP	O7-C23	2.12	1.40	1.34
2	C	602	QNP	O1-C14	-2.11	1.16	1.22
2	D	602	QNP	O1-C14	-2.11	1.16	1.22
2	B	601	QNP	O1-C14	-2.09	1.16	1.22
2	A	601	QNP	O1-C14	-2.07	1.16	1.22

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	QNJ	C21-C20-C22	-6.11	100.79	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	601	QNJ	C21-C20-C22	-6.11	100.79	110.36
3	C	601	QNJ	C21-C20-C22	-6.11	100.79	110.36
3	A	602	QNJ	C21-C20-C22	-6.11	100.79	110.36
3	B	602	QNJ	C4-C5-C10	4.90	117.87	112.66
3	D	601	QNJ	C4-C5-C10	4.90	117.87	112.66
3	C	601	QNJ	C4-C5-C10	4.90	117.87	112.66
3	A	602	QNJ	C4-C5-C10	4.90	117.87	112.66
3	B	602	QNJ	C5-C4-C3	3.98	118.61	112.76
3	D	601	QNJ	C5-C4-C3	3.98	118.61	112.76
3	C	601	QNJ	C5-C4-C3	3.98	118.61	112.76
3	A	602	QNJ	C5-C4-C3	3.98	118.61	112.76
3	B	602	QNJ	C21-C20-C17	3.93	118.93	112.92
3	D	601	QNJ	C21-C20-C17	3.93	118.93	112.92
3	C	601	QNJ	C21-C20-C17	3.93	118.93	112.92
3	A	602	QNJ	C21-C20-C17	3.93	118.93	112.92
3	B	602	QNJ	C11-C9-C10	-3.76	109.58	113.91
3	D	601	QNJ	C11-C9-C10	-3.76	109.58	113.91
3	C	601	QNJ	C11-C9-C10	-3.76	109.58	113.91
3	A	602	QNJ	C11-C9-C10	-3.76	109.58	113.91
2	A	601	QNP	O7-C23-C24	3.52	119.08	111.50
2	C	602	QNP	O7-C23-C24	3.51	119.07	111.50
2	B	601	QNP	O7-C23-C24	3.49	119.02	111.50
2	D	602	QNP	O7-C23-C24	3.48	119.00	111.50
