



Full wwPDB EM Validation Report ⓘ

Nov 9, 2025 – 12:18 AM JST

PDB ID : 9UC8 / pdb_00009uc8
EMDB ID : EMD-64038
Title : structure of human KCNQ1-KCNE1-CaM complex with PIP2
Authors : Hou, P.P.; Zhang, J.; Wan, S.Y.; Cheng, X.Y.; Zhong, L.; Hu, B.
Deposited on : 2025-04-03
Resolution : 3.36 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

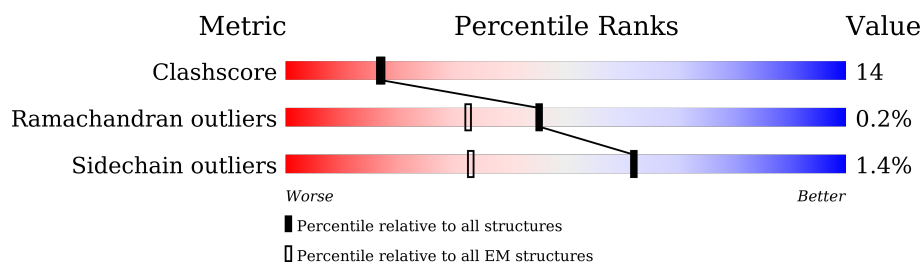
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.36 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	35% 14% . 50%
1	D	676	35% 14% . 50%
1	G	676	35% 13% . 50%
1	J	676	35% 14% . 50%
2	B	149	89% 8% .
2	E	149	89% 8% .
2	H	149	88% 9% .
2	K	149	89% 8% .
3	C	30	90% 10%

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Mol	Chain	Length	Quality of chain
3	F	30	 90%10%
3	I	30	 90%10%
3	L	30	 90%10%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 15595 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	339	Total	C	N	O	S	0	0
			2734	1797	479	447	11		
1	D	339	Total	C	N	O	S	0	0
			2734	1797	479	447	11		
1	G	339	Total	C	N	O	S	0	0
			2734	1797	479	447	11		
1	J	339	Total	C	N	O	S	0	0
			2734	1797	479	447	11		

- Molecule 2 is a protein called Calmodulin-1.

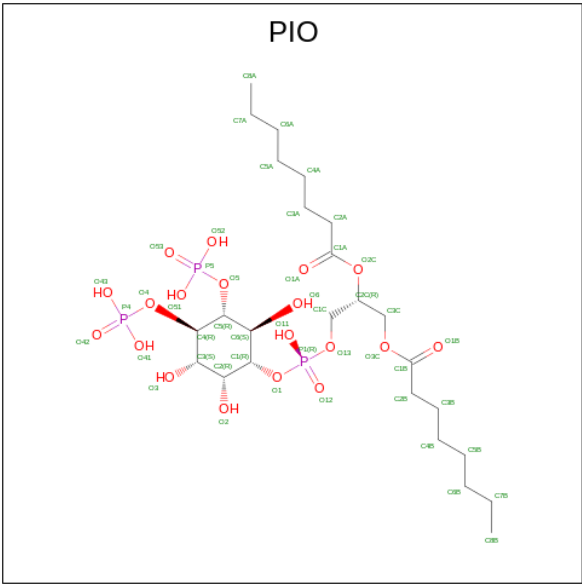
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	144	Total	C	N	O	S	0	0
			831	522	154	152	3		
2	E	144	Total	C	N	O	S	0	0
			831	522	154	152	3		
2	H	144	Total	C	N	O	S	0	0
			831	522	154	152	3		
2	K	144	Total	C	N	O	S	0	0
			831	522	154	152	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	30	Total	C	N	O	S	0	0
			239	164	34	39	2		
3	F	30	Total	C	N	O	S	0	0
			239	164	34	39	2		
3	I	30	Total	C	N	O	S	0	0
			239	164	34	39	2		
3	L	30	Total	C	N	O	S	0	0
			239	164	34	39	2		

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

) -4,5-diphosphonooxy-cyclohexyl]oxy-phosphoryl]oxy-propyl] octanoate (CCD ID: PIO) (formula: C₂₅H₄₉O₁₉P₃) (labeled as "Ligand of Interest" by depositor).




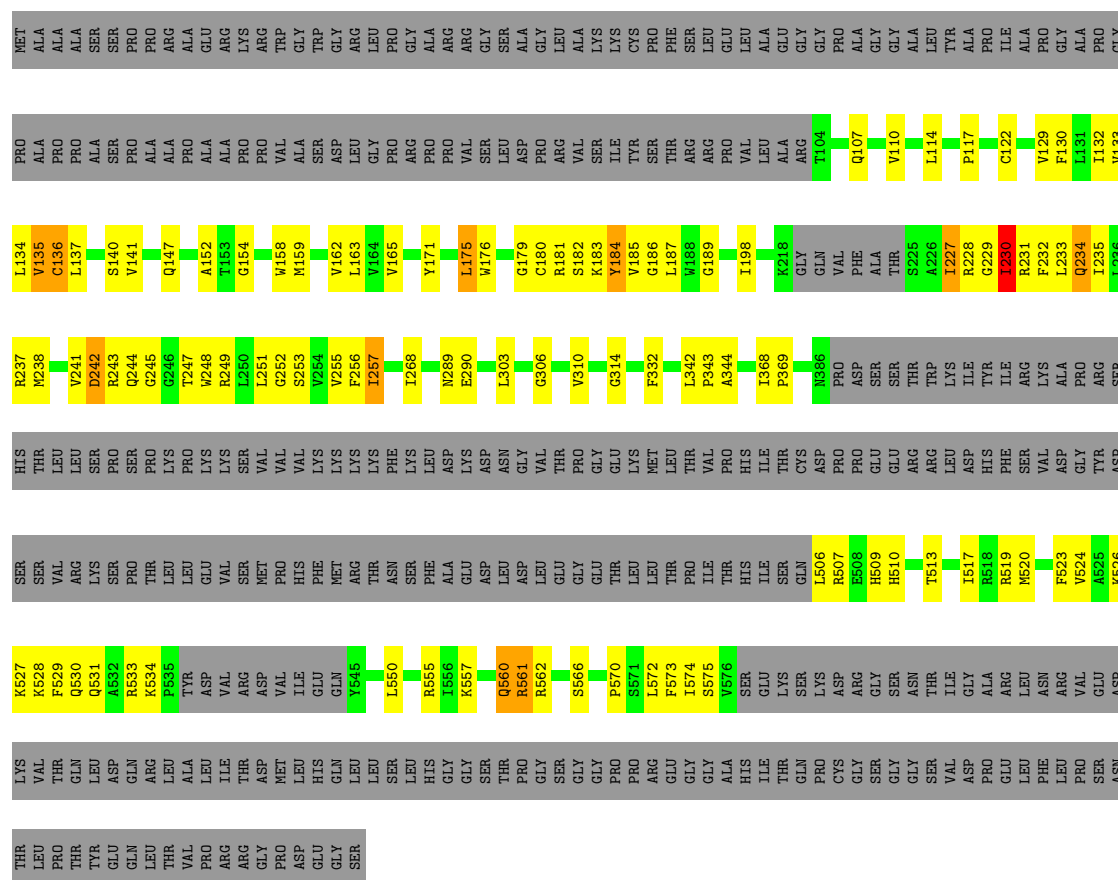
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	O	P	0
			47	25	19	3	
4	C	1	Total	C	O	P	0
			47	25	19	3	
4	D	1	Total	C	O	P	0
			47	25	19	3	
4	F	1	Total	C	O	P	0
			47	25	19	3	
4	G	1	Total	C	O	P	0
			47	25	19	3	
4	I	1	Total	C	O	P	0
			47	25	19	3	
4	J	1	Total	C	O	P	0
			47	25	19	3	
4	L	1	Total	C	O	P	0
			47	25	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	3	Total	K	0
			3	3	



Chain J:  35% 14% 50%



• Molecule 2: Calmodulin-1

Chain B:  89% 8%




• Molecule 2: Calmodulin-1

Chain E:  89% 8%




• Molecule 2: Calmodulin-1

Chain H:  88% 9%



• Molecule 2: Calmodulin-1

Chain K:  89% 8%




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

Chain C:  90% 10%




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

Chain F:  90% 10%




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

Chain I:  90% 10%



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

Chain L:  90% 10%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	168370	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 ($e^-/\text{\AA}^2$)	50.73	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: K, PIO

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	0.61	5/2800 (0.2%)	0.81	10/3784 (0.3%)
1	D	0.61	5/2800 (0.2%)	0.81	10/3784 (0.3%)
1	G	0.61	5/2800 (0.2%)	0.81	10/3784 (0.3%)
1	J	0.61	5/2800 (0.2%)	0.81	10/3784 (0.3%)
2	B	0.16	0/841	0.45	0/1155
2	E	0.16	0/841	0.45	0/1155
2	H	0.17	0/841	0.46	0/1155
2	K	0.17	0/841	0.46	0/1155
3	C	0.33	0/244	0.52	0/326
3	F	0.33	0/244	0.51	0/326
3	I	0.33	0/244	0.52	0/326
3	L	0.33	0/244	0.51	0/326
All	All	0.53	20/15540 (0.1%)	0.73	40/21060 (0.2%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	158	TRP	C-N	-8.09	1.23	1.33
1	G	158	TRP	C-N	-8.09	1.23	1.33
1	J	158	TRP	C-N	-8.09	1.23	1.33
1	A	560	GLN	C-N	-8.05	1.23	1.33
1	D	560	GLN	C-N	-8.05	1.23	1.33
1	J	560	GLN	C-N	-8.03	1.23	1.33
1	D	158	TRP	C-N	-8.03	1.23	1.33
1	G	560	GLN	C-N	-8.00	1.23	1.33
1	A	184	TYR	C-N	7.97	1.43	1.33
1	G	184	TYR	C-N	7.97	1.43	1.33
1	J	184	TYR	C-N	7.95	1.43	1.33
1	D	184	TYR	C-N	7.95	1.43	1.33
1	D	561	ARG	C-N	6.41	1.41	1.33
1	G	561	ARG	C-N	6.41	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	561	ARG	C-N	6.41	1.41	1.33
1	A	561	ARG	C-N	6.39	1.41	1.33
1	A	159	MET	C-N	5.86	1.41	1.33
1	G	159	MET	C-N	5.86	1.41	1.33
1	J	159	MET	C-N	5.86	1.41	1.33
1	D	159	MET	C-N	5.81	1.41	1.33

