Full wwPDB EM Validation Report ⓘ

Jul 7, 2024 – 12:10 AM JST

PDB ID	:	8X43
EMDB ID	:	EMD-38041
Title	:	human KCNQ2-CaM-Ebio1-S1 complex in the presence of PIP2
Authors	:	Ma, D.; Guo, J.
Deposited on	:	2023-11-15
Resolution	:	3.00 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

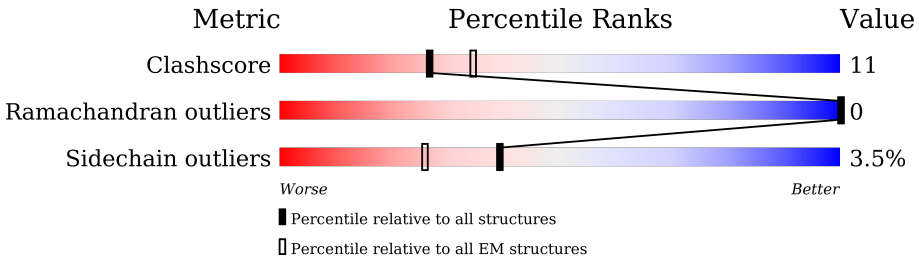
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.00 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	656	38% 11% 50%
1	C	656	37% 13% 50%
1	E	656	37% 12% • 50%
1	G	656	37% 12% 50%
2	B	149	72% 21% • •
2	D	149	69% 26% • •
2	F	149	64% 30% • •
2	H	149	69% 26% • •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 30224 atoms, of which 15044 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 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	327	Total	C	H	N	O	S	0	0
			5389	1751	2723	463	439	13		
1	C	327	Total	C	H	N	O	S	0	0
			5389	1751	2723	463	439	13		
1	E	327	Total	C	H	N	O	S	0	0
			5389	1751	2723	463	439	13		
1	G	327	Total	C	H	N	O	S	0	0
			5389	1751	2723	463	439	13		

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	63	MET	-	initiating methionine	UNP O43526
A	703	VAL	-	expression tag	UNP O43526
A	704	GLU	-	expression tag	UNP O43526
A	705	GLY	-	expression tag	UNP O43526
A	706	GLY	-	expression tag	UNP O43526
A	707	SER	-	expression tag	UNP O43526
A	708	SER	-	expression tag	UNP O43526
A	709	GLY	-	expression tag	UNP O43526
A	710	GLY	-	expression tag	UNP O43526
A	711	TRP	-	expression tag	UNP O43526
A	712	SER	-	expression tag	UNP O43526
A	713	HIS	-	expression tag	UNP O43526
A	714	PRO	-	expression tag	UNP O43526
A	715	GLN	-	expression tag	UNP O43526
A	716	PHE	-	expression tag	UNP O43526
A	717	GLU	-	expression tag	UNP O43526
A	718	LYS	-	expression tag	UNP O43526
C	63	MET	-	initiating methionine	UNP O43526
C	703	VAL	-	expression tag	UNP O43526
C	704	GLU	-	expression tag	UNP O43526
C	705	GLY	-	expression tag	UNP O43526
C	706	GLY	-	expression tag	UNP O43526