2	A	601	QNP	C17-C16-C15	-3.38	103.79	111.79
2	B	601	QNP	C17-C16-C15	-3.38	103.80	111.79
2	C	602	QNP	C17-C16-C15	-3.36	103.83	111.79
2	D	602	QNP	C17-C16-C15	-3.36	103.84	111.79
2	D	602	QNP	O2-C14-C13	3.26	122.14	111.91
2	A	601	QNP	O2-C14-C13	3.26	122.14	111.91
2	B	601	QNP	O2-C14-C13	3.26	122.14	111.91
2	C	602	QNP	O2-C14-C13	3.24	122.09	111.91
3	B	602	QNJ	C1-C10-C5	3.09	112.34	107.77
3	D	601	QNJ	C1-C10-C5	3.09	112.34	107.77
3	C	601	QNJ	C1-C10-C5	3.09	112.34	107.77
3	A	602	QNJ	C1-C10-C5	3.09	112.34	107.77
3	B	602	QNJ	C16-C17-C20	-3.09	107.36	112.15
3	D	601	QNJ	C16-C17-C20	-3.09	107.36	112.15
3	C	601	QNJ	C16-C17-C20	-3.09	107.36	112.15
3	A	602	QNJ	C16-C17-C20	-3.09	107.36	112.15
3	B	602	QNJ	C13-C14-C8	-2.98	109.96	114.38
3	D	601	QNJ	C13-C14-C8	-2.98	109.96	114.38
3	C	601	QNJ	C13-C14-C8	-2.98	109.96	114.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	QNJ	C13-C14-C8	-2.98	109.96	114.38
2	A	601	QNP	O3-P1-O5	2.84	114.43	106.47
2	D	602	QNP	O3-P1-O5	2.83	114.42	106.47
2	C	602	QNP	O3-P1-O5	2.83	114.41	106.47
2	B	601	QNP	O3-P1-O5	2.82	114.38	106.47
3	B	602	QNJ	C19-C10-C5	-2.76	105.68	110.36
3	D	601	QNJ	C19-C10-C5	-2.76	105.68	110.36
3	C	601	QNJ	C19-C10-C5	-2.76	105.68	110.36
3	A	602	QNJ	C19-C10-C5	-2.76	105.68	110.36