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	257	ILE	N-CA-C	6.36	116.53	110.42
1	J	257	ILE	N-CA-C	6.35	116.52	110.42
1	A	257	ILE	N-CA-C	6.33	116.50	110.42
1	D	257	ILE	N-CA-C	6.32	116.49	110.42
1	J	141	VAL	N-CA-C	-6.22	104.62	113.07
1	A	141	VAL	N-CA-C	-6.20	104.63	113.07
1	D	141	VAL	N-CA-C	-6.20	104.63	113.07
1	G	141	VAL	N-CA-C	-6.20	104.64	113.07
1	G	242	ASP	N-CA-C	-6.20	104.30	113.72
1	A	242	ASP	N-CA-C	-6.20	104.30	113.72
1	D	242	ASP	N-CA-C	-6.19	104.31	113.72
1	J	242	ASP	N-CA-C	-6.19	104.31	113.72
1	G	560	GLN	O-C-N	-6.00	115.79	122.03
1	A	560	GLN	O-C-N	-5.95	115.84	122.03
1	D	560	GLN	O-C-N	-5.95	115.84	122.03
1	J	560	GLN	O-C-N	-5.91	115.89	122.03
1	J	227	ILE	CB-CA-C	-5.80	104.27	111.70
1	A	227	ILE	CB-CA-C	-5.76	104.32	111.70
1	G	227	ILE	CB-CA-C	-5.76	104.32	111.70
1	D	227	ILE	CB-CA-C	-5.74	104.35	111.70
1	G	183	LYS	N-CA-C	-5.64	106.10	112.87
1	A	183	LYS	N-CA-C	-5.63	106.11	112.87
1	D	183	LYS	N-CA-C	-5.61	106.13	112.87
1	J	183	LYS	N-CA-C	-5.59	106.16	112.87
1	A	230	ILE	CA-C-N	-5.24	112.86	120.29
1	A	230	ILE	C-N-CA	-5.24	112.86	120.29
1	G	230	ILE	CA-C-N	-5.24	112.86	120.29
1	G	230	ILE	C-N-CA	-5.24	112.86	120.29
1	J	230	ILE	CA-C-N	-5.24	112.86	120.29
1	J	230	ILE	C-N-CA	-5.24	112.86	120.29
1	D	230	ILE	CA-C-N	-5.22	112.88	120.29
1	D	230	ILE	C-N-CA	-5.22	112.88	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	136	CYS	N-CA-C	5.20	116.95	111.28
1	D	136	CYS	N-CA-C	5.20	116.95	111.28
1	A	136	CYS	N-CA-C	5.15	116.89	111.28
1	G	136	CYS	N-CA-C	5.15	116.89	111.28
1	A	158	TRP	O-C-N	-5.05	116.39	122.15
1	G	158	TRP	O-C-N	-5.05	116.39	122.15
1	J	158	TRP	O-C-N	-5.05	116.39	122.15
1	D	158	TRP	O-C-N	-5.01	116.44	122.15

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	2734	0	2820	103	0
1	D	2734	0	2820	102	0
1	G	2734	0	2820	101	0
1	J	2734	0	2820	100	0
2	B	831	0	556	9	0
2	E	831	0	556	9	0
2	H	831	0	556	10	0
2	K	831	0	556	9	0
3	C	239	0	247	3	0
3	F	239	0	247	3	0
3	I	239	0	247	3	0
3	L	239	0	247	3	0
4	A	47	0	44	6	0
4	C	47	0	44	1	0
4	D	47	0	44	4	0
4	F	47	0	44	1	0
4	G	47	0	44	4	0
4	I	47	0	44	1	0
4	J	47	0	44	4	0
4	L	47	0	44	1	0
5	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	15595	0	14844	416	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 14.

