



Full wwPDB EM Validation Report ⓘ

Nov 9, 2025 – 12:19 AM JST

PDB ID : 9U7F / pdb_00009u7f
EMDB ID : EMD-63935
Title : structure of human KCNQ1-KCNE1-CaM complex
Authors : Hou, P.P.; Zhang, J.; Wan, S.Y.; Cheng, X.Y.; Zhong, L.; Hu, B.
Deposited on : 2025-03-24
Resolution : 2.90 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:

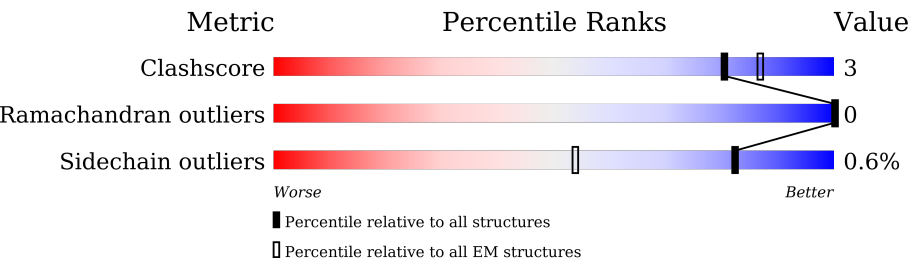
EMDB validation analysis : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

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 2.90 Å.

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






Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	676	<div><div>48%5%47%</div></div>
1	D	676	<div><div>47%5%47%</div></div>
1	G	676	<div><div>48%5%47%</div></div>
1	J	676	<div><div>47%5%47%</div></div>
2	B	149	<div><div>90%6%..</div></div>
2	E	149	<div><div>90%6%..</div></div>
2	H	149	<div><div>90%6%..</div></div>
2	K	149	<div><div>90%6%..</div></div>
3	C	129	<div><div>21%.78%</div></div>

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Mol	Chain	Length	Quality of chain
3	F	129	 21% 78%
3	I	129	 21% 78%
3	L	129	 21% 78%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 17224 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 voltage-gated channel subfamily KQT member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	360	Total	C	N	O	S	0	0
			2907	1905	507	484	11		
1	D	360	Total	C	N	O	S	0	0
			2907	1905	507	484	11		
1	G	360	Total	C	N	O	S	0	0
			2907	1905	507	484	11		
1	J	360	Total	C	N	O	S	0	0
			2907	1905	507	484	11		

- Molecule 2 is a protein called Calmodulin-1.

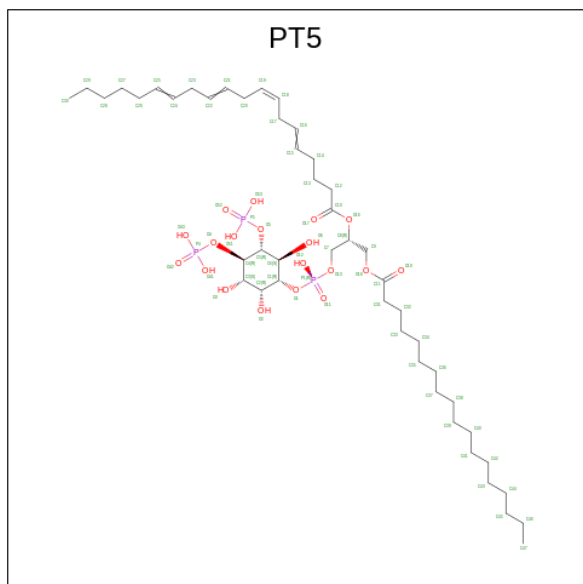
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	144	Total	C	N	O	S	0	0
			1105	681	180	235	9		
2	E	144	Total	C	N	O	S	0	0
			1105	681	180	235	9		
2	H	144	Total	C	N	O	S	0	0
			1105	681	180	235	9		
2	K	144	Total	C	N	O	S	0	0
			1105	681	180	235	9		

- Molecule 3 is a protein called Potassium voltage-gated channel subfamily E member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	28	Total	C	N	O	S	0	0
			222	155	29	36	2		
3	F	28	Total	C	N	O	S	0	0
			222	155	29	36	2		
3	I	28	Total	C	N	O	S	0	0
			222	155	29	36	2		
3	L	28	Total	C	N	O	S	0	0
			222	155	29	36	2		

- Molecule 4 is [(2R)-1-octadecanoyloxy-3-[oxidanyl]-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxida

nyl)-4,5-diphosphonoxy-cyclohexyl]oxy-phospho ryl]oxy-propan-2-yl] (8Z)-icosa-5,8,11,14-tetraenoate (CCD ID: PT5) (formula: $C_{47}H_{85}O_{19}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	O	P	0
			69	47	19	3	
4	D	1	Total	C	O	P	0
			69	47	19	3	
4	G	1	Total	C	O	P	0
			69	47	19	3	
4	J	1	Total	C	O	P	0
			69	47	19	3	

- Molecule 5 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	A	4	Total	K	0
			4	4	

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
6	B	2	Total	Ca	0
			2	2	
6	E	2	Total	Ca	0
			2	2	