3	B	602	QNJ	C9-C10-C5	2.53	112.13	108.58
3	D	601	QNJ	C9-C10-C5	2.53	112.13	108.58
3	C	601	QNJ	C9-C10-C5	2.53	112.13	108.58
3	A	602	QNJ	C9-C10-C5	2.53	112.13	108.58
3	B	602	QNJ	C6-C7-C8	2.19	115.74	112.14
3	D	601	QNJ	C6-C7-C8	2.19	115.74	112.14
3	C	601	QNJ	C6-C7-C8	2.19	115.74	112.14
3	A	602	QNJ	C6-C7-C8	2.19	115.74	112.14
3	B	602	QNJ	C16-C17-C13	-2.09	101.33	103.84
3	D	601	QNJ	C16-C17-C13	-2.09	101.33	103.84
3	C	601	QNJ	C16-C17-C13	-2.09	101.33	103.84
3	A	602	QNJ	C16-C17-C13	-2.09	101.33	103.84
2	C	602	QNP	O1-C14-C13	-2.02	115.86	123.73
2	A	601	QNP	O1-C14-C13	-2.02	115.86	123.73
2	D	602	QNP	O1-C14-C13	-2.02	115.87	123.73
2	B	601	QNP	O1-C14-C13	-2.01	115.88	123.73

There are no chirality outliers.

All (96) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	QNP	C24-C23-O7-C16
2	A	601	QNP	C17-O3-P1-O4
2	A	601	QNP	C17-O3-P1-O5
2	A	601	QNP	C17-O3-P1-O6
2	C	602	QNP	C24-C23-O7-C16
2	C	602	QNP	C17-O3-P1-O4
2	C	602	QNP	C17-O3-P1-O5
2	C	602	QNP	C17-O3-P1-O6
2	D	602	QNP	C24-C23-O7-C16
2	D	602	QNP	C17-O3-P1-O4
2	D	602	QNP	C17-O3-P1-O5
2	D	602	QNP	C17-O3-P1-O6

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Mol	Chain	Res	Type	Atoms
2	B	601	QNP	C24-C23-O7-C16
2	B	601	QNP	C17-O3-P1-O4
2	B	601	QNP	C17-O3-P1-O5
2	B	601	QNP	C17-O3-P1-O6