All (416) 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:557:LYS:HG3	1:D:561:ARG:NH1	1.30	1.46
1:J:557:LYS:HG3	1:J:561:ARG:NH1	1.30	1.46
1:A:557:LYS:HG3	1:A:561:ARG:NH1	1.30	1.43
1:G:557:LYS:HG3	1:G:561:ARG:NH1	1.30	1.41
1:A:557:LYS:CG	1:A:561:ARG:HH12	1.52	1.23
1:J:557:LYS:CG	1:J:561:ARG:HH12	1.52	1.22
1:D:557:LYS:CG	1:D:561:ARG:HH12	1.52	1.22
1:G:557:LYS:CG	1:G:561:ARG:HH12	1.52	1.22
1:A:344:ALA:HB1	1:J:342:LEU:HD23	1.52	0.92
1:G:342:LEU:HD23	1:J:344:ALA:HB1	1.53	0.90
1:A:342:LEU:HD23	1:D:344:ALA:HB1	1.53	0.90
1:D:342:LEU:HD23	1:G:344:ALA:HB1	1.52	0.90
1:G:557:LYS:CG	1:G:561:ARG:NH1	2.23	0.89
1:D:557:LYS:HG3	1:D:561:ARG:HH12	0.73	0.88
1:A:557:LYS:HG3	1:A:561:ARG:HH12	0.73	0.85
1:A:557:LYS:CG	1:A:561:ARG:NH1	2.23	0.85
1:J:557:LYS:CG	1:J:561:ARG:NH1	2.23	0.84
1:D:557:LYS:CG	1:D:561:ARG:NH1	2.23	0.83
1:A:249:ARG:HG2	4:A:701:PIO:H2B	1.63	0.79
1:D:249:ARG:HG2	4:D:701:PIO:H2B	1.65	0.78
1:G:249:ARG:HG2	4:G:701:PIO:H2B	1.65	0.77
1:J:249:ARG:HG2	4:J:701:PIO:H2B	1.65	0.77
1:D:249:ARG:HE	4:D:701:PIO:H3CA	1.51	0.76
1:J:249:ARG:HE	4:J:701:PIO:H3CA	1.51	0.75
1:G:249:ARG:HE	4:G:701:PIO:H3CA	1.51	0.75
1:A:147:GLN:HG2	3:C:39:ASP:HB3	1.67	0.75
1:G:147:GLN:HG2	3:I:39:ASP:HB3	1.67	0.75
1:D:147:GLN:HG2	3:F:39:ASP:HB3	1.67	0.74
1:A:344:ALA:HB1	1:J:342:LEU:CD2	2.18	0.73
1:J:147:GLN:HG2	3:L:39:ASP:HB3	1.67	0.73
1:G:342:LEU:CD2	1:J:344:ALA:HB1	2.19	0.72
1:A:342:LEU:CD2	1:D:344:ALA:HB1	2.19	0.72
1:D:342:LEU:CD2	1:G:344:ALA:HB1	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:524:VAL:HG12	1:D:528:LYS:HE2	1.72	0.72
1:A:524:VAL:HG12	1:A:528:LYS:HE2	1.72	0.72
1:J:524:VAL:HG12	1:J:528:LYS:HE2	1.72	0.71
1:G:524:VAL:HG12	1:G:528:LYS:HE2	1.72	0.71
1:J:179:GLY:CA	1:J:185:VAL:HB	2.22	0.70
1:A:247:THR:O	1:A:251:LEU:HG	1.93	0.69
1:D:247:THR:O	1:D:251:LEU:HG	1.93	0.69
1:G:179:GLY:CA	1:G:185:VAL:HB	2.22	0.69
1:A:179:GLY:CA	1:A:185:VAL:HB	2.22	0.69
1:J:247:THR:O	1:J:251:LEU:HG	1.93	0.69
1:A:249:ARG:HE	4:A:701:PIO:H3CA	1.57	0.68
1:D:132:ILE:HG21	1:D:163:LEU:HD11	1.76	0.68
1:G:247:THR:O	1:G:251:LEU:HG	1.93	0.68
1:D:179:GLY:CA	1:D:185:VAL:HB	2.22	0.68
1:A:132:ILE:HG21	1:A:163:LEU:HD11	1.76	0.67
1:G:132:ILE:HG21	1:G:163:LEU:HD11	1.76	0.67
1:J:132:ILE:HG21	1:J:163:LEU:HD11	1.76	0.66
1:D:241:VAL:C	1:D:243:ARG:H	2.03	0.66
1:J:557:LYS:HG3	1:J:561:ARG:HH12	0.73	0.66
1:A:140:SER:HB3	1:A:231:ARG:CZ	2.27	0.65
1:G:140:SER:HB3	1:G:231:ARG:CZ	2.27	0.65
1:G:241:VAL:C	1:G:243:ARG:H	2.03	0.65
1:J:140:SER:HB3	1:J:231:ARG:CZ	2.27	0.65
1:D:140:SER:HB3	1:D:231:ARG:CZ	2.27	0.64
1:J:117:PRO:HG2	1:J:122:CYS:HB2	1.80	0.64
1:J:241:VAL:C	1:J:243:ARG:H	2.03	0.64
1:A:241:VAL:C	1:A:243:ARG:H	2.04	0.64
1:G:117:PRO:HG2	1:G:122:CYS:HB2	1.80	0.64
1:D:163:LEU:HD23	1:D:237:ARG:NH1	2.13	0.64
1:D:117:PRO:HG2	1:D:122:CYS:HB2	1.80	0.63
1:J:163:LEU:HD23	1:J:237:ARG:NH1	2.13	0.63
1:G:163:LEU:HD23	1:G:237:ARG:NH1	2.13	0.63
1:A:163:LEU:HD23	1:A:237:ARG:NH1	2.13	0.63
1:A:117:PRO:HG2	1:A:122:CYS:HB2	1.80	0.62
1:A:248:TRP:CD1	4:A:701:PIO:H4A	2.35	0.62
1:D:198:ILE:HD13	1:D:241:VAL:HG13	1.80	0.62
1:J:198:ILE:HD13	1:J:241:VAL:HG13	1.80	0.62
2:K:66:PHE:HA	2:K:69:PHE:HD2	1.65	0.62
1:G:198:ILE:HD13	1:G:241:VAL:HG13	1.80	0.62
1:G:557:LYS:HG3	1:G:561:ARG:HH12	0.73	0.62
1:A:198:ILE:HD13	1:A:241:VAL:HG13	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:66:PHE:HA	2:H:69:PHE:HD2	1.65	0.61
2:B:66:PHE:HA	2:B:69:PHE:HD2	1.65	0.61
1:G:198:ILE:HD13	1:G:241:VAL:CG1	2.33	0.59
2:E:66:PHE:HA	2:E:69:PHE:HD2	1.65	0.59
1:J:198:ILE:HD13	1:J:241:VAL:CG1	2.33	0.59
1:A:306:GLY:O	1:A:310:VAL:HG23	2.03	0.58
1:D:306:GLY:O	1:D:310:VAL:HG23	2.03	0.58
1:D:198:ILE:HD13	1:D:241:VAL:CG1	2.32	0.58
1:D:107:GLN:OE1	1:D:180:CYS:HB3	2.04	0.58
1:A:198:ILE:HD13	1:A:241:VAL:CG1	2.32	0.58
1:D:241:VAL:C	1:D:243:ARG:N	2.60	0.58
1:G:107:GLN:OE1	1:G:180:CYS:HB3	2.04	0.58
1:A:107:GLN:OE1	1:A:180:CYS:HB3	2.04	0.58
1:J:306:GLY:O	1:J:310:VAL:HG23	2.03	0.57
1:G:306:GLY:O	1:G:310:VAL:HG23	2.03	0.57
1:J:520:MET:O	1:J:524:VAL:HG23	2.04	0.57
1:A:241:VAL:C	1:A:243:ARG:N	2.60	0.57
1:A:520:MET:O	1:A:524:VAL:HG23	2.04	0.57
1:D:520:MET:O	1:D:524:VAL:HG23	2.04	0.57
1:G:520:MET:O	1:G:524:VAL:HG23	2.04	0.57
1:G:241:VAL:C	1:G:243:ARG:N	2.60	0.56
1:J:107:GLN:OE1	1:J:180:CYS:HB3	2.04	0.56
1:D:249:ARG:HH21	4:D:701:PIO:H1CA	1.72	0.55
1:A:110:VAL:HG21	1:A:176:TRP:HZ2	1.69	0.55
1:J:228:ARG:NH2	1:J:229:GLY:HA2	2.22	0.55
1:A:228:ARG:NH2	1:A:229:GLY:HA2	2.22	0.55
1:G:228:ARG:NH2	1:G:229:GLY:HA2	2.22	0.55
1:G:249:ARG:HH21	4:G:701:PIO:H1CA	1.72	0.55
1:A:249:ARG:HH21	4:A:701:PIO:H1CA	1.71	0.55
1:A:513:THR:O	1:A:517:ILE:HG12	2.07	0.55
1:J:513:THR:O	1:J:517:ILE:HG12	2.07	0.54
1:D:228:ARG:NH2	1:D:229:GLY:HA2	2.22	0.54
1:J:132:ILE:HA	1:J:135:VAL:HG13	1.90	0.54
1:A:132:ILE:HA	1:A:135:VAL:HG13	1.90	0.54
1:G:513:THR:O	1:G:517:ILE:HG12	2.07	0.54
1:J:241:VAL:C	1:J:243:ARG:N	2.60	0.54
1:D:110:VAL:HG21	1:D:176:TRP:HZ2	1.72	0.54
1:J:249:ARG:HH21	4:J:701:PIO:H1CA	1.71	0.54
1:J:507:ARG:HA	1:J:510:HIS:CD2	2.43	0.54
1:A:176:TRP:H	1:A:176:TRP:CD1	2.25	0.53
1:A:507:ARG:HA	1:A:510:HIS:CD2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:110:VAL:HG21	1:G:176:TRP:HZ2	1.72	0.53
1:D:513:THR:O	1:D:517:ILE:HG12	2.07	0.53
1:D:507:ARG:HA	1:D:510:HIS:CD2	2.43	0.53
1:G:507:ARG:HA	1:G:510:HIS:CD2	2.43	0.53
1:J:134:LEU:O	1:J:135:VAL:C	2.51	0.53
2:B:89:ALA:O	2:B:92:VAL:HG12	2.08	0.53
2:H:89:ALA:O	2:H:92:VAL:HG12	2.08	0.53
1:J:137:LEU:HA	1:J:231:ARG:NH2	2.24	0.53
1:G:137:LEU:HA	1:G:231:ARG:NH2	2.24	0.53
1:A:574:ILE:HG21	1:D:573:PHE:CG	2.44	0.53
2:E:89:ALA:O	2:E:92:VAL:HG12	2.08	0.53
2:K:89:ALA:O	2:K:92:VAL:HG12	2.08	0.53
1:A:137:LEU:HA	1:A:231:ARG:NH2	2.24	0.52
1:D:132:ILE:HA	1:D:135:VAL:HG13	1.90	0.52
1:D:184:TYR:HB3	1:D:189:GLY:CA	2.39	0.52
1:G:132:ILE:HA	1:G:135:VAL:HG13	1.90	0.52
1:J:110:VAL:HG21	1:J:176:TRP:HZ2	1.73	0.52
1:J:182:SER:C	1:J:184:TYR:N	2.67	0.52
1:D:137:LEU:HA	1:D:231:ARG:NH2	2.24	0.52
1:A:527:LYS:HA	1:A:530:GLN:NE2	2.25	0.52
1:G:182:SER:C	1:G:184:TYR:N	2.67	0.52
1:J:184:TYR:HB3	1:J:189:GLY:CA	2.39	0.52
1:J:527:LYS:HA	1:J:530:GLN:NE2	2.25	0.52
1:A:184:TYR:HB3	1:A:189:GLY:CA	2.39	0.51
1:D:230:ILE:HG23	1:D:234:GLN:NE2	2.26	0.51
1:G:184:TYR:HB3	1:G:189:GLY:CA	2.39	0.51
1:G:303:LEU:HD12	3:L:47:VAL:HG12	1.92	0.51
1:D:527:LYS:HA	1:D:530:GLN:NE2	2.25	0.51
1:G:527:LYS:HA	1:G:530:GLN:NE2	2.25	0.51
1:G:230:ILE:HG23	1:G:234:GLN:NE2	2.25	0.51
1:G:531:GLN:HA	1:G:534:LYS:HE3	1.93	0.51
1:A:230:ILE:HG23	1:A:234:GLN:NE2	2.25	0.51
1:D:303:LEU:HD12	3:I:47:VAL:HG12	1.92	0.51
1:D:531:GLN:HA	1:D:534:LYS:HE3	1.93	0.51
1:A:134:LEU:O	1:A:135:VAL:C	2.52	0.51
1:A:342:LEU:N	1:A:343:PRO:CD	2.74	0.51
1:A:531:GLN:HA	1:A:534:LYS:HE3	1.93	0.51
1:D:342:LEU:N	1:D:343:PRO:CD	2.74	0.51
1:G:241:VAL:O	1:G:242:ASP:HB2	2.11	0.51
1:A:241:VAL:O	1:A:242:ASP:HB2	2.11	0.51
1:G:342:LEU:N	1:G:343:PRO:CD	2.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:107:GLN:NE2	1:J:181:ARG:HB3	2.26	0.51
1:J:526:LYS:HE3	1:J:530:GLN:OE1	2.11	0.51
1:D:107:GLN:NE2	1:D:181:ARG:HB3	2.26	0.50
1:D:179:GLY:HA2	1:D:185:VAL:HB	1.93	0.50
1:G:526:LYS:HE3	1:G:530:GLN:OE1	2.11	0.50
1:A:303:LEU:HD12	3:F:47:VAL:HG12	1.92	0.50
1:A:179:GLY:HA2	1:A:185:VAL:HB	1.93	0.50
1:D:526:LYS:HE3	1:D:530:GLN:OE1	2.11	0.50
1:J:176:TRP:CD1	1:J:176:TRP:H	2.29	0.50
1:D:176:TRP:H	1:D:176:TRP:CD1	2.30	0.50
1:G:574:ILE:HG21	1:J:573:PHE:CG	2.46	0.50
1:A:107:GLN:NE2	1:A:181:ARG:HB3	2.26	0.50
1:G:107:GLN:NE2	1:G:181:ARG:HB3	2.26	0.50
1:J:519:ARG:HG3	1:J:523:PHE:CE2	2.47	0.50
1:D:241:VAL:O	1:D:242:ASP:HB2	2.11	0.50
1:D:574:ILE:HG21	1:G:573:PHE:CG	2.46	0.50
1:G:133:VAL:HG13	1:G:237:ARG:HE	1.77	0.50
1:J:133:VAL:HG13	1:J:237:ARG:HE	1.77	0.50
1:J:342:LEU:N	1:J:343:PRO:CD	2.74	0.50
1:A:573:PHE:CG	1:J:574:ILE:HG21	2.47	0.50
1:G:176:TRP:CD1	1:G:176:TRP:H	2.29	0.50
1:J:230:ILE:HG23	1:J:234:GLN:NE2	2.26	0.50
1:A:519:ARG:HG3	1:A:523:PHE:CE2	2.47	0.50
1:J:531:GLN:HA	1:J:534:LYS:HE3	1.93	0.50
1:G:179:GLY:HA2	1:G:185:VAL:HB	1.93	0.49
1:D:134:LEU:O	1:D:135:VAL:C	2.52	0.49
1:G:519:ARG:HG3	1:G:523:PHE:CE2	2.47	0.49
1:A:227:ILE:O	1:A:228:ARG:C	2.55	0.49
1:D:133:VAL:HG13	1:D:237:ARG:HE	1.77	0.49
3:C:47:VAL:HG12	1:J:303:LEU:HD12	1.93	0.49
1:A:133:VAL:HG13	1:A:237:ARG:HE	1.77	0.49
1:A:526:LYS:HE3	1:A:530:GLN:OE1	2.11	0.49
1:J:241:VAL:O	1:J:242:ASP:HB2	2.11	0.49
1:A:560:GLN:O	1:A:561:ARG:C	2.54	0.49
1:G:227:ILE:O	1:G:228:ARG:C	2.55	0.49
1:D:519:ARG:HG3	1:D:523:PHE:CE2	2.47	0.49
1:D:572:LEU:O	1:D:575:SER:OG	2.30	0.49
2:E:66:PHE:N	2:E:67:PRO:HD2	2.28	0.49
2:K:66:PHE:N	2:K:67:PRO:HD2	2.28	0.48
1:D:560:GLN:O	1:D:561:ARG:C	2.54	0.48
1:G:134:LEU:O	1:G:135:VAL:C	2.52	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:179:GLY:HA2	1:J:185:VAL:HB	1.93	0.48
2:B:66:PHE:N	2:B:67:PRO:HD2	2.28	0.48
1:D:114:LEU:O	1:D:243:ARG:NH2	2.47	0.48
1:G:117:PRO:HD2	1:G:122:CYS:SG	2.54	0.48
2:K:132:ASP:HA	2:K:142:PHE:HZ	1.78	0.48
2:H:66:PHE:N	2:H:67:PRO:HD2	2.28	0.48
1:J:117:PRO:HD2	1:J:122:CYS:SG	2.54	0.48
1:A:114:LEU:O	1:A:243:ARG:NH2	2.47	0.48
1:A:368:ILE:HB	1:A:369:PRO:HD3	1.95	0.48
1:J:114:LEU:O	1:J:243:ARG:NH2	2.47	0.48
1:J:368:ILE:HB	1:J:369:PRO:HD3	1.95	0.48
1:A:251:LEU:HD11	1:J:268:ILE:HD11	1.96	0.48
2:B:132:ASP:HA	2:B:142:PHE:HZ	1.78	0.48
1:D:228:ARG:NH2	1:D:232:PHE:HB3	2.29	0.48
1:D:248:TRP:CD1	4:D:701:PIO:H4A	2.49	0.48
2:E:132:ASP:HA	2:E:142:PHE:HZ	1.78	0.48
1:G:268:ILE:HD11	1:J:251:LEU:HD11	1.96	0.48