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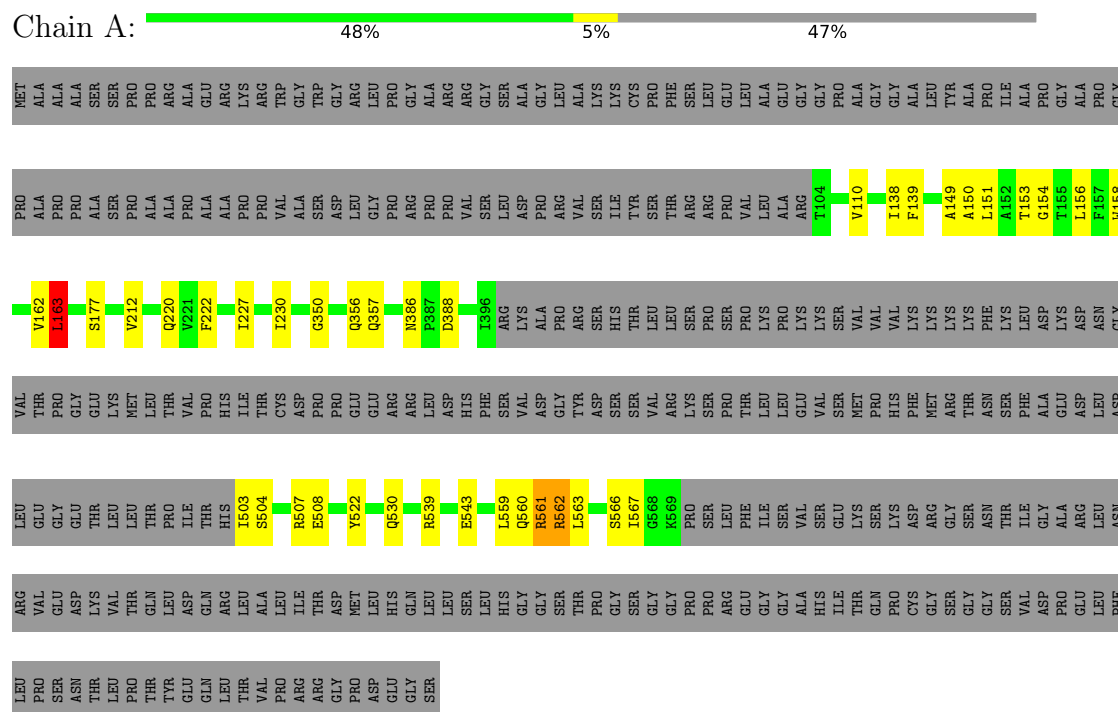
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Mol	Chain	Residues	Atoms		AltConf
6	H	2	Total 2	Ca 2	0
6	K	2	Total 2	Ca 2	0

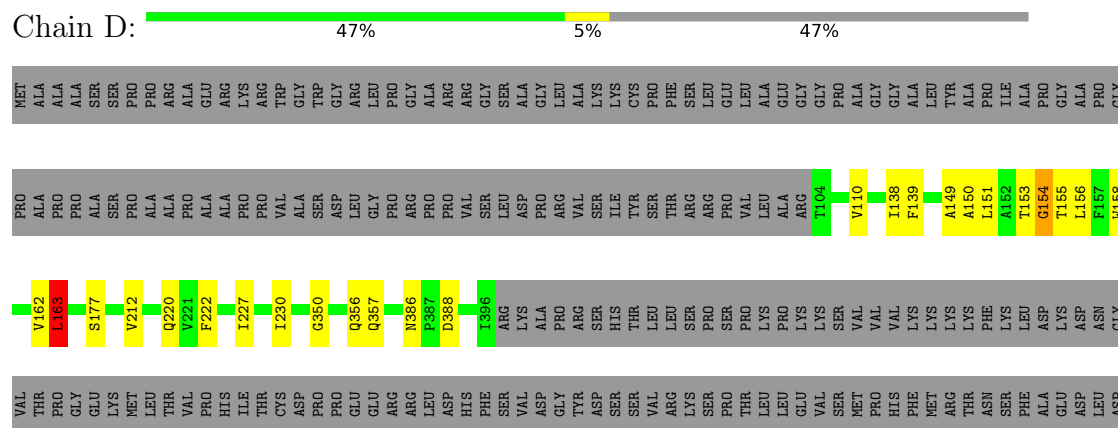
3 Residue-property plots

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: Potassium voltage-gated channel subfamily KQT member 1



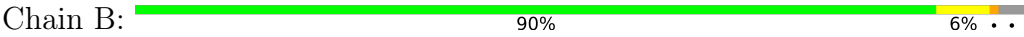
- Molecule 1: Potassium voltage-gated channel subfamily KQT member 1



LEU ASN ARG VAL GLU ASP LYS VAL THR GLN LEU ASP GLN ARG LEU ALA LEU ILE ARG THR ASP MET HIS GLN LEU SER LEU HIS GLY GLY THR PRO GLY SER GLY PRO ARG GLU GLY ALA HIS THR GLN PRO CYS GLY SER GLY VAL ASP PRO GLU

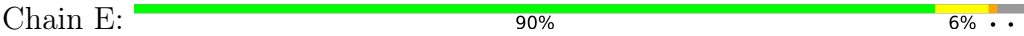
LEU PHE LEU PRO SER ASN THR LEU PRO THR TYR GLU LEU THR VAL PRO ARG GLY PRO ASP GLY SER

● Molecule 2: Calmodulin-1



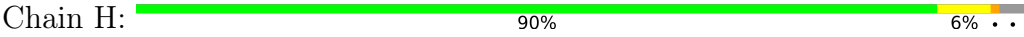
MET ALA ASP GLN LEU T6 Q9 E12 M77 K78 D79 T80 E84 E85 I86 R87 V143 T147 A148 K149

● Molecule 2: Calmodulin-1



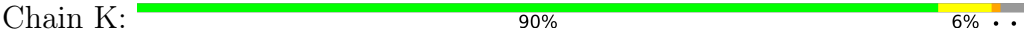
MET ALA ASP GLN LEU T6 Q9 E12 M77 K78 D79 T80 E84 E85 I86 R87 V143 T147 A148 K149