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Chain	Residue	Modelled	Actual	Comment	Reference
C	707	SER	-	expression tag	UNP O43526
C	708	SER	-	expression tag	UNP O43526
C	709	GLY	-	expression tag	UNP O43526
C	710	GLY	-	expression tag	UNP O43526
C	711	TRP	-	expression tag	UNP O43526
C	712	SER	-	expression tag	UNP O43526
C	713	HIS	-	expression tag	UNP O43526
C	714	PRO	-	expression tag	UNP O43526
C	715	GLN	-	expression tag	UNP O43526
C	716	PHE	-	expression tag	UNP O43526
C	717	GLU	-	expression tag	UNP O43526
C	718	LYS	-	expression tag	UNP O43526
E	63	MET	-	initiating methionine	UNP O43526
E	703	VAL	-	expression tag	UNP O43526
E	704	GLU	-	expression tag	UNP O43526
E	705	GLY	-	expression tag	UNP O43526
E	706	GLY	-	expression tag	UNP O43526
E	707	SER	-	expression tag	UNP O43526
E	708	SER	-	expression tag	UNP O43526
E	709	GLY	-	expression tag	UNP O43526
E	710	GLY	-	expression tag	UNP O43526
E	711	TRP	-	expression tag	UNP O43526
E	712	SER	-	expression tag	UNP O43526
E	713	HIS	-	expression tag	UNP O43526
E	714	PRO	-	expression tag	UNP O43526
E	715	GLN	-	expression tag	UNP O43526
E	716	PHE	-	expression tag	UNP O43526
E	717	GLU	-	expression tag	UNP O43526
E	718	LYS	-	expression tag	UNP O43526
G	63	MET	-	initiating methionine	UNP O43526
G	703	VAL	-	expression tag	UNP O43526
G	704	GLU	-	expression tag	UNP O43526
G	705	GLY	-	expression tag	UNP O43526
G	706	GLY	-	expression tag	UNP O43526
G	707	SER	-	expression tag	UNP O43526
G	708	SER	-	expression tag	UNP O43526
G	709	GLY	-	expression tag	UNP O43526
G	710	GLY	-	expression tag	UNP O43526
G	711	TRP	-	expression tag	UNP O43526
G	712	SER	-	expression tag	UNP O43526
G	713	HIS	-	expression tag	UNP O43526
G	714	PRO	-	expression tag	UNP O43526

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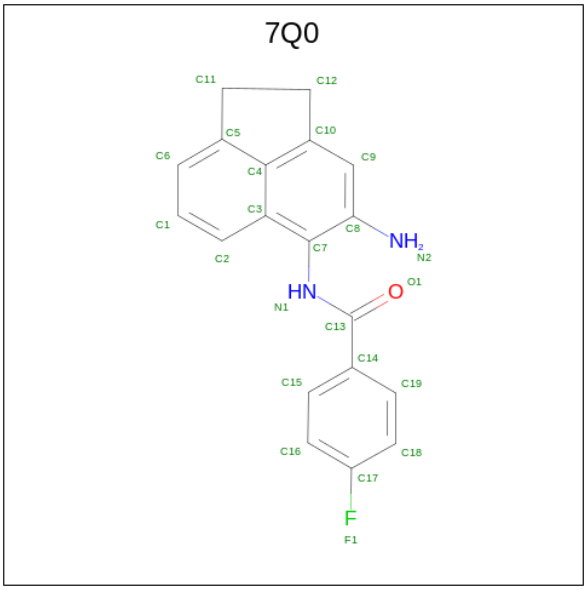
Chain	Residue	Modelled	Actual	Comment	Reference
G	715	GLN	-	expression tag	UNP O43526
G	716	PHE	-	expression tag	UNP O43526
G	717	GLU	-	expression tag	UNP O43526
G	718	LYS	-	expression tag	UNP O43526

- Molecule 2 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	143	Total	C	H	N	O	S	0	0
			2129	681	1023	178	238	9		
2	D	143	Total	C	H	N	O	S	0	0
			2129	681	1023	178	238	9		
2	F	143	Total	C	H	N	O	S	0	0
			2129	681	1023	178	238	9		
2	H	143	Total	C	H	N	O	S	0	0
			2129	681	1023	178	238	9		

- Molecule 3 is N-(4-azanyl-1,2-dihydroacenaphthylen-5-yl)-4-fluoranyl-benzamide (three-letter code: 7Q0) (formula: $C_{19}H_{15}FN_2O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total	C	F	H	N	O	0
			38	19	1	15	2	1	
3	C	1	Total	C	F	H	N	O	0
			38	19	1	15	2	1	
3	E	1	Total	C	F	H	N	O	0
			38	19	1	15	2	1	