1:A:117:PRO:HD2	1:A:122:CYS:SG	2.54	0.48
1:A:228:ARG:NH2	1:A:232:PHE:HB3	2.29	0.48
1:A:550:LEU:HD12	1:A:550:LEU:H	1.79	0.48
1:D:227:ILE:O	1:D:228:ARG:C	2.55	0.48
1:J:248:TRP:CD1	4:J:701:PIO:H4A	2.49	0.48
1:D:368:ILE:HB	1:D:369:PRO:HD3	1.95	0.47
1:D:550:LEU:HD12	1:D:550:LEU:H	1.79	0.47
1:D:107:GLN:CD	1:D:181:ARG:HB3	2.39	0.47
1:D:117:PRO:HD2	1:D:122:CYS:SG	2.54	0.47
1:D:182:SER:C	1:D:184:TYR:H	2.21	0.47
1:G:248:TRP:CD1	4:G:701:PIO:H4A	2.49	0.47
1:A:182:SER:C	1:A:184:TYR:N	2.67	0.47
1:A:253:SER:O	1:A:257:ILE:HG13	2.15	0.47
1:G:114:LEU:O	1:G:243:ARG:NH2	2.47	0.47
1:G:550:LEU:HD12	1:G:550:LEU:H	1.80	0.47
1:J:162:VAL:O	1:J:165:VAL:HG12	2.14	0.47
1:A:107:GLN:CD	1:A:181:ARG:HB3	2.39	0.47
1:A:162:VAL:O	1:A:165:VAL:HG12	2.14	0.47
1:A:268:ILE:HD11	1:D:251:LEU:HD11	1.97	0.47
1:G:135:VAL:HG22	1:G:136:CYS:N	2.29	0.47
1:J:253:SER:O	1:J:257:ILE:HG13	2.15	0.47
1:A:176:TRP:H	1:A:176:TRP:HD1	1.60	0.47
1:G:228:ARG:NH2	1:G:232:PHE:HB3	2.29	0.47
1:G:252:GLY:O	1:G:253:SER:C	2.56	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:368:ILE:HB	1:G:369:PRO:HD3	1.95	0.47
2:H:132:ASP:HA	2:H:142:PHE:HZ	1.78	0.47
1:A:135:VAL:HG22	1:A:136:CYS:N	2.29	0.47
1:A:251:LEU:HD11	1:J:268:ILE:CD1	2.45	0.47
1:A:519:ARG:NH1	2:B:72:MET:O	2.48	0.47
1:G:107:GLN:CD	1:G:181:ARG:HB3	2.39	0.47
1:G:182:SER:C	1:G:184:TYR:H	2.21	0.47
1:D:162:VAL:O	1:D:165:VAL:HG12	2.14	0.47
1:D:253:SER:O	1:D:257:ILE:HG13	2.15	0.47
1:G:519:ARG:NH1	2:H:72:MET:O	2.48	0.47
1:J:107:GLN:CD	1:J:181:ARG:HB3	2.39	0.47
1:J:550:LEU:H	1:J:550:LEU:HD12	1.80	0.47
1:J:566:SER:O	1:J:570:PRO:HD2	2.14	0.47
1:A:182:SER:C	1:A:184:TYR:H	2.21	0.47
1:D:566:SER:O	1:D:570:PRO:HD2	2.14	0.47
1:G:566:SER:O	1:G:570:PRO:HD2	2.14	0.47
1:A:252:GLY:O	1:A:253:SER:C	2.56	0.47
1:D:230:ILE:HG22	1:D:231:ARG:HD2	1.97	0.47
1:J:182:SER:C	1:J:184:TYR:H	2.21	0.47
1:A:566:SER:O	1:A:570:PRO:HD2	2.14	0.46
1:D:342:LEU:CD2	1:G:344:ALA:CB	2.93	0.46
1:D:509:HIS:O	1:D:513:THR:HG23	2.15	0.46
1:J:252:GLY:O	1:J:253:SER:C	2.56	0.46
1:D:182:SER:C	1:D:184:TYR:N	2.67	0.46
1:D:268:ILE:CD1	1:G:251:LEU:HD11	2.46	0.46
1:D:519:ARG:NH1	2:E:72:MET:O	2.48	0.46
1:G:253:SER:O	1:G:257:ILE:HG13	2.15	0.46
1:G:509:HIS:O	1:G:513:THR:HG23	2.15	0.46
1:J:135:VAL:HG22	1:J:136:CYS:N	2.29	0.46
1:G:230:ILE:HG22	1:G:231:ARG:HD2	1.97	0.46
1:G:268:ILE:CD1	1:J:251:LEU:HD11	2.45	0.46
1:J:228:ARG:NH2	1:J:232:PHE:HB3	2.29	0.46
1:J:519:ARG:NH1	2:K:72:MET:O	2.48	0.46
1:A:268:ILE:CD1	1:D:251:LEU:HD11	2.46	0.46
1:D:268:ILE:HD11	1:G:251:LEU:HD11	1.97	0.46
1:G:232:PHE:O	1:G:232:PHE:CG	2.69	0.46
2:K:139:TYR:O	2:K:143:VAL:HG13	2.16	0.46
3:L:67:ARG:NH2	4:L:101:PIO:O42	2.49	0.46
2:H:139:TYR:O	2:H:143:VAL:HG13	2.16	0.46
1:G:572:LEU:O	1:G:575:SER:OG	2.30	0.46
1:J:232:PHE:O	1:J:232:PHE:CG	2.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:243:ARG:O	1:J:244:GLN:HB2	2.16	0.46
1:A:243:ARG:O	1:A:244:GLN:HB2	2.16	0.46
1:A:527:LYS:O	1:A:531:GLN:HG3	2.16	0.46
1:G:560:GLN:O	1:G:561:ARG:C	2.54	0.46
1:J:509:HIS:O	1:J:513:THR:HG23	2.16	0.46
1:A:230:ILE:HG22	1:A:231:ARG:HD2	1.97	0.45
1:G:162:VAL:O	1:G:165:VAL:HG12	2.14	0.45
1:G:527:LYS:O	1:G:531:GLN:HG3	2.17	0.45
1:A:344:ALA:CB	1:J:342:LEU:CD2	2.92	0.45
3:F:67:ARG:NH2	4:F:101:PIO:O42	2.49	0.45
1:A:509:HIS:O	1:A:513:THR:HG23	2.15	0.45
1:A:529:PHE:HE1	1:A:533:ARG:HH21	1.64	0.45
1:D:135:VAL:HG22	1:D:136:CYS:N	2.29	0.45
1:D:232:PHE:O	1:D:232:PHE:CG	2.69	0.45
2:E:139:TYR:O	2:E:143:VAL:HG13	2.16	0.45
1:J:230:ILE:HG22	1:J:231:ARG:HD2	1.97	0.45
1:J:244:GLN:HG2	1:J:245:GLY:H	1.82	0.45
1:D:252:GLY:O	1:D:253:SER:C	2.56	0.45
2:H:132:ASP:HA	2:H:142:PHE:CZ	2.52	0.45
1:A:342:LEU:CD2	1:D:344:ALA:CB	2.93	0.45
1:D:243:ARG:O	1:D:244:GLN:HB2	2.16	0.45
1:D:529:PHE:HE1	1:D:533:ARG:HH21	1.64	0.45
3:I:67:ARG:NH2	4:I:101:PIO:O42	2.49	0.45
1:J:527:LYS:O	1:J:531:GLN:HG3	2.17	0.45
1:A:230:ILE:HG23	1:A:234:GLN:HE21	1.81	0.45
1:D:244:GLN:HG2	1:D:245:GLY:H	1.82	0.45
1:J:227:ILE:O	1:J:228:ARG:C	2.55	0.45
1:A:110:VAL:HG21	1:A:176:TRP:CZ2	2.50	0.45
1:J:230:ILE:HG23	1:J:234:GLN:HE21	1.81	0.45
1:A:232:PHE:O	1:A:232:PHE:CG	2.69	0.45
2:B:139:TYR:O	2:B:143:VAL:HG13	2.16	0.45
1:D:230:ILE:HG23	1:D:234:GLN:HE21	1.82	0.45
1:J:529:PHE:HE1	1:J:533:ARG:HH21	1.64	0.45
2:K:132:ASP:HA	2:K:142:PHE:CZ	2.52	0.45
2:E:132:ASP:HA	2:E:142:PHE:CZ	2.52	0.45
1:G:557:LYS:HE3	1:G:561:ARG:HH11	1.82	0.45
1:J:228:ARG:HH21	1:J:229:GLY:HA2	1.82	0.45
1:J:572:LEU:O	1:J:575:SER:OG	2.30	0.45
1:A:557:LYS:HE3	1:A:561:ARG:HH11	1.82	0.44
1:D:176:TRP:H	1:D:176:TRP:HD1	1.65	0.44
1:D:527:LYS:O	1:D:531:GLN:HG3	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:243:ARG:O	1:G:244:GLN:HB2	2.16	0.44
1:G:529:PHE:HE1	1:G:533:ARG:HH21	1.64	0.44
2:B:132:ASP:HA	2:B:142:PHE:CZ	2.52	0.44
1:G:131:LEU:HD12	1:G:131:LEU:HA	1.79	0.44
1:J:186:GLY:O	1:J:187:LEU:C	2.60	0.44
1:D:163:LEU:HD23	1:D:237:ARG:HH12	1.82	0.44
1:D:557:LYS:HE3	1:D:561:ARG:HH11	1.82	0.44
1:G:176:TRP:H	1:G:176:TRP:HD1	1.65	0.44
1:G:228:ARG:HH21	1:G:229:GLY:HA2	1.82	0.44
1:G:244:GLN:HG2	1:G:245:GLY:H	1.82	0.44
1:G:555:ARG:HD2	1:G:555:ARG:HA	1.88	0.44
1:J:176:TRP:H	1:J:176:TRP:HD1	1.65	0.44
1:J:555:ARG:HD2	1:J:555:ARG:HA	1.88	0.44
1:A:186:GLY:O	1:A:187:LEU:C	2.60	0.44
1:A:228:ARG:HH21	1:A:229:GLY:HA2	1.83	0.44
1:D:186:GLY:O	1:D:187:LEU:C	2.60	0.44
1:G:230:ILE:HG23	1:G:234:GLN:HE21	1.81	0.44
1:J:557:LYS:HE3	1:J:561:ARG:HH11	1.82	0.44
3:C:67:ARG:NH2	4:C:101:PIO:O42	2.51	0.44
1:G:186:GLY:O	1:G:187:LEU:C	2.60	0.43
1:D:310:VAL:HG22	1:D:332:PHE:HZ	1.84	0.43
1:J:560:GLN:O	1:J:561:ARG:C	2.54	0.43
1:A:244:GLN:HG2	1:A:245:GLY:H	1.82	0.43
1:D:185:VAL:N	1:D:189:GLY:HA3	2.33	0.43
1:G:163:LEU:HD23	1:G:237:ARG:HH12	1.82	0.43
1:A:185:VAL:N	1:A:189:GLY:HA3	2.33	0.43
1:G:185:VAL:N	1:G:189:GLY:HA3	2.33	0.43
1:J:310:VAL:HG22	1:J:332:PHE:HZ	1.84	0.43
1:D:131:LEU:HD12	1:D:131:LEU:HA	1.79	0.43
1:J:171:TYR:CZ	1:J:175:LEU:HD21	2.54	0.43
1:J:185:VAL:N	1:J:189:GLY:HA3	2.33	0.42
1:A:133:VAL:HB	1:A:238:MET:SD	2.60	0.42
1:A:310:VAL:HG22	1:A:332:PHE:HZ	1.84	0.42
1:D:228:ARG:HH21	1:D:229:GLY:HA2	1.83	0.42
2:E:103:ALA:C	2:E:105:GLU:N	2.77	0.42
1:G:310:VAL:HG22	1:G:332:PHE:HZ	1.84	0.42
1:G:342:LEU:CD2	1:J:344:ALA:CB	2.94	0.42
1:J:133:VAL:HB	1:J:238:MET:SD	2.59	0.42
1:A:248:TRP:CG	4:A:701:PIO:H4A	2.53	0.42
1:G:133:VAL:HB	1:G:238:MET:SD	2.60	0.42
2:B:103:ALA:C	2:B:105:GLU:N	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171:TYR:CZ	1:D:175:LEU:HD21	2.54	0.42
1:D:557:LYS:HA	1:D:557:LYS:HD2	1.89	0.42
1:A:129:VAL:O	1:A:130:PHE:C	2.61	0.42
1:A:151:LEU:HD23	1:A:151:LEU:HA	1.85	0.42
1:G:171:TYR:CZ	1:G:175:LEU:HD21	2.55	0.42
1:A:114:LEU:HB3	1:A:174:ARG:NH2	2.35	0.42
2:B:103:ALA:C	2:B:105:GLU:H	2.28	0.42
1:D:110:VAL:HG21	1:D:176:TRP:CZ2	2.55	0.42
1:D:133:VAL:HB	1:D:238:MET:SD	2.60	0.42
2:H:103:ALA:C	2:H:105:GLU:N	2.77	0.42
1:J:129:VAL:O	1:J:130:PHE:C	2.61	0.42
1:G:229:GLY:O	1:G:230:ILE:C	2.63	0.41
2:K:103:ALA:C	2:K:105:GLU:N	2.77	0.41
2:K:103:ALA:C	2:K:105:GLU:H	2.28	0.41
1:D:129:VAL:O	1:D:130:PHE:C	2.61	0.41
1:G:506:LEU:HD12	1:G:506:LEU:O	2.20	0.41
2:H:103:ALA:C	2:H:105:GLU:H	2.28	0.41
2:H:117:LEU:HD12	2:H:117:LEU:HA	1.97	0.41
1:A:234:GLN:O	1:A:235:ILE:C	2.63	0.41
2:E:103:ALA:C	2:E:105:GLU:H	2.28	0.41
1:G:310:VAL:HG22	1:G:332:PHE:CZ	2.56	0.41
1:G:560:GLN:HE22	1:J:562:ARG:NE	2.19	0.41
1:J:152:ALA:C	1:J:154:GLY:H	2.29	0.41
1:J:310:VAL:HG22	1:J:332:PHE:CZ	2.56	0.41
1:J:506:LEU:O	1:J:506:LEU:HD12	2.21	0.41
1:A:152:ALA:C	1:A:154:GLY:H	2.29	0.41
1:A:289:ASN:OD1	1:A:290:GLU:N	2.49	0.41
1:D:152:ALA:C	1:D:154:GLY:H	2.29	0.41
1:D:234:GLN:O	1:D:235:ILE:C	2.63	0.41
1:A:163:LEU:HD23	1:A:237:ARG:HH12	1.82	0.41
1:A:574:ILE:HG21	1:D:573:PHE:CD1	2.55	0.41
1:D:190:ARG:HE	1:D:190:ARG:HB3	1.77	0.41
1:J:234:GLN:O	1:J:235:ILE:C	2.64	0.41
1:A:111:TYR:O	1:A:115:GLU:HB2	2.21	0.41
1:A:310:VAL:HG22	1:A:332:PHE:CZ	2.56	0.41
1:D:310:VAL:HG22	1:D:332:PHE:CZ	2.56	0.41
1:G:179:GLY:N	1:G:184:TYR:O	2.54	0.41
1:G:557:LYS:HA	1:G:557:LYS:HD2	1.89	0.41
1:J:289:ASN:OD1	1:J:290:GLU:N	2.49	0.41
1:J:163:LEU:HD23	1:J:237:ARG:HH12	1.82	0.41
1:G:129:VAL:O	1:G:130:PHE:C	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:152:ALA:C	1:G:154:GLY:H	2.29	0.40
1:G:234:GLN:N	1:G:234:GLN:OE1	2.55	0.40
1:A:179:GLY:N	1:A:184:TYR:O	2.54	0.40
1:D:234:GLN:N	1:D:234:GLN:OE1	2.55	0.40
1:G:111:TYR:O	1:G:115:GLU:HB2	2.21	0.40
1:J:526:LYS:HA	1:J:526:LYS:HD2	1.82	0.40
1:A:255:VAL:HG23	1:A:256:PHE:N	2.37	0.40
1:A:506:LEU:O	1:A:506:LEU:HD12	2.21	0.40
1:D:138:ILE:HA	1:D:141:VAL:HG22	2.04	0.40
1:J:234:GLN:N	1:J:234:GLN:OE1	2.54	0.40
1:J:255:VAL:HG23	1:J:256:PHE:N	2.37	0.40
1:A:248:TRP:HB3	4:A:701:PIO:H6B	2.03	0.40
1:A:560:GLN:HE22	1:D:562:ARG:NE	2.19	0.40
1:D:255:VAL:HG23	1:D:256:PHE:N	2.37	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	331/676 (49%)	311 (94%)	19 (6%)	1 (0%)	37	65
1	D	331/676 (49%)	311 (94%)	19 (6%)	1 (0%)	37	65
1	G	331/676 (49%)	311 (94%)	19 (6%)	1 (0%)	37	65
1	J	331/676 (49%)	311 (94%)	19 (6%)	1 (0%)	37	65
2	B	142/149 (95%)	133 (94%)	9 (6%)	0	100	100
2	E	142/149 (95%)	133 (94%)	9 (6%)	0	100	100
2	H	142/149 (95%)	133 (94%)	9 (6%)	0	100	100
2	K	142/149 (95%)	133 (94%)	9 (6%)	0	100	100
3	C	28/30 (93%)	28 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	F	28/30 (93%)	28 (100%)	0	0	100	100
3	I	28/30 (93%)	28 (100%)	0	0	100	100
3	L	28/30 (93%)	28 (100%)	0	0	100	100
All	All	2004/3420 (59%)	1888 (94%)	112 (6%)	4 (0%)	45	71