● Molecule 2: Calmodulin-1



MET ALA ASP GLN LEU T6 Q9 E12 M77 K78 D79 T80 E84 E85 I86 R87 V143 T147 A148 K149

● Molecule 2: Calmodulin-1



MET ALA ASP GLN LEU T6 Q9 E12 M77 K78 D79 T80 E84 E85 I86 R87 V143 T147 A148 K149

● Molecule 3: Potassium voltage-gated channel subfamily E member 1



MET ILE LEU SER ASN THR THR ALA VAL THR PRO PHE LEU THR LYS TRP GLN ARG GLU THR VAL GLN GLY GLY ASN MET HIS LEU ALA ARG ARG ARG SER PRO THR ARG SER SER D39 T66 ARG SER LYS LYS LEU GLU HIS SER ASN ASP PRO PHE ASN VAL TYR ILE GLU SER ASP

ALA TRP GLN SER LYS ASP THR ALA VAL THR PRO PHE ARG VAL LEU LEU TRP TYR ARG SER CYS VAL GLN VAL GLY GLY ASN MET HIS LEU ALA GLU GLN ARG ARG ARG SER PRO THR ARG SER SER D39 T66 ARG SER LYS LYS LEU GLU HIS SER ASN ASP PRO PHE ASN VAL TYR ILE GLU SER ASP

● Molecule 3: Potassium voltage-gated channel subfamily E member 1



MET ILE LEU SER ASN THR THR ALA VAL THR PRO PHE ARG VAL LEU LEU TRP TYR ARG SER CYS VAL GLN VAL GLY GLY ASN MET HIS LEU ALA GLU GLN ARG ARG ARG SER PRO THR ARG SER SER D39 T66 ARG SER LYS LYS LEU GLU HIS SER ASN ASP PRO PHE ASN VAL TYR ILE GLU SER ASP

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	152699	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI SPIRIT	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51.45	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (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: CA, K, PT5

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	0.63	8/2979 (0.3%)	0.75	22/4033 (0.5%)
1	D	0.63	8/2979 (0.3%)	0.74	20/4033 (0.5%)
1	G	0.62	7/2979 (0.2%)	0.74	21/4033 (0.5%)
1	J	0.63	8/2979 (0.3%)	0.75	20/4033 (0.5%)
2	B	0.43	1/1117 (0.1%)	0.50	1/1503 (0.1%)
2	E	0.43	1/1117 (0.1%)	0.50	1/1503 (0.1%)
2	H	0.43	1/1117 (0.1%)	0.50	1/1503 (0.1%)
2	K	0.43	1/1117 (0.1%)	0.50	1/1503 (0.1%)
3	C	0.14	0/227	0.35	0/304
3	F	0.14	0/227	0.35	0/304
3	I	0.14	0/227	0.35	0/304
3	L	0.14	0/227	0.35	0/304
All	All	0.57	35/17292 (0.2%)	0.67	87/23360 (0.4%)

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	79	ASP	C-N	10.88	1.50	1.33
2	H	79	ASP	C-N	10.88	1.50	1.33
2	K	79	ASP	C-N	10.88	1.50	1.33
2	B	79	ASP	C-N	10.85	1.50	1.33
1	D	154	GLY	C-O	9.88	1.35	1.23
1	A	154	GLY	C-O	9.87	1.35	1.23
1	G	154	GLY	C-O	9.85	1.35	1.23
1	J	154	GLY	C-O	9.80	1.35	1.23
1	A	150	ALA	C-O	9.06	1.37	1.23
1	J	150	ALA	C-O	9.06	1.37	1.23
1	D	150	ALA	C-O	9.02	1.37	1.23
1	G	150	ALA	C-O	9.02	1.37	1.23
1	J	153	THR	C-O	8.04	1.33	1.24
1	D	153	THR	C-O	8.01	1.33	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	153	THR	C-O	8.01	1.33	1.24
1	A	153	THR	C-O	7.95	1.33	1.24
1	A	151	LEU	C-O	6.62	1.31	1.24
1	G	151	LEU	C-O	6.62	1.31	1.24
1	D	151	LEU	C-O	6.62	1.31	1.24
1	J	151	LEU	C-O	6.54	1.31	1.24
1	J	230	ILE	C-N	-6.08	1.23	1.33
1	D	230	ILE	C-N	-6.03	1.23	1.33
1	A	230	ILE	C-N	-6.02	1.23	1.33
1	A	561	ARG	CA-C	-5.83	1.45	1.52
1	D	561	ARG	CA-C	-5.83	1.45	1.52
1	G	561	ARG	CA-C	-5.83	1.45	1.52
1	J	561	ARG	CA-C	-5.82	1.45	1.52
1	J	563	LEU	N-CA	5.18	1.52	1.46
1	A	563	LEU	N-CA	5.13	1.52	1.46
1	D	563	LEU	N-CA	5.13	1.52	1.46
1	G	563	LEU	N-CA	5.13	1.52	1.46
1	D	154	GLY	CA-C	5.12	1.57	1.52
1	G	154	GLY	CA-C	5.12	1.57	1.52
1	J	154	GLY	CA-C	5.12	1.57	1.52
1	A	154	GLY	CA-C	5.12	1.57	1.52