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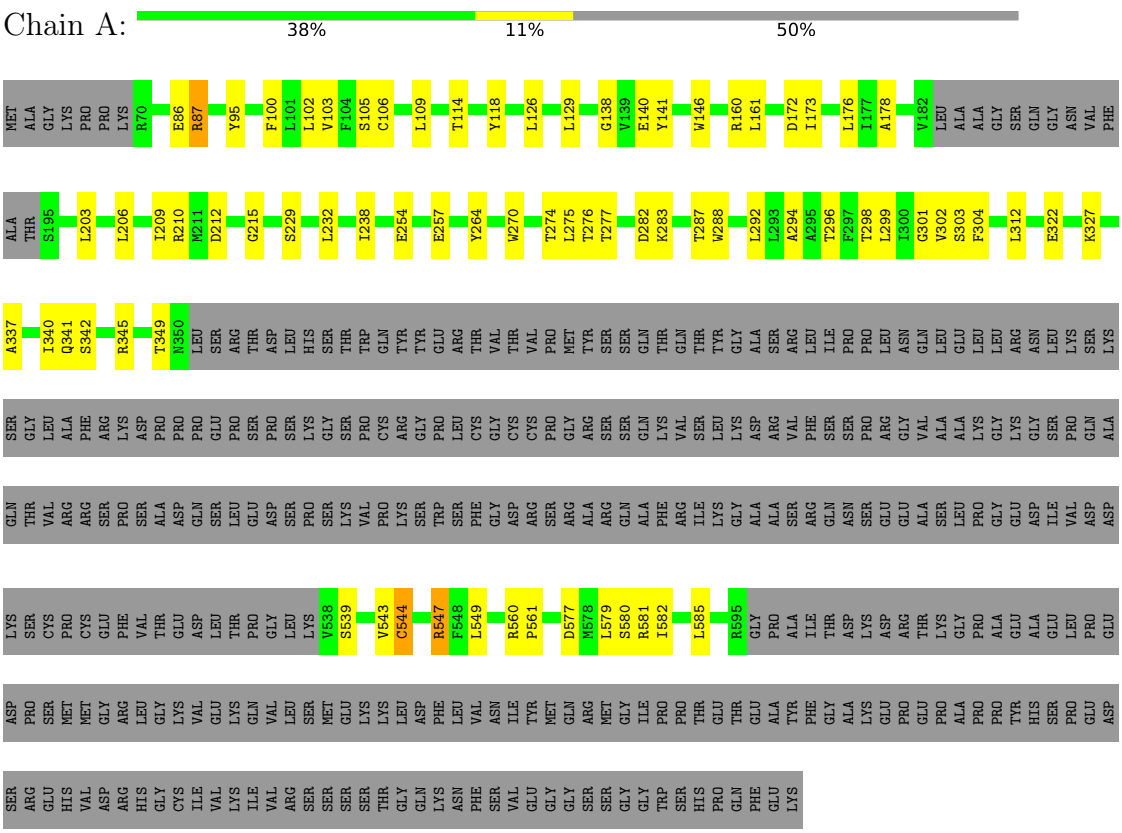
Mol	Chain	Residues	Atoms						AltConf
3	G	1	Total	C	F	H	N	O	0
			38	19	1	15	2	1	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

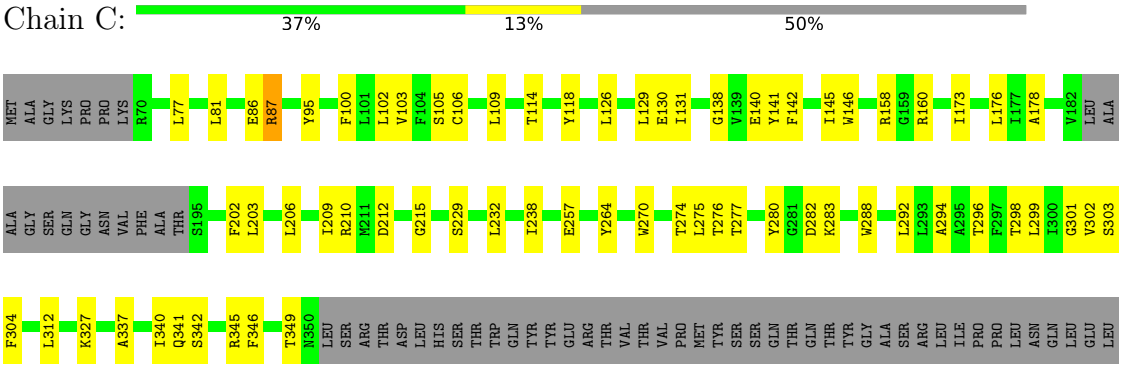
• Molecule 1: Potassium voltage-gated channel subfamily KQT member 2