2	A	601	QNP	O8-C23-O7-C16
2	C	602	QNP	O8-C23-O7-C16
2	D	602	QNP	O8-C23-O7-C16
2	B	601	QNP	O8-C23-O7-C16
2	A	601	QNP	C13-C14-O2-C15
2	C	602	QNP	C13-C14-O2-C15
2	D	602	QNP	C13-C14-O2-C15
2	B	601	QNP	C13-C14-O2-C15
2	A	601	QNP	O1-C14-O2-C15
2	C	602	QNP	O1-C14-O2-C15
2	D	602	QNP	O1-C14-O2-C15
2	B	601	QNP	O1-C14-O2-C15
3	B	602	QNJ	C17-C20-C22-C23
3	D	601	QNJ	C17-C20-C22-C23
3	C	601	QNJ	C17-C20-C22-C23
3	A	602	QNJ	C17-C20-C22-C23
3	B	602	QNJ	C21-C20-C22-C23
3	D	601	QNJ	C21-C20-C22-C23
3	C	601	QNJ	C21-C20-C22-C23
3	A	602	QNJ	C21-C20-C22-C23
2	A	601	QNP	C23-C24-C25-C26
2	C	602	QNP	C23-C24-C25-C26
2	D	602	QNP	C23-C24-C25-C26
2	B	601	QNP	C23-C24-C25-C26
3	B	602	QNJ	C16-C17-C20-C22
3	D	601	QNJ	C16-C17-C20-C22
3	C	601	QNJ	C16-C17-C20-C22
3	A	602	QNJ	C16-C17-C20-C22
2	A	601	QNP	C9-C10-C11-C12
2	C	602	QNP	C9-C10-C11-C12
2	D	602	QNP	C9-C10-C11-C12
2	B	601	QNP	C9-C10-C11-C12
2	A	601	QNP	C7-C8-C9-C10
2	C	602	QNP	C7-C8-C9-C10
2	D	602	QNP	C7-C8-C9-C10
2	B	601	QNP	C7-C8-C9-C10
2	A	601	QNP	C24-C25-C26-C27
2	C	602	QNP	C24-C25-C26-C27

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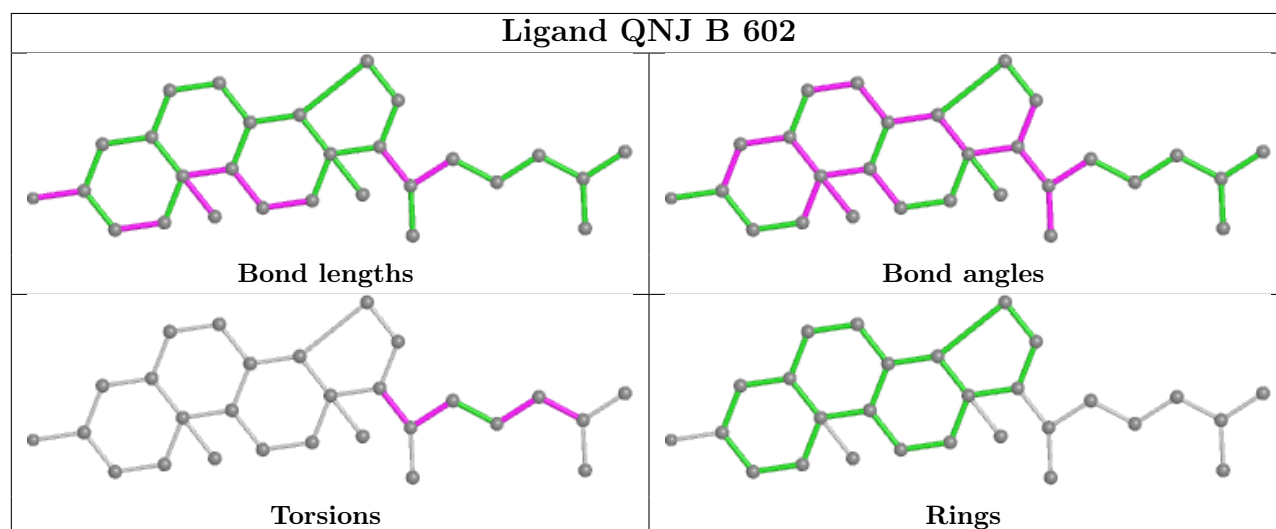
Mol	Chain	Res	Type	Atoms
2	D	602	QNP	C24-C25-C26-C27
2	B	601	QNP	C24-C25-C26-C27
2	A	601	QNP	C31-C32-C33-C34