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	162	VAL	N-CA-C	9.18	119.98	110.62
1	G	162	VAL	N-CA-C	9.15	119.95	110.62
1	J	162	VAL	N-CA-C	9.15	119.95	110.62
1	D	162	VAL	N-CA-C	9.13	119.93	110.62
1	J	562	ARG	O-C-N	-8.53	113.08	122.12
1	D	562	ARG	O-C-N	-8.49	113.12	122.12
1	A	562	ARG	O-C-N	-8.48	113.13	122.12
1	G	562	ARG	O-C-N	-8.48	113.13	122.12
1	A	563	LEU	N-CA-C	7.65	119.25	111.07
1	D	563	LEU	N-CA-C	7.65	119.25	111.07
1	G	563	LEU	N-CA-C	7.65	119.25	111.07
1	J	563	LEU	N-CA-C	7.64	119.25	111.07
1	J	158	TRP	N-CA-C	7.15	119.15	111.36
1	A	158	TRP	N-CA-C	7.11	119.11	111.36
1	G	158	TRP	N-CA-C	7.08	119.08	111.36
1	D	158	TRP	N-CA-C	7.07	119.06	111.36
1	A	138	ILE	O-C-N	-7.03	115.05	121.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	138	ILE	O-C-N	-7.03	115.05	121.87
1	G	138	ILE	O-C-N	-7.03	115.05	121.87
1	J	138	ILE	O-C-N	-6.98	115.09	121.87
2	H	79	ASP	O-C-N	6.41	130.54	122.65
2	K	79	ASP	O-C-N	6.41	130.54	122.65
2	E	79	ASP	O-C-N	6.39	130.51	122.65
2	B	79	ASP	O-C-N	6.38	130.49	122.65
1	J	504	SER	N-CA-C	6.19	119.49	109.40
1	G	504	SER	N-CA-C	6.10	119.35	109.40
1	G	357	GLN	N-CA-C	6.00	120.29	113.15
1	G	163	LEU	CA-C-N	5.96	130.47	121.65
1	G	163	LEU	C-N-CA	5.96	130.47	121.65
1	G	149	ALA	N-CA-C	5.94	120.23	112.92
1	A	149	ALA	N-CA-C	5.93	120.22	112.92
1	A	163	LEU	CA-C-N	5.93	130.42	121.65
1	A	163	LEU	C-N-CA	5.93	130.42	121.65
1	D	163	LEU	CA-C-N	5.92	130.41	121.65
1	D	163	LEU	C-N-CA	5.92	130.41	121.65
1	D	149	ALA	N-CA-C	5.92	120.20	112.92
1	J	163	LEU	CA-C-N	5.90	130.38	121.65
1	J	163	LEU	C-N-CA	5.90	130.38	121.65
1	D	357	GLN	N-CA-C	5.88	120.14	113.15
1	A	357	GLN	N-CA-C	5.87	120.13	113.15
1	J	357	GLN	N-CA-C	5.85	120.11	113.15
1	J	149	ALA	N-CA-C	5.83	120.09	112.92
1	J	350	GLY	N-CA-C	5.80	119.23	112.50
1	A	350	GLY	N-CA-C	5.79	119.22	112.50
1	D	350	GLY	N-CA-C	5.78	119.21	112.50
1	A	504	SER	N-CA-C	5.77	118.80	109.40
1	D	504	SER	N-CA-C	5.76	118.79	109.40
1	A	230	ILE	O-C-N	-5.71	116.49	122.20
1	D	230	ILE	O-C-N	-5.70	116.50	122.20
1	J	230	ILE	O-C-N	-5.69	116.51	122.20
1	G	350	GLY	N-CA-C	5.59	118.98	112.50
1	J	150	ALA	CA-C-O	5.53	126.03	119.67
1	D	150	ALA	CA-C-O	5.51	126.00	119.67
1	A	150	ALA	CA-C-O	5.51	126.00	119.67
1	G	150	ALA	CA-C-O	5.46	125.95	119.67
1	D	154	GLY	CA-C-O	5.40	126.83	121.00
1	J	154	GLY	CA-C-O	5.39	126.82	121.00
1	A	154	GLY	CA-C-O	5.38	126.81	121.00
1	A	162	VAL	CB-CA-C	-5.37	104.89	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	154	GLY	CA-C-O	5.37	126.80	121.00
1	G	162	VAL	CB-CA-C	-5.31	104.97	112.14
1	A	154	GLY	N-CA-C	5.29	118.63	112.50
1	G	154	GLY	N-CA-C	5.28	118.63	112.50
1	J	154	GLY	N-CA-C	5.28	118.63	112.50
1	D	162	VAL	CB-CA-C	-5.28	105.01	112.14
1	D	154	GLY	N-CA-C	5.27	118.62	112.50
1	J	162	VAL	CB-CA-C	-5.27	105.02	112.14
1	D	139	PHE	CA-C-N	-5.09	112.58	120.31
1	D	139	PHE	C-N-CA	-5.09	112.58	120.31
1	G	139	PHE	CA-C-N	-5.09	112.58	120.31
1	G	139	PHE	C-N-CA	-5.09	112.58	120.31
1	J	139	PHE	CA-C-N	-5.09	112.58	120.31
1	J	139	PHE	C-N-CA	-5.09	112.58	120.31
1	G	153	THR	CA-C-N	-5.07	114.31	119.94
1	G	153	THR	C-N-CA	-5.07	114.31	119.94
1	J	153	THR	CA-C-N	-5.07	114.31	119.94
1	J	153	THR	C-N-CA	-5.07	114.31	119.94
1	A	139	PHE	CA-C-N	-5.06	112.61	120.31
1	A	139	PHE	C-N-CA	-5.06	112.61	120.31
1	A	154	GLY	CA-C-N	-5.04	113.52	120.28
1	A	154	GLY	C-N-CA	-5.04	113.52	120.28
1	G	154	GLY	CA-C-N	-5.03	113.54	120.28
1	G	154	GLY	C-N-CA	-5.03	113.54	120.28
1	A	153	THR	CA-C-N	-5.02	114.37	119.94
1	A	153	THR	C-N-CA	-5.02	114.37	119.94
1	D	153	THR	CA-C-N	-5.02	114.37	119.94
1	D	153	THR	C-N-CA	-5.02	114.37	119.94