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	314	GLY
1	D	314	GLY
1	G	314	GLY
1	J	314	GLY

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	288/567 (51%)	283 (98%)	5 (2%)	56	74
1	D	288/567 (51%)	283 (98%)	5 (2%)	56	74
1	G	288/567 (51%)	283 (98%)	5 (2%)	56	74
1	J	288/567 (51%)	283 (98%)	5 (2%)	56	74
2	B	32/127 (25%)	32 (100%)	0	100	100
2	E	32/127 (25%)	32 (100%)	0	100	100
2	H	32/127 (25%)	32 (100%)	0	100	100
2	K	32/127 (25%)	32 (100%)	0	100	100
3	C	25/25 (100%)	25 (100%)	0	100	100
3	F	25/25 (100%)	25 (100%)	0	100	100
3	I	25/25 (100%)	25 (100%)	0	100	100
3	L	25/25 (100%)	25 (100%)	0	100	100
All	All	1380/2876 (48%)	1360 (99%)	20 (1%)	62	78

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	VAL
1	A	175	LEU
1	A	230	ILE
1	A	233	LEU
1	A	234	GLN
1	D	135	VAL
1	D	175	LEU
1	D	230	ILE
1	D	233	LEU
1	D	234	GLN
1	G	135	VAL
1	G	175	LEU
1	G	230	ILE
1	G	233	LEU
1	G	234	GLN
1	J	135	VAL
1	J	175	LEU
1	J	230	ILE
1	J	233	LEU
1	J	234	GLN

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

Mol	Chain	Res	Type
1	A	240	HIS
1	A	376	GLN
1	A	531	GLN
1	A	560	GLN
1	D	386	ASN
1	D	531	GLN
1	D	560	GLN
1	G	240	HIS
1	G	531	GLN
1	G	560	GLN
1	J	376	GLN
1	J	386	ASN
1	J	531	GLN
1	J	560	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 11 ligands modelled in this entry, 3 are monoatomic - leaving 8 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	PIO	J	701	-	47,47,47	1.17	6 (12%)	61,65,65	0.98	3 (4%)
4	PIO	I	101	-	47,47,47	1.19	6 (12%)	61,65,65	1.08	4 (6%)
4	PIO	F	101	-	47,47,47	1.20	6 (12%)	61,65,65	1.08	4 (6%)
4	PIO	G	701	-	47,47,47	1.17	6 (12%)	61,65,65	0.98	3 (4%)
4	PIO	A	701	-	47,47,47	1.18	6 (12%)	61,65,65	0.98	3 (4%)
4	PIO	C	101	-	47,47,47	1.19	6 (12%)	61,65,65	1.08	4 (6%)
4	PIO	D	701	-	47,47,47	1.18	6 (12%)	61,65,65	0.98	3 (4%)
4	PIO	L	101	-	47,47,47	1.19	6 (12%)	61,65,65	1.08	4 (6%)

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	PIO	J	701	-	-	15/44/68/68	0/1/1/1
4	PIO	I	101	-	-	21/44/68/68	0/1/1/1
4	PIO	F	101	-	-	21/44/68/68	0/1/1/1
4	PIO	G	701	-	-	14/44/68/68	0/1/1/1
4	PIO	A	701	-	-	15/44/68/68	0/1/1/1
4	PIO	C	101	-	-	21/44/68/68	0/1/1/1
4	PIO	D	701	-	-	15/44/68/68	0/1/1/1
4	PIO	L	101	-	-	21/44/68/68	0/1/1/1

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	101	PIO	P5-O5	3.28	1.65	1.59
4	C	101	PIO	P5-O5	3.25	1.65	1.59
4	I	101	PIO	P5-O5	3.25	1.65	1.59
4	L	101	PIO	P5-O5	3.24	1.65	1.59
4	A	701	PIO	P5-O5	3.20	1.65	1.59
4	J	701	PIO	P5-O5	3.18	1.65	1.59
4	G	701	PIO	P5-O5	3.16	1.65	1.59
4	D	701	PIO	P5-O5	3.16	1.65	1.59
4	F	101	PIO	P4-O4	3.08	1.65	1.59
4	C	101	PIO	P4-O4	3.05	1.65	1.59
4	I	101	PIO	P4-O4	3.04	1.65	1.59
4	L	101	PIO	P4-O4	3.04	1.65	1.59
4	D	701	PIO	P4-O4	3.00	1.65	1.59
4	A	701	PIO	P4-O4	2.98	1.64	1.59
4	J	701	PIO	P4-O4	2.94	1.64	1.59
4	G	701	PIO	P4-O4	2.94	1.64	1.59
4	D	701	PIO	O2C-C2C	-2.61	1.40	1.46
4	A	701	PIO	O2C-C2C	-2.59	1.40	1.46
4	I	101	PIO	O2C-C2C	-2.59	1.40	1.46
4	C	101	PIO	O2C-C2C	-2.59	1.40	1.46
4	G	701	PIO	O2C-C2C	-2.58	1.40	1.46
4	L	101	PIO	O2C-C2C	-2.57	1.40	1.46
4	J	701	PIO	O2C-C2C	-2.57	1.40	1.46
4	F	101	PIO	O2C-C2C	-2.56	1.40	1.46
4	L	101	PIO	O3C-C1B	2.46	1.40	1.33
4	C	101	PIO	O3C-C1B	2.46	1.40	1.33
4	F	101	PIO	O3C-C1B	2.46	1.40	1.33
4	I	101	PIO	O3C-C1B	2.45	1.40	1.33
4	D	701	PIO	O3C-C1B	2.31	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	701	PIO	O3C-C1B	2.31	1.40	1.33
4	J	701	PIO	O3C-C1B	2.31	1.40	1.33
4	A	701	PIO	O3C-C1B	2.31	1.40	1.33
4	J	701	PIO	O3C-C3C	-2.25	1.40	1.45
4	A	701	PIO	O3C-C3C	-2.22	1.40	1.45
4	D	701	PIO	O3C-C3C	-2.21	1.40	1.45
4	G	701	PIO	O3C-C3C	-2.21	1.40	1.45
4	L	101	PIO	O3C-C3C	-2.10	1.40	1.45
4	C	101	PIO	O3C-C3C	-2.10	1.40	1.45
4	I	101	PIO	O3C-C3C	-2.10	1.40	1.45
4	F	101	PIO	O3C-C3C	-2.09	1.40	1.45
4	I	101	PIO	O2C-C1A	2.05	1.40	1.34
4	C	101	PIO	O2C-C1A	2.05	1.40	1.34
4	L	101	PIO	O2C-C1A	2.03	1.40	1.34
4	F	101	PIO	O2C-C1A	2.03	1.40	1.34
4	A	701	PIO	O2C-C1A	2.02	1.40	1.34
4	G	701	PIO	O2C-C1A	2.02	1.40	1.34
4	D	701	PIO	O2C-C1A	2.02	1.40	1.34
4	J	701	PIO	O2C-C1A	2.02	1.40	1.34

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	701	PIO	O2C-C1A-C2A	4.25	120.67	111.50
4	D	701	PIO	O2C-C1A-C2A	4.25	120.66	111.50
4	J	701	PIO	O2C-C1A-C2A	4.25	120.66	111.50
4	G	701	PIO	O2C-C1A-C2A	4.23	120.62	111.50
4	L	101	PIO	O2C-C1A-C2A	4.22	120.59	111.50
4	C	101	PIO	O2C-C1A-C2A	4.20	120.56	111.50
4	I	101	PIO	O2C-C1A-C2A	4.20	120.56	111.50
4	F	101	PIO	O2C-C1A-C2A	4.20	120.56	111.50
4	I	101	PIO	O3C-C1B-C2B	2.81	120.72	111.91
4	L	101	PIO	O3C-C1B-C2B	2.80	120.71	111.91
4	C	101	PIO	O3C-C1B-C2B	2.80	120.69	111.91
4	F	101	PIO	O3C-C1B-C2B	2.79	120.67	111.91
4	J	701	PIO	O3C-C1B-C2B	2.55	119.91	111.91
4	D	701	PIO	O3C-C1B-C2B	2.55	119.90	111.91
4	A	701	PIO	O3C-C1B-C2B	2.55	119.90	111.91
4	G	701	PIO	O3C-C1B-C2B	2.54	119.86	111.91
4	L	101	PIO	C3-C4-C5	-2.44	106.08	111.66
4	F	101	PIO	C3-C4-C5	-2.44	106.08	111.66
4	I	101	PIO	C3-C4-C5	-2.44	106.08	111.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	101	PIO	C3-C4-C5	-2.44	106.08	111.66
4	I	101	PIO	C6-C5-C4	-2.36	106.27	111.66
4	L	101	PIO	C6-C5-C4	-2.36	106.27	111.66
4	C	101	PIO	C6-C5-C4	-2.36	106.27	111.66
4	F	101	PIO	C6-C5-C4	-2.35	106.30	111.66
4	D	701	PIO	C2C-O2C-C1A	-2.17	112.44	117.79
4	G	701	PIO	C2C-O2C-C1A	-2.17	112.45	117.79
4	J	701	PIO	C2C-O2C-C1A	-2.16	112.46	117.79
4	A	701	PIO	C2C-O2C-C1A	-2.16	112.47	117.79

There are no chirality outliers.