2	C	602	QNP	C31-C32-C33-C34
2	D	602	QNP	C31-C32-C33-C34
2	B	601	QNP	C31-C32-C33-C34
2	A	601	QNP	C30-C31-C32-C33
2	C	602	QNP	C30-C31-C32-C33
2	D	602	QNP	C30-C31-C32-C33
2	B	601	QNP	C30-C31-C32-C33
2	A	601	QNP	C11-C10-C9-C8
2	C	602	QNP	C11-C10-C9-C8
2	D	602	QNP	C11-C10-C9-C8
2	B	601	QNP	C11-C10-C9-C8
2	A	601	QNP	C29-C30-C31-C32
2	C	602	QNP	C28-C29-C30-C31
2	A	601	QNP	C28-C29-C30-C31
2	C	602	QNP	C29-C30-C31-C32
2	D	602	QNP	C28-C29-C30-C31
2	D	602	QNP	C29-C30-C31-C32
2	B	601	QNP	C28-C29-C30-C31
2	B	601	QNP	C29-C30-C31-C32
2	A	601	QNP	C6-C7-C8-C9
2	C	602	QNP	C6-C7-C8-C9
2	D	602	QNP	C6-C7-C8-C9
2	B	601	QNP	C6-C7-C8-C9
2	A	601	QNP	C17-C16-O7-C23
2	C	602	QNP	C17-C16-O7-C23
2	D	602	QNP	C17-C16-O7-C23
2	B	601	QNP	C17-C16-O7-C23
3	B	602	QNJ	C22-C23-C24-C25
3	D	601	QNJ	C22-C23-C24-C25
3	C	601	QNJ	C22-C23-C24-C25
3	A	602	QNJ	C22-C23-C24-C25
2	A	601	QNP	C15-C16-C17-O3
2	C	602	QNP	C15-C16-C17-O3
2	D	602	QNP	C15-C16-C17-O3
2	B	601	QNP	C15-C16-C17-O3
3	B	602	QNJ	C23-C24-C25-C27
3	D	601	QNJ	C23-C24-C25-C27
3	C	601	QNJ	C23-C24-C25-C27
3	A	602	QNJ	C23-C24-C25-C27

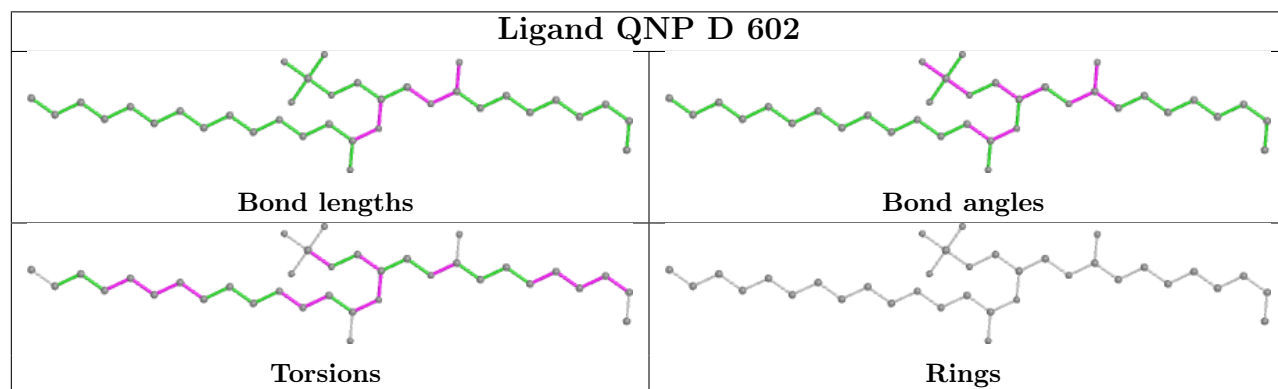
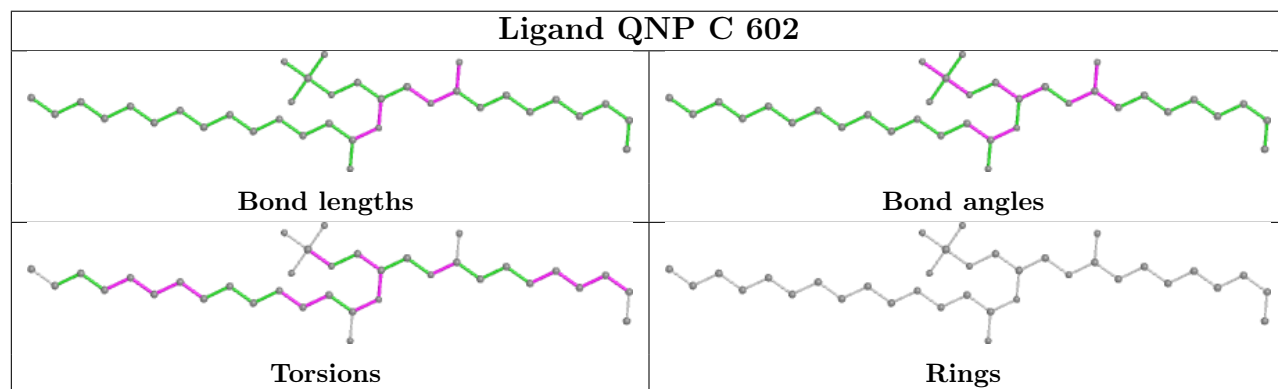
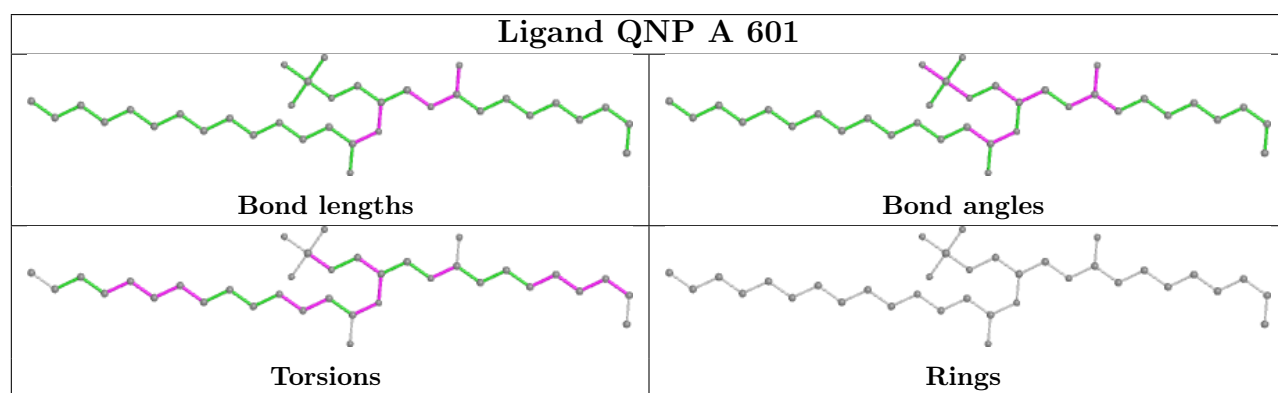
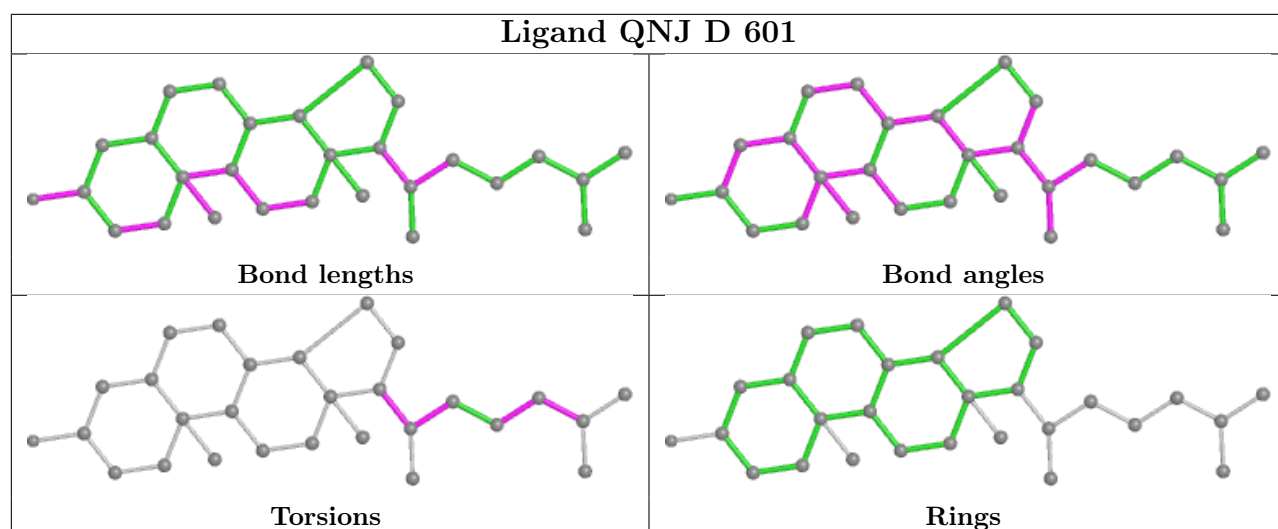
There are no ring outliers.