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	2907	0	2974	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2907	0	2974	15	0
1	G	2907	0	2974	15	0
1	J	2907	0	2974	15	0
2	B	1105	0	1020	8	0
2	E	1105	0	1020	8	0
2	H	1105	0	1020	8	0
2	K	1105	0	1020	8	0
3	C	222	0	229	1	0
3	F	222	0	229	1	0
3	I	222	0	229	1	0
3	L	222	0	229	1	0
4	A	69	0	80	1	0
4	D	69	0	80	1	0
4	G	69	0	80	1	0
4	J	69	0	80	1	0
5	A	4	0	0	0	0
6	B	2	0	0	0	0
6	E	2	0	0	0	0
6	H	2	0	0	0	0
6	K	2	0	0	0	0
All	All	17224	0	17212	87	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 (87) 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:D:530:GLN:NE2	2:E:85:GLU:OE2	2.32	0.63
1:G:530:GLN:NE2	2:H:85:GLU:OE2	2.32	0.63
1:J:530:GLN:NE2	2:K:85:GLU:OE2	2.32	0.63
1:A:530:GLN:NE2	2:B:85:GLU:OE2	2.32	0.62
1:D:566:SER:O	1:D:567:ILE:C	2.46	0.59
1:J:566:SER:O	1:J:567:ILE:C	2.45	0.57
1:G:566:SER:O	1:G:567:ILE:C	2.46	0.55
1:A:566:SER:O	1:A:567:ILE:C	2.45	0.55
2:H:79:ASP:CG	2:H:80:THR:N	2.66	0.54
2:B:79:ASP:CG	2:B:80:THR:N	2.66	0.54
2:E:79:ASP:CG	2:E:80:THR:N	2.66	0.53
2:K:79:ASP:CG	2:K:80:THR:N	2.66	0.53
1:J:212:VAL:HG11	1:J:227:ILE:HG21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:212:VAL:HG11	1:D:227:ILE:HG21	1.91	0.53
2:K:79:ASP:OD1	2:K:80:THR:N	2.40	0.52
1:A:212:VAL:HG11	1:A:227:ILE:HG21	1.91	0.52
1:G:212:VAL:HG11	1:G:227:ILE:HG21	1.91	0.51
2:H:79:ASP:OD1	2:H:80:THR:N	2.40	0.51
2:E:143:VAL:O	2:E:147:THR:HG22	2.12	0.50
2:B:79:ASP:CG	2:B:80:THR:H	2.19	0.50
2:E:79:ASP:CG	2:E:80:THR:H	2.19	0.50
2:B:143:VAL:O	2:B:147:THR:HG22	2.12	0.50
1:D:507:ARG:HG3	1:D:508:GLU:HG2	1.94	0.49
1:A:507:ARG:HG3	1:A:508:GLU:HG2	1.94	0.49
2:H:79:ASP:CG	2:H:80:THR:H	2.19	0.49
1:J:507:ARG:HG3	1:J:508:GLU:HG2	1.94	0.49
2:H:143:VAL:O	2:H:147:THR:HG22	2.12	0.49
2:K:79:ASP:CG	2:K:80:THR:H	2.19	0.48
1:J:522:TYR:CE2	2:K:77:MET:HE2	2.49	0.48
1:A:356:GLN:O	1:A:356:GLN:HG2	2.14	0.48
2:K:143:VAL:O	2:K:147:THR:HG22	2.12	0.48
1:G:507:ARG:HG3	1:G:508:GLU:HG2	1.94	0.48
1:A:522:TYR:CE2	2:B:77:MET:HE2	2.49	0.48
1:G:522:TYR:CE2	2:H:77:MET:HE2	2.49	0.48
1:D:522:TYR:CE2	2:E:77:MET:HE2	2.49	0.48
1:D:356:GLN:O	1:D:356:GLN:HG2	2.14	0.47
2:H:9:GLN:HA	2:H:12:GLU:HG2	1.96	0.47
4:A:701:PT5:H25	4:A:701:PT5:H28	1.69	0.47
2:E:9:GLN:HA	2:E:12:GLU:HG2	1.96	0.47
1:J:561:ARG:O	1:J:562:ARG:C	2.58	0.47
1:A:561:ARG:O	1:A:562:ARG:C	2.58	0.47
4:D:701:PT5:H28	4:D:701:PT5:H25	1.69	0.47
4:G:701:PT5:H25	4:G:701:PT5:H28	1.69	0.47
1:G:220:GLN:HG3	1:G:222:PHE:H	1.80	0.46
1:J:356:GLN:HG2	1:J:356:GLN:O	2.14	0.46
1:D:220:GLN:HG3	1:D:222:PHE:H	1.80	0.46
1:G:356:GLN:O	1:G:356:GLN:HG2	2.14	0.46
2:K:9:GLN:HA	2:K:12:GLU:HG2	1.96	0.46
4:J:701:PT5:H25	4:J:701:PT5:H28	1.69	0.46
2:B:9:GLN:HA	2:B:12:GLU:HG2	1.96	0.46
1:A:386:ASN:ND2	1:A:388:ASP:OD1	2.49	0.46