All (143) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	701	PIO	C1C-O13-P1-O11
4	A	701	PIO	C6-C5-O5-P5
4	A	701	PIO	C5-O5-P5-O53
4	C	101	PIO	C2-C1-O1-P1
4	C	101	PIO	C6-C1-O1-P1
4	C	101	PIO	C1C-O13-P1-O11
4	C	101	PIO	C1C-O13-P1-O12
4	C	101	PIO	C4-O4-P4-O42
4	C	101	PIO	C5-O5-P5-O53
4	C	101	PIO	O1A-C1A-O2C-C2C
4	C	101	PIO	C2A-C1A-O2C-C2C
4	C	101	PIO	O1B-C1B-O3C-C3C
4	C	101	PIO	C2B-C1B-O3C-C3C
4	D	701	PIO	C1C-O13-P1-O11
4	D	701	PIO	C6-C5-O5-P5
4	D	701	PIO	C5-O5-P5-O53
4	F	101	PIO	C2-C1-O1-P1
4	F	101	PIO	C6-C1-O1-P1
4	F	101	PIO	C1C-O13-P1-O11
4	F	101	PIO	C1C-O13-P1-O12
4	F	101	PIO	C4-O4-P4-O42
4	F	101	PIO	C5-O5-P5-O53
4	F	101	PIO	O1A-C1A-O2C-C2C
4	F	101	PIO	C2A-C1A-O2C-C2C
4	F	101	PIO	O1B-C1B-O3C-C3C
4	F	101	PIO	C2B-C1B-O3C-C3C
4	G	701	PIO	C1C-O13-P1-O11
4	G	701	PIO	C6-C5-O5-P5

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Mol	Chain	Res	Type	Atoms
4	G	701	PIO	C5-O5-P5-O53
4	I	101	PIO	C2-C1-O1-P1
4	I	101	PIO	C6-C1-O1-P1
4	I	101	PIO	C1C-O13-P1-O11
4	I	101	PIO	C1C-O13-P1-O12
4	I	101	PIO	C4-O4-P4-O42
4	I	101	PIO	C5-O5-P5-O53
4	I	101	PIO	O1A-C1A-O2C-C2C
4	I	101	PIO	C2A-C1A-O2C-C2C
4	I	101	PIO	O1B-C1B-O3C-C3C
4	I	101	PIO	C2B-C1B-O3C-C3C
4	J	701	PIO	C1C-O13-P1-O11
4	J	701	PIO	C6-C5-O5-P5
4	J	701	PIO	C5-O5-P5-O53
4	L	101	PIO	C2-C1-O1-P1
4	L	101	PIO	C6-C1-O1-P1
4	L	101	PIO	C1C-O13-P1-O11
4	L	101	PIO	C1C-O13-P1-O12
4	L	101	PIO	C4-O4-P4-O42
4	L	101	PIO	C5-O5-P5-O53
4	L	101	PIO	O1A-C1A-O2C-C2C
4	L	101	PIO	C2A-C1A-O2C-C2C
4	L	101	PIO	O1B-C1B-O3C-C3C
4	L	101	PIO	C2B-C1B-O3C-C3C
4	A	701	PIO	O1B-C1B-O3C-C3C
4	D	701	PIO	O1B-C1B-O3C-C3C
4	G	701	PIO	O1B-C1B-O3C-C3C
4	J	701	PIO	O1B-C1B-O3C-C3C
4	A	701	PIO	C2B-C1B-O3C-C3C
4	D	701	PIO	C2B-C1B-O3C-C3C
4	G	701	PIO	C2B-C1B-O3C-C3C
4	J	701	PIO	C2B-C1B-O3C-C3C
4	A	701	PIO	C1-O1-P1-O13
4	D	701	PIO	C1-O1-P1-O13
4	G	701	PIO	C1-O1-P1-O13
4	J	701	PIO	C1-O1-P1-O13
4	A	701	PIO	C1A-C2A-C3A-C4A
4	D	701	PIO	C1A-C2A-C3A-C4A
4	G	701	PIO	C1A-C2A-C3A-C4A
4	J	701	PIO	C1A-C2A-C3A-C4A
4	A	701	PIO	C1C-O13-P1-O1
4	C	101	PIO	C1C-O13-P1-O1

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Mol	Chain	Res	Type	Atoms
4	D	701	PIO	C1C-O13-P1-O1
4	F	101	PIO	C1C-O13-P1-O1
4	G	701	PIO	C1C-O13-P1-O1
4	I	101	PIO	C1C-O13-P1-O1
4	J	701	PIO	C1C-O13-P1-O1
4	L	101	PIO	C1C-O13-P1-O1
4	A	701	PIO	C2A-C1A-O2C-C2C
4	D	701	PIO	C2A-C1A-O2C-C2C
4	G	701	PIO	C2A-C1A-O2C-C2C
4	J	701	PIO	C2A-C1A-O2C-C2C
4	A	701	PIO	O1A-C1A-O2C-C2C
4	D	701	PIO	O1A-C1A-O2C-C2C
4	G	701	PIO	O1A-C1A-O2C-C2C
4	J	701	PIO	O1A-C1A-O2C-C2C
4	C	101	PIO	C2A-C3A-C4A-C5A
4	I	101	PIO	C2A-C3A-C4A-C5A
4	L	101	PIO	C2A-C3A-C4A-C5A
4	F	101	PIO	C2A-C3A-C4A-C5A
4	A	701	PIO	C1C-O13-P1-O12
4	D	701	PIO	C1C-O13-P1-O12
4	G	701	PIO	C1C-O13-P1-O12
4	J	701	PIO	C1C-O13-P1-O12
4	C	101	PIO	C1B-C2B-C3B-C4B
4	F	101	PIO	C1B-C2B-C3B-C4B
4	I	101	PIO	C1B-C2B-C3B-C4B
4	L	101	PIO	C1B-C2B-C3B-C4B
4	C	101	PIO	C2C-C1C-O13-P1
4	F	101	PIO	C2C-C1C-O13-P1
4	I	101	PIO	C2C-C1C-O13-P1
4	L	101	PIO	C2C-C1C-O13-P1
4	A	701	PIO	C1-O1-P1-O11
4	D	701	PIO	C1-O1-P1-O11
4	G	701	PIO	C1-O1-P1-O11
4	J	701	PIO	C1-O1-P1-O11
4	C	101	PIO	C4A-C5A-C6A-C7A
4	F	101	PIO	C4A-C5A-C6A-C7A
4	I	101	PIO	C4A-C5A-C6A-C7A
4	L	101	PIO	C4A-C5A-C6A-C7A
4	A	701	PIO	C4-C5-O5-P5
4	D	701	PIO	C4-C5-O5-P5
4	G	701	PIO	C4-C5-O5-P5
4	J	701	PIO	C4-C5-O5-P5

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Mol	Chain	Res	Type	Atoms
4	C	101	PIO	C1-O1-P1-O13
4	F	101	PIO	C1-O1-P1-O13
4	I	101	PIO	C1-O1-P1-O13
4	L	101	PIO	C1-O1-P1-O13
4	C	101	PIO	O3C-C1B-C2B-C3B
4	F	101	PIO	O3C-C1B-C2B-C3B
4	I	101	PIO	O3C-C1B-C2B-C3B
4	L	101	PIO	O3C-C1B-C2B-C3B
4	C	101	PIO	O2C-C2C-C3C-O3C
4	F	101	PIO	O2C-C2C-C3C-O3C
4	I	101	PIO	O2C-C2C-C3C-O3C
4	L	101	PIO	O2C-C2C-C3C-O3C
4	C	101	PIO	C4-O4-P4-O43
4	C	101	PIO	C5-O5-P5-O51
4	F	101	PIO	C4-O4-P4-O43
4	F	101	PIO	C5-O5-P5-O51
4	I	101	PIO	C4-O4-P4-O43
4	I	101	PIO	C5-O5-P5-O51
4	L	101	PIO	C4-O4-P4-O43
4	L	101	PIO	C5-O5-P5-O51
4	F	101	PIO	O1B-C1B-C2B-C3B
4	C	101	PIO	O1B-C1B-C2B-C3B
4	I	101	PIO	O1B-C1B-C2B-C3B
4	L	101	PIO	O1B-C1B-C2B-C3B
4	D	701	PIO	O3C-C1B-C2B-C3B
4	G	701	PIO	O3C-C1B-C2B-C3B
4	A	701	PIO	O3C-C1B-C2B-C3B
4	J	701	PIO	O3C-C1B-C2B-C3B
4	A	701	PIO	O1B-C1B-C2B-C3B
4	J	701	PIO	O1B-C1B-C2B-C3B
4	D	701	PIO	O1B-C1B-C2B-C3B

There are no ring outliers.