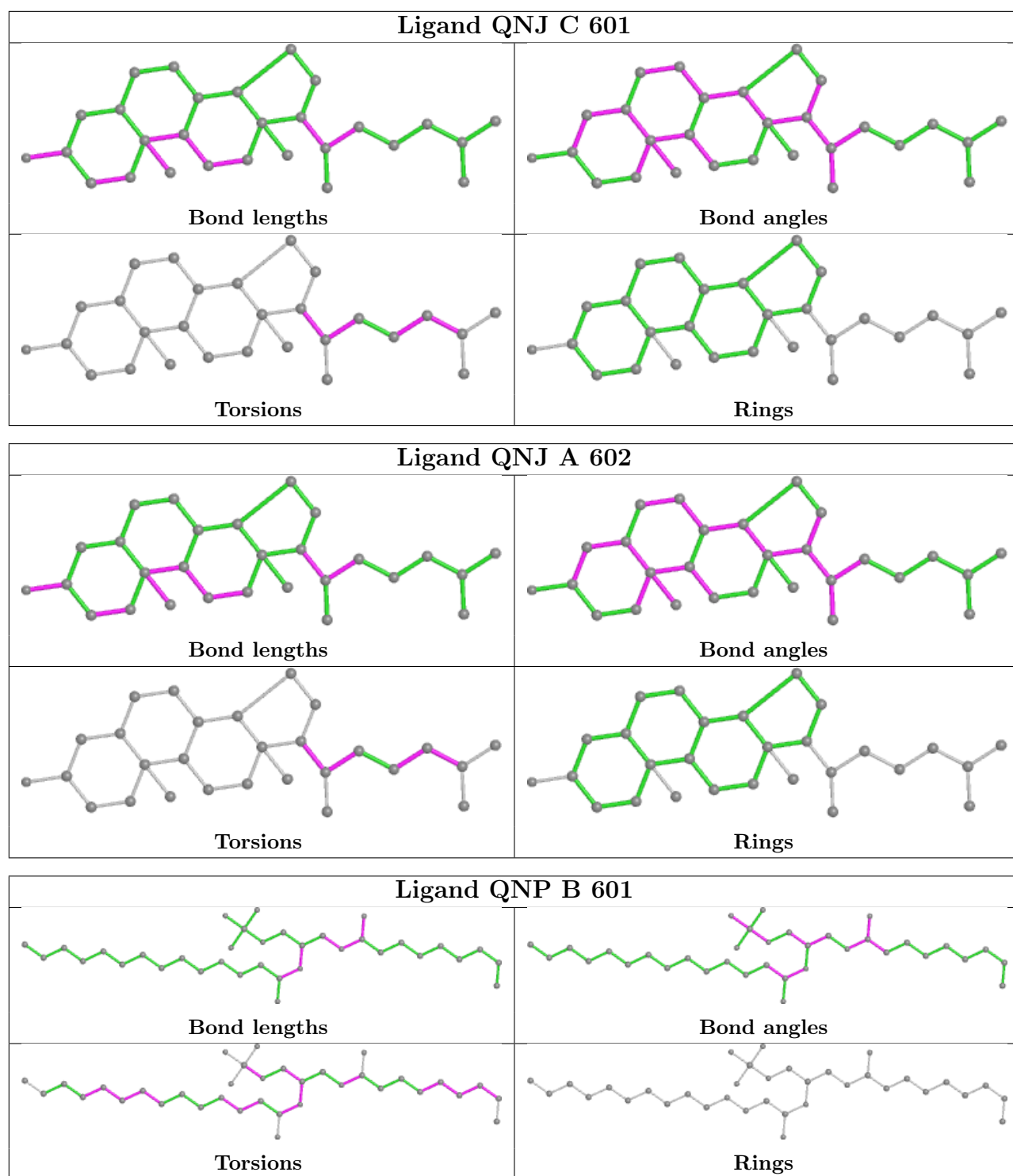
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	QNP	1	0
2	C	602	QNP	1	0
2	D	602	QNP	1	0
2	B	601	QNP	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 ⓘ

There are no chain breaks in this entry.