1:G:386:ASN:ND2	1:G:388:ASP:OD1	2.49	0.46
1:D:386:ASN:ND2	1:D:388:ASP:OD1	2.49	0.45
1:J:386:ASN:ND2	1:J:388:ASP:OD1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:ARG:O	1:A:543:GLU:HG3	2.16	0.45
1:G:539:ARG:O	1:G:543:GLU:HG3	2.16	0.45
1:D:539:ARG:O	1:D:543:GLU:HG3	2.16	0.45
1:D:561:ARG:O	1:D:562:ARG:C	2.58	0.45
1:J:539:ARG:O	1:J:543:GLU:HG3	2.16	0.45
1:J:220:GLN:HG3	1:J:222:PHE:H	1.80	0.45
1:A:220:GLN:HG3	1:A:222:PHE:H	1.80	0.44
2:E:79:ASP:OD1	2:E:80:THR:N	2.40	0.44
1:G:163:LEU:O	1:G:163:LEU:HG	2.18	0.43
1:G:561:ARG:O	1:G:562:ARG:C	2.58	0.43
1:A:163:LEU:HG	1:A:163:LEU:O	2.18	0.43
3:I:39:ASP:OD1	3:I:39:ASP:N	2.52	0.43
3:F:39:ASP:N	3:F:39:ASP:OD1	2.52	0.43
1:D:163:LEU:O	1:D:163:LEU:HG	2.18	0.42
2:B:79:ASP:OD1	2:B:80:THR:N	2.40	0.42
3:L:39:ASP:N	3:L:39:ASP:OD1	2.52	0.42
1:A:559:LEU:HD13	1:J:560:GLN:HG2	2.02	0.42
1:A:560:GLN:HG2	1:D:559:LEU:HD13	2.02	0.42
1:D:110:VAL:HG23	1:D:177:SER:HB2	2.02	0.42
1:D:560:GLN:HG2	1:G:559:LEU:HD13	2.02	0.42
1:A:110:VAL:HG23	1:A:177:SER:HB2	2.02	0.41
2:B:84:GLU:OE1	2:B:87:ARG:NH1	2.54	0.41
1:G:110:VAL:HG23	1:G:177:SER:HB2	2.02	0.41
1:D:154:GLY:O	1:D:155:THR:C	2.63	0.41
2:E:84:GLU:OE1	2:E:87:ARG:NH1	2.54	0.41
1:J:154:GLY:O	1:J:155:THR:C	2.63	0.41
1:G:560:GLN:HG2	1:J:559:LEU:HD13	2.03	0.41
2:K:84:GLU:OE1	2:K:87:ARG:NH1	2.54	0.41
3:C:39:ASP:OD1	3:C:39:ASP:N	2.52	0.41
1:J:110:VAL:HG23	1:J:177:SER:HB2	2.02	0.41
1:G:160:GLU:O	1:G:161:ILE:C	2.64	0.40
1:J:160:GLU:O	1:J:161:ILE:C	2.64	0.40
2:H:84:GLU:OE1	2:H:87:ARG:NH1	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	356/676 (53%)	346 (97%)	10 (3%)	0	100	100
1	D	356/676 (53%)	346 (97%)	10 (3%)	0	100	100
1	G	356/676 (53%)	346 (97%)	10 (3%)	0	100	100
1	J	356/676 (53%)	346 (97%)	10 (3%)	0	100	100
2	B	142/149 (95%)	136 (96%)	6 (4%)	0	100	100
2	E	142/149 (95%)	136 (96%)	6 (4%)	0	100	100
2	H	142/149 (95%)	137 (96%)	5 (4%)	0	100	100
2	K	142/149 (95%)	137 (96%)	5 (4%)	0	100	100
3	C	26/129 (20%)	25 (96%)	1 (4%)	0	100	100
3	F	26/129 (20%)	25 (96%)	1 (4%)	0	100	100
3	I	26/129 (20%)	25 (96%)	1 (4%)	0	100	100
3	L	26/129 (20%)	25 (96%)	1 (4%)	0	100	100
All	All	2096/3816 (55%)	2030 (97%)	66 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	306/567 (54%)	303 (99%)	3 (1%)	73	91
1	D	306/567 (54%)	303 (99%)	3 (1%)	73	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	306/567 (54%)	304 (99%)	2 (1%)	81	94
1	J	306/567 (54%)	304 (99%)	2 (1%)	81	94
2	B	114/127 (90%)	114 (100%)	0	100	100
2	E	114/127 (90%)	114 (100%)	0	100	100
2	H	114/127 (90%)	114 (100%)	0	100	100
2	K	114/127 (90%)	114 (100%)	0	100	100
3	C	23/115 (20%)	23 (100%)	0	100	100
3	F	23/115 (20%)	23 (100%)	0	100	100
3	I	23/115 (20%)	23 (100%)	0	100	100
3	L	23/115 (20%)	23 (100%)	0	100	100
All	All	1772/3236 (55%)	1762 (99%)	10 (1%)	82	95