8 monomers are involved in 22 short contacts:

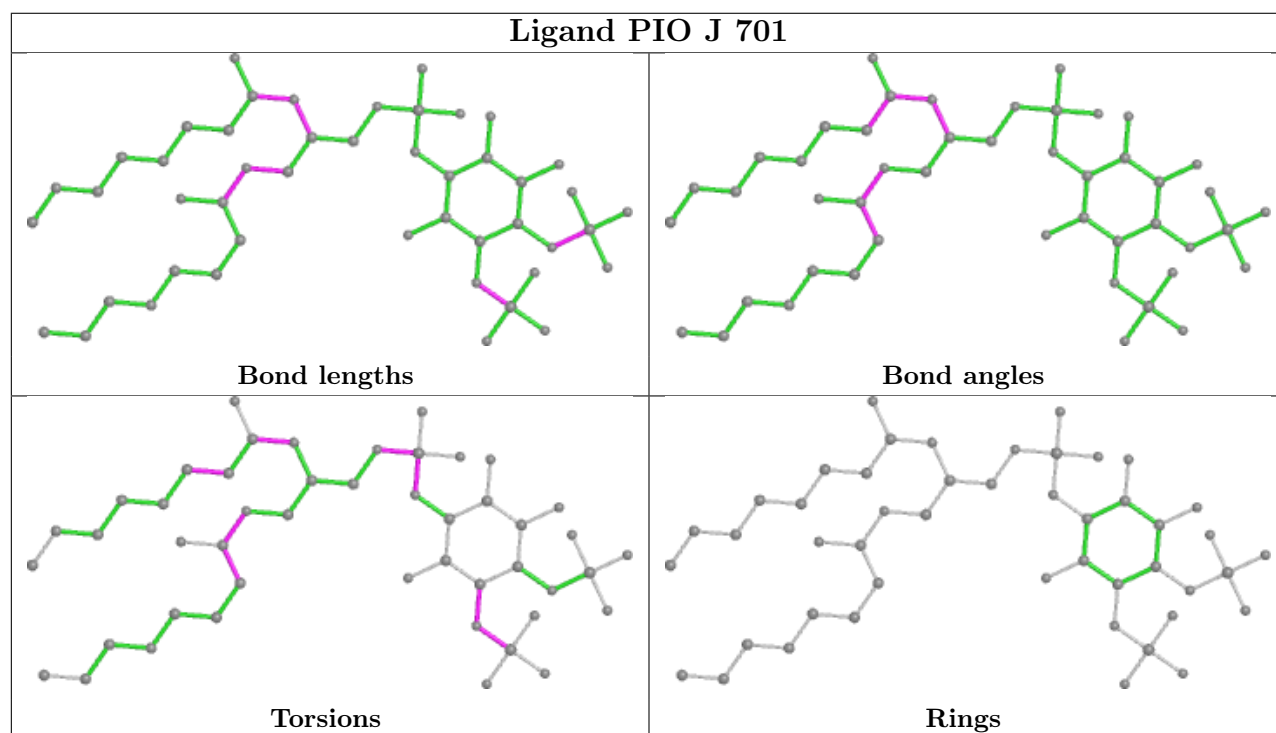
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	701	PIO	4	0
4	I	101	PIO	1	0
4	F	101	PIO	1	0
4	G	701	PIO	4	0
4	A	701	PIO	6	0
4	C	101	PIO	1	0

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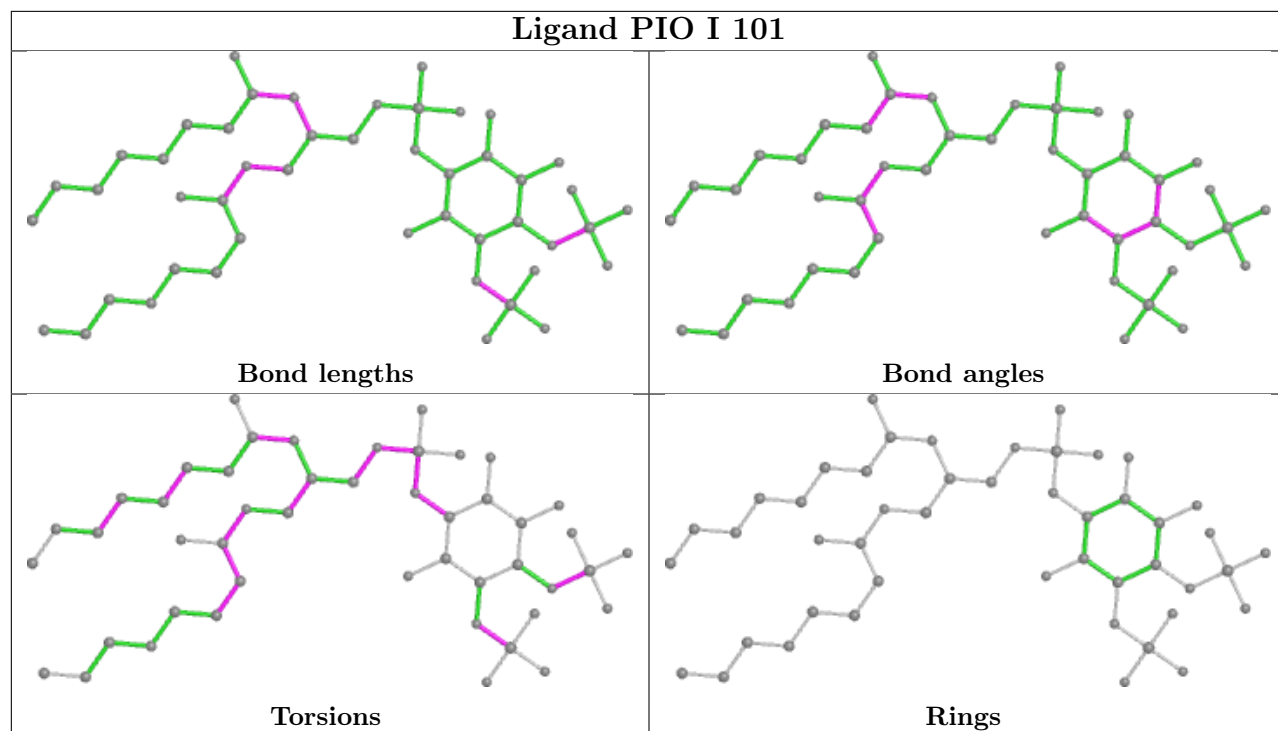
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	701	PIO	4	0
4	L	101	PIO	1	0

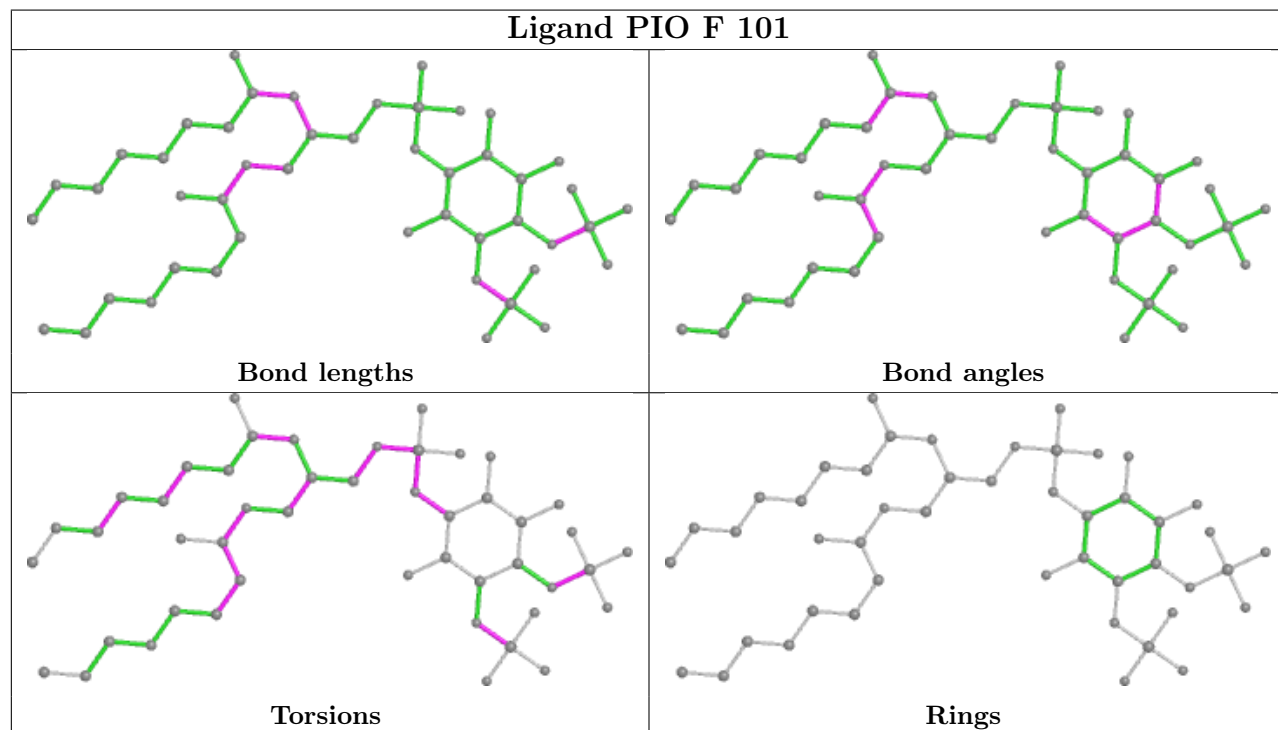
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

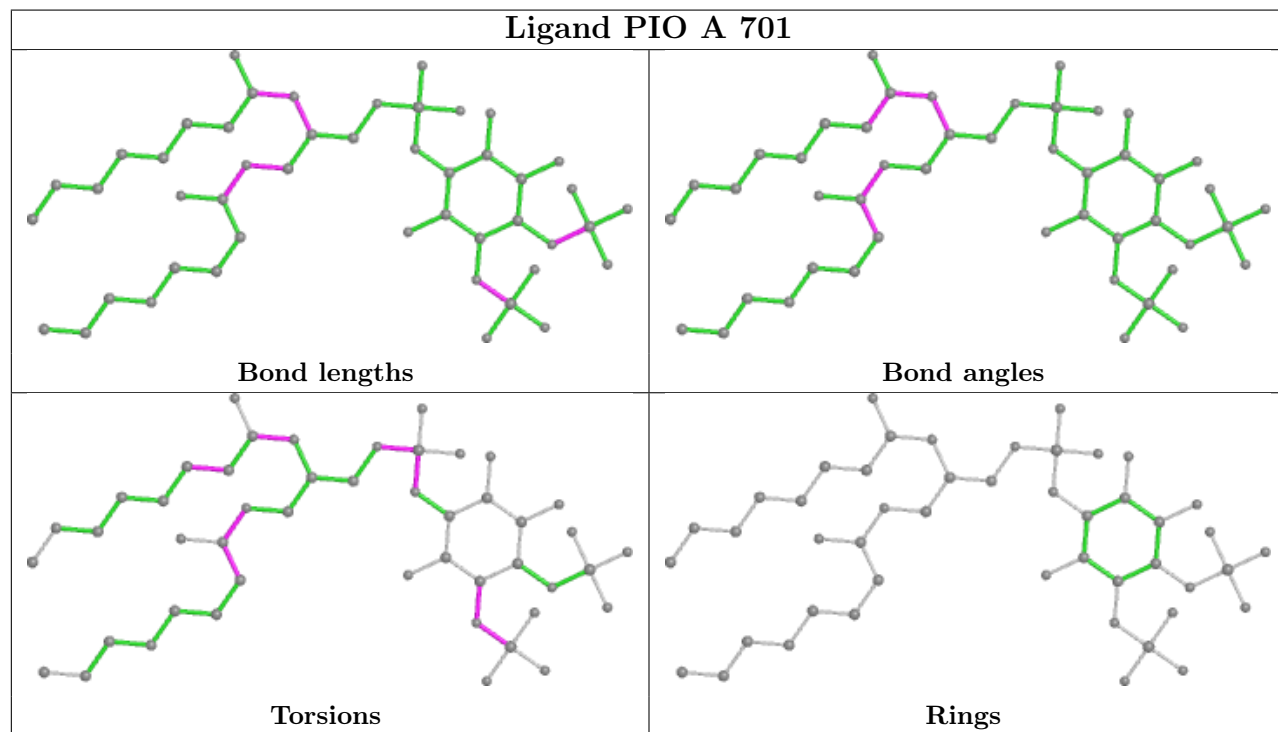
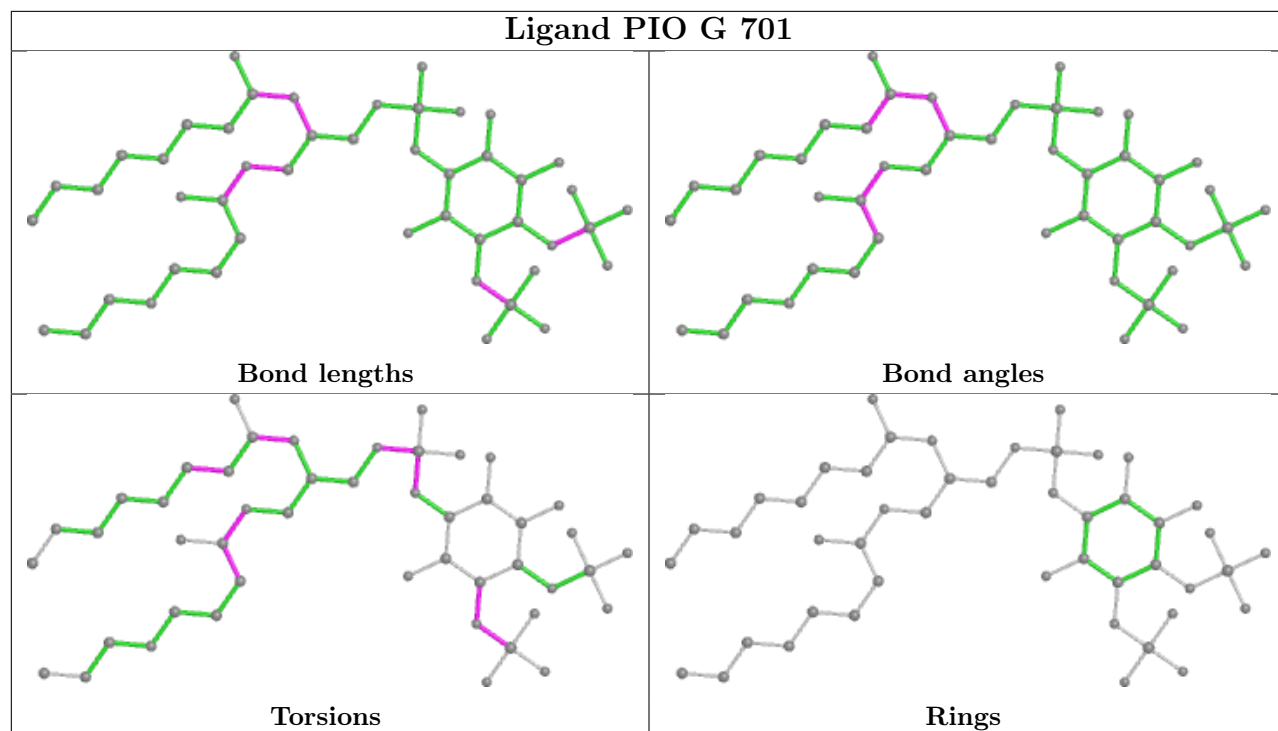