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	156	LEU
1	A	163	LEU
1	A	503	ILE
1	D	156	LEU
1	D	163	LEU
1	D	503	ILE
1	G	156	LEU
1	G	163	LEU
1	J	156	LEU
1	J	163	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	220	GLN
1	A	240	HIS
1	A	560	GLN
2	B	42	GLN
2	B	108	HIS
2	B	136	GLN
1	D	220	GLN
1	D	240	HIS

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Mol	Chain	Res	Type
1	D	560	GLN
2	E	42	GLN
2	E	108	HIS
2	E	136	GLN
2	E	138	ASN
1	G	220	GLN
1	G	240	HIS
1	G	560	GLN
2	H	42	GLN
2	H	136	GLN
2	H	138	ASN
1	J	220	GLN
1	J	240	HIS
1	J	560	GLN
2	K	42	GLN
2	K	108	HIS
2	K	136	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 12 are monoatomic - leaving 4 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
4	PT5	D	701	-	69,69,69	0.84	2 (2%)	83,87,87	1.03	3 (3%)
4	PT5	J	701	-	69,69,69	0.84	2 (2%)	83,87,87	1.03	3 (3%)
4	PT5	G	701	-	69,69,69	0.84	2 (2%)	83,87,87	1.02	3 (3%)
4	PT5	A	701	-	69,69,69	0.84	2 (2%)	83,87,87	1.03	3 (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
4	PT5	D	701	-	-	4/66/90/90	0/1/1/1
4	PT5	J	701	-	-	4/66/90/90	0/1/1/1
4	PT5	G	701	-	-	4/66/90/90	0/1/1/1
4	PT5	A	701	-	-	4/66/90/90	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	701	PT5	O18-C11	4.20	1.45	1.33
4	J	701	PT5	O18-C11	4.20	1.45	1.33
4	D	701	PT5	O18-C11	4.19	1.45	1.33
4	G	701	PT5	O18-C11	4.19	1.45	1.33
4	J	701	PT5	O16-C10	4.12	1.45	1.34
4	A	701	PT5	O16-C10	4.10	1.45	1.34
4	D	701	PT5	O16-C10	4.10	1.45	1.34
4	G	701	PT5	O16-C10	4.10	1.45	1.34

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	701	PT5	O16-C10-C12	4.13	120.41	111.50
4	A	701	PT5	O16-C10-C12	4.12	120.39	111.50
4	D	701	PT5	O16-C10-C12	4.12	120.39	111.50
4	G	701	PT5	O16-C10-C12	4.11	120.35	111.50
4	A	701	PT5	C8-O16-C10	-2.71	111.12	117.79
4	D	701	PT5	C8-O16-C10	-2.69	111.16	117.79
4	G	701	PT5	C8-O16-C10	-2.69	111.16	117.79
4	J	701	PT5	C8-O16-C10	-2.69	111.17	117.79
4	D	701	PT5	O18-C11-C31	2.37	119.36	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	701	PT5	O18-C11-C31	2.37	119.36	111.91
4	J	701	PT5	O18-C11-C31	2.37	119.34	111.91
4	A	701	PT5	O18-C11-C31	2.36	119.33	111.91

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	701	PT5	C19-C20-C21-C22
4	D	701	PT5	C19-C20-C21-C22
4	G	701	PT5	C19-C20-C21-C22
4	J	701	PT5	C19-C20-C21-C22
4	J	701	PT5	O13-C7-C8-O16
4	A	701	PT5	O13-C7-C8-C9
4	D	701	PT5	O13-C7-C8-C9
4	G	701	PT5	O13-C7-C8-C9
4	J	701	PT5	O13-C7-C8-C9
4	A	701	PT5	O13-C7-C8-O16
4	D	701	PT5	O13-C7-C8-O16
4	G	701	PT5	O13-C7-C8-O16
4	A	701	PT5	C4-O4-P4-O41
4	D	701	PT5	C4-O4-P4-O41
4	G	701	PT5	C4-O4-P4-O41
4	J	701	PT5	C4-O4-P4-O41

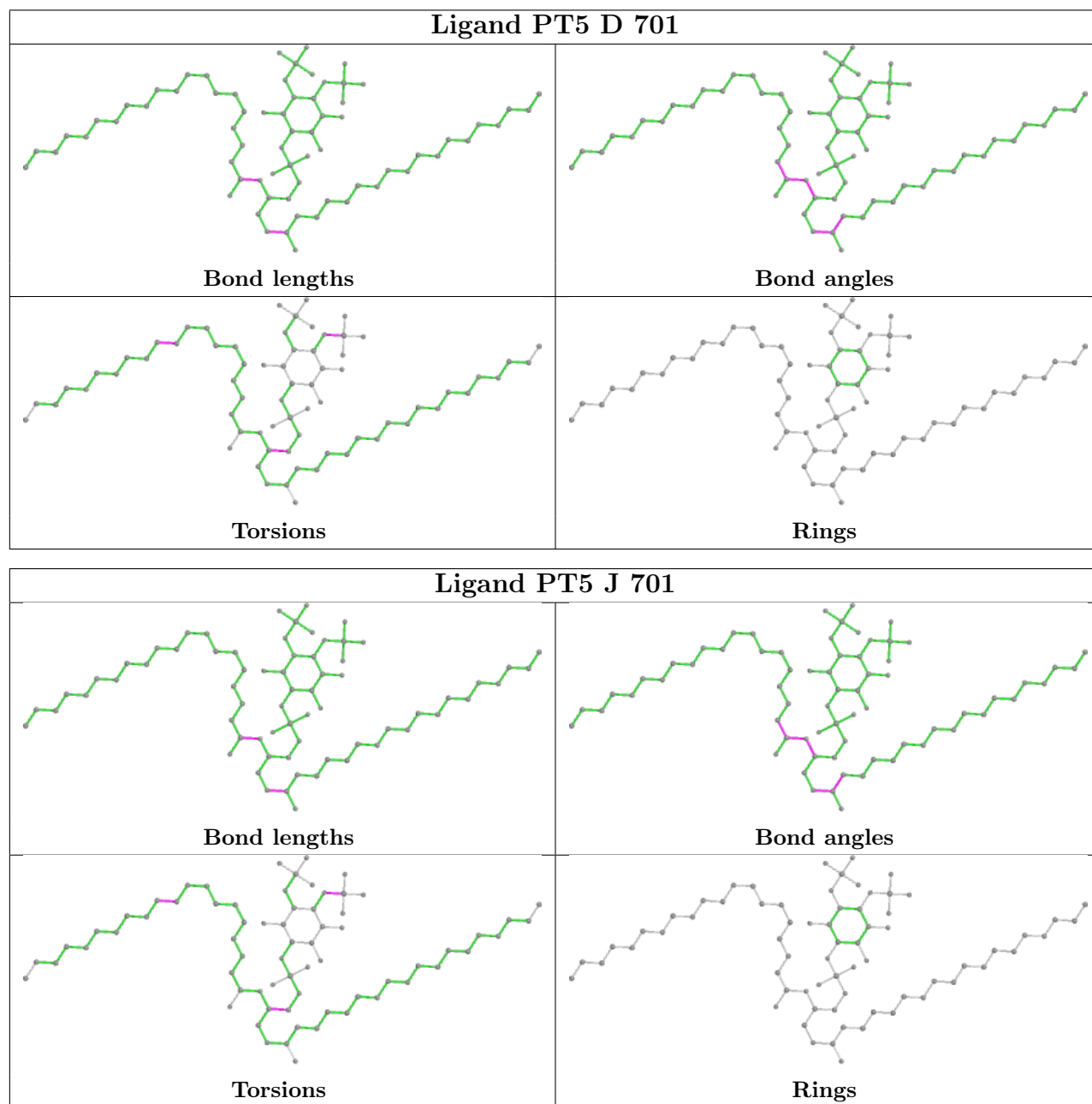
There are no ring outliers.