Ligand PIO I 101

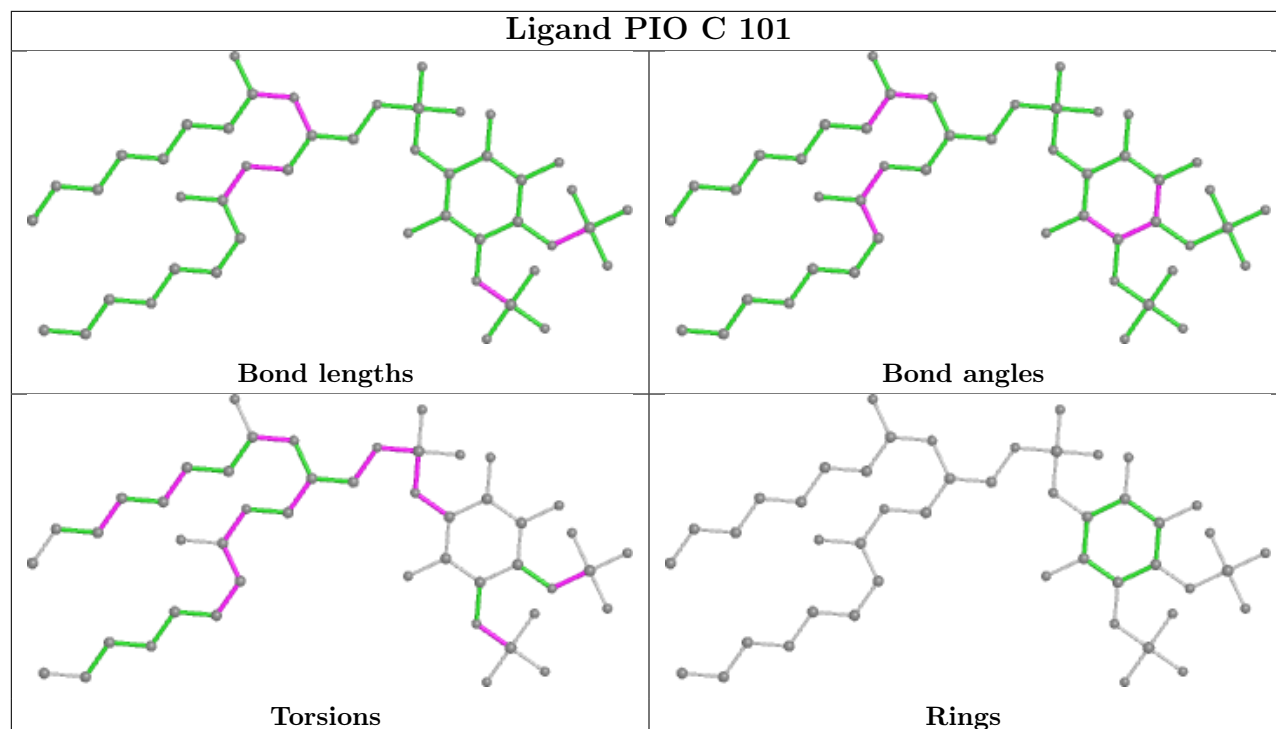


Ligand PIO F 101

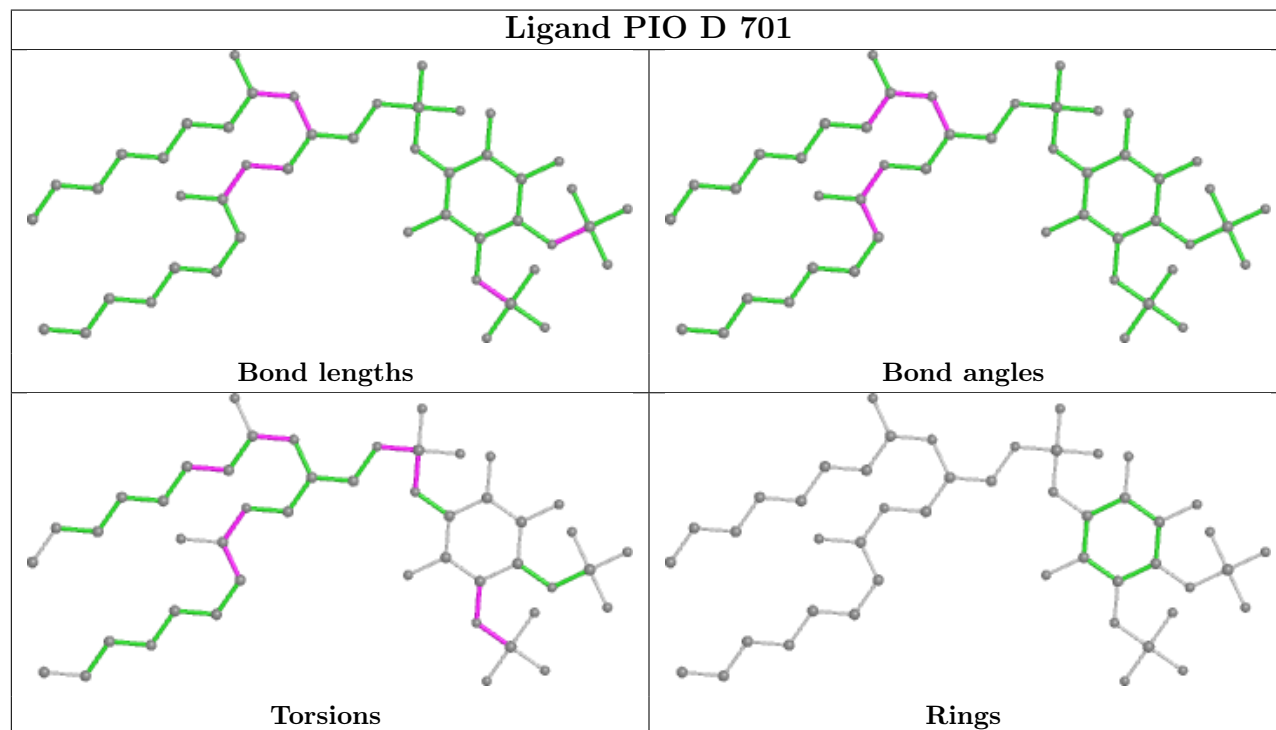


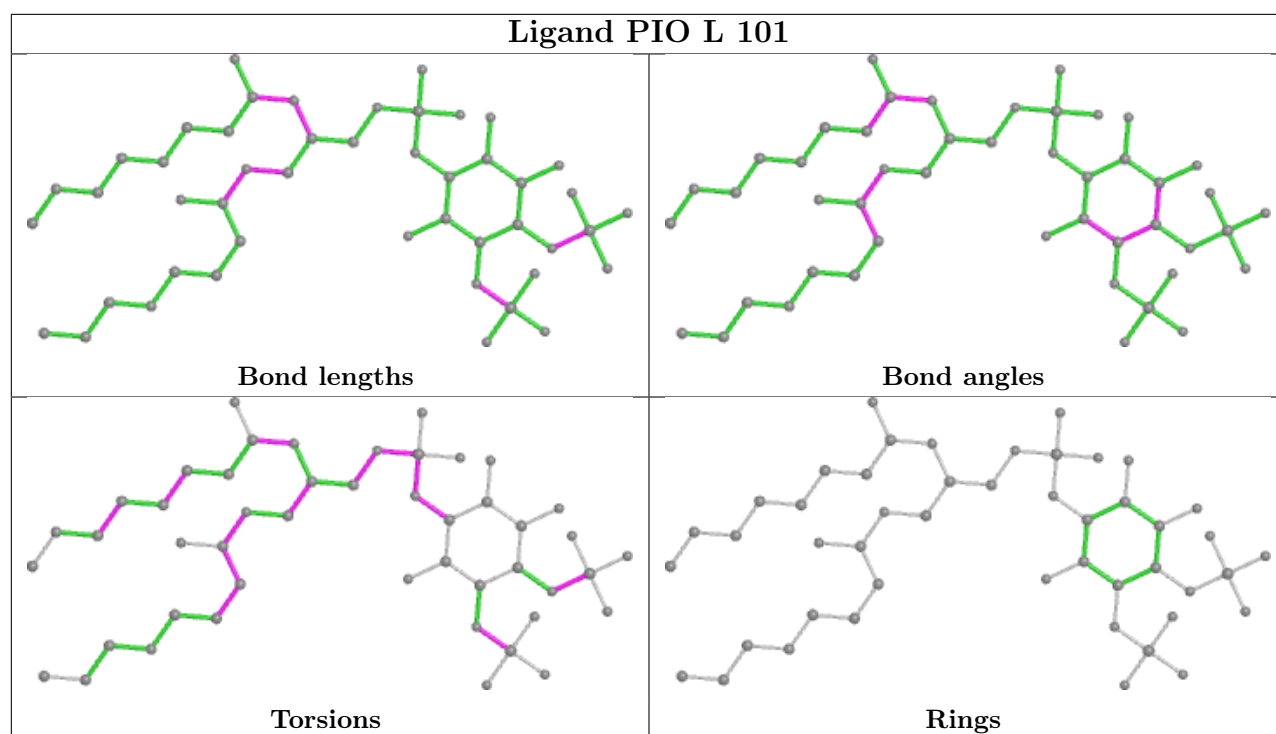


Ligand PIO C 101



Ligand PIO D 701





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.