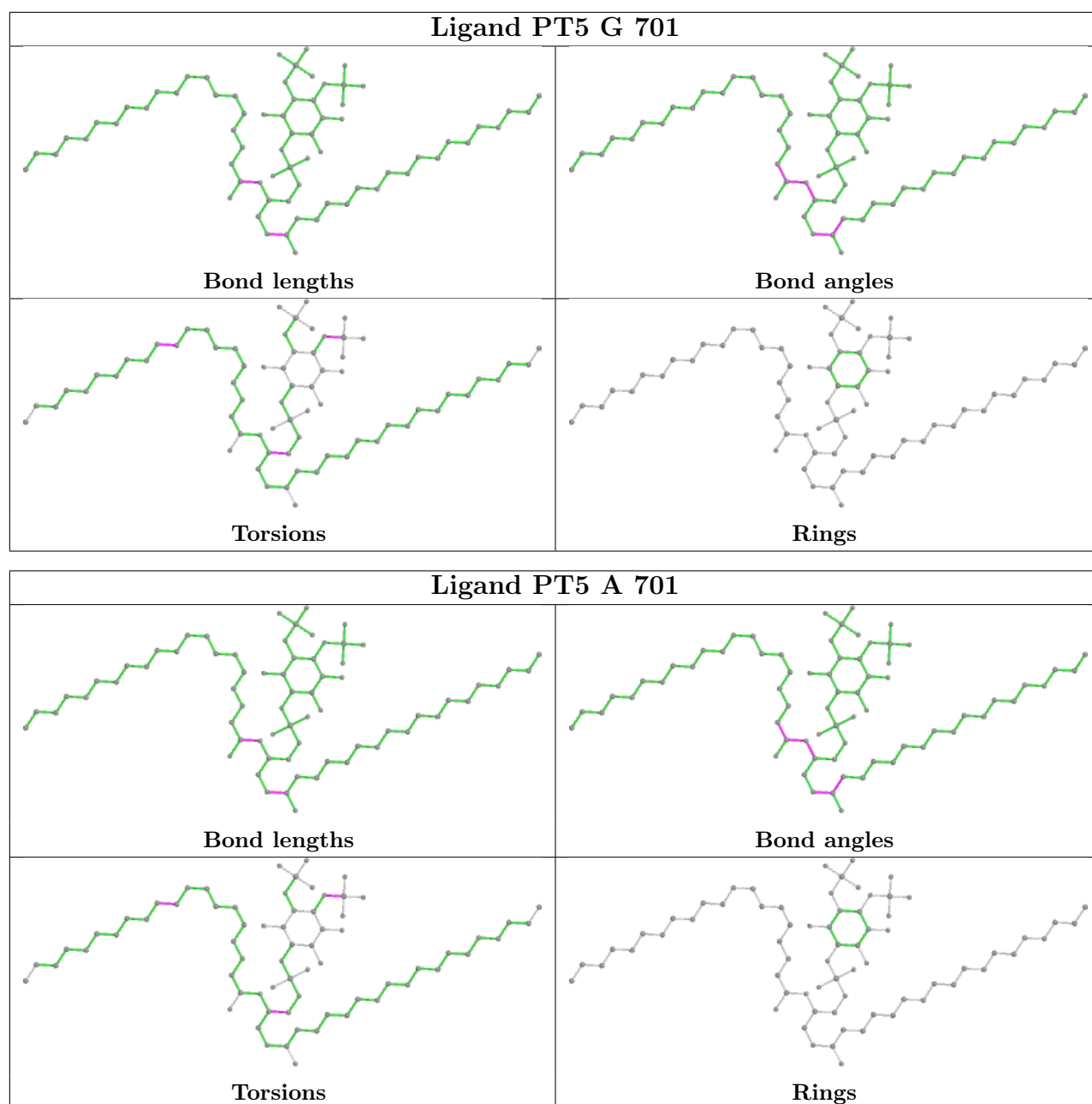
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	701	PT5	1	0
4	J	701	PT5	1	0
4	G	701	PT5	1	0
4	A	701	PT5	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.