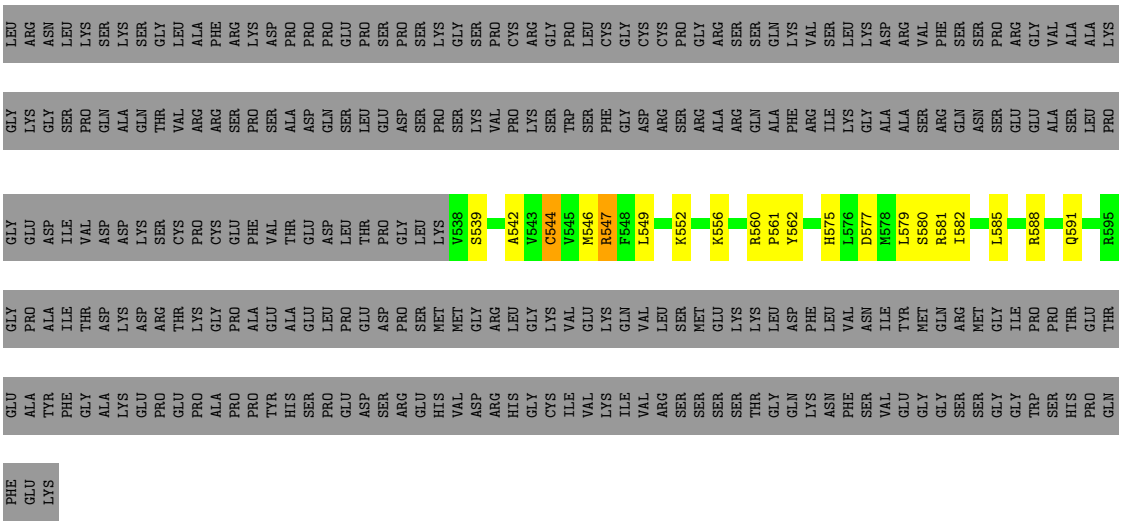
Chain A:



• Molecule 1: Potassium voltage-gated channel subfamily KQT member 2

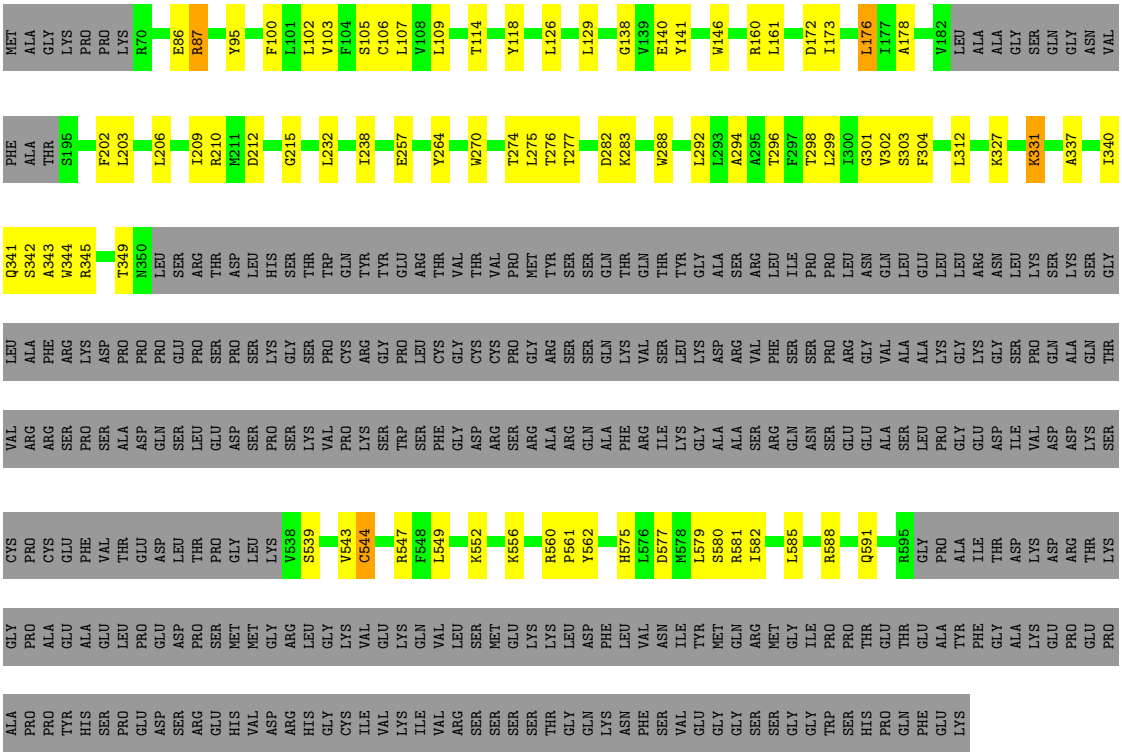
Chain C:





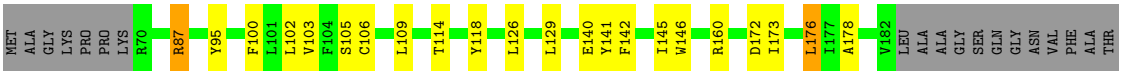
• Molecule 1: Potassium voltage-gated channel subfamily KQT member 2

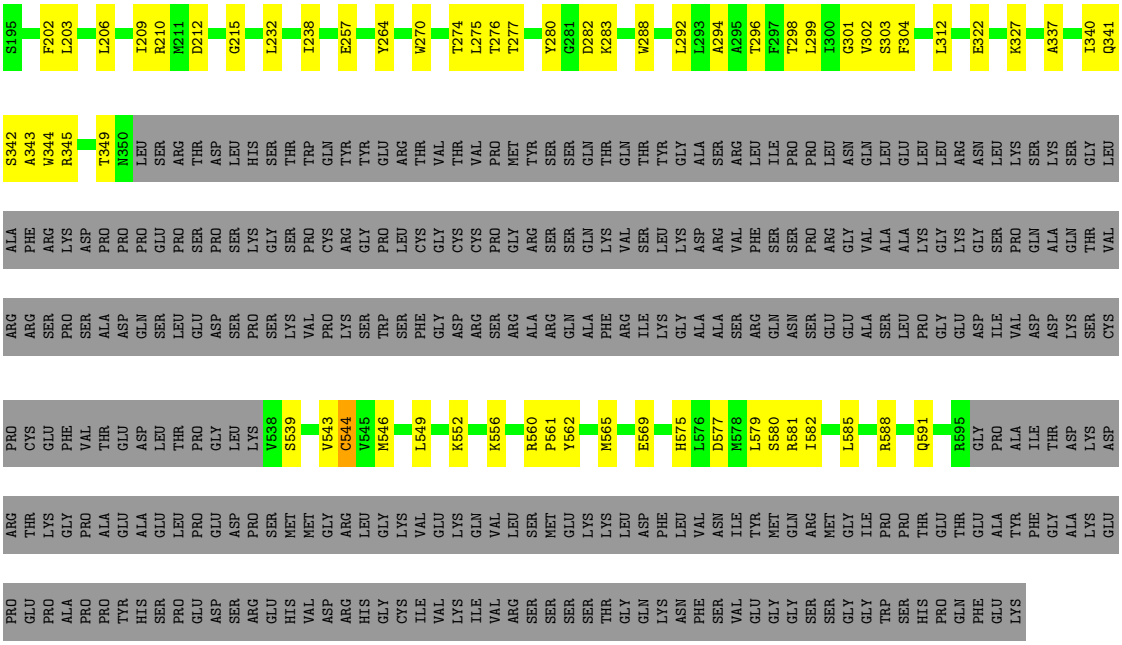
Chain E:



• Molecule 1: Potassium voltage-gated channel subfamily KQT member 2

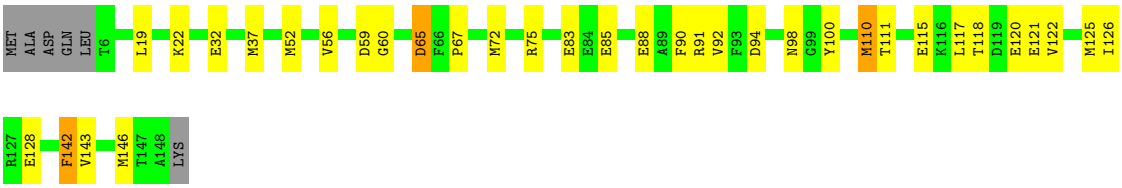
Chain G:





• Molecule 2: Calmodulin-1

Chain B:



• Molecule 2: Calmodulin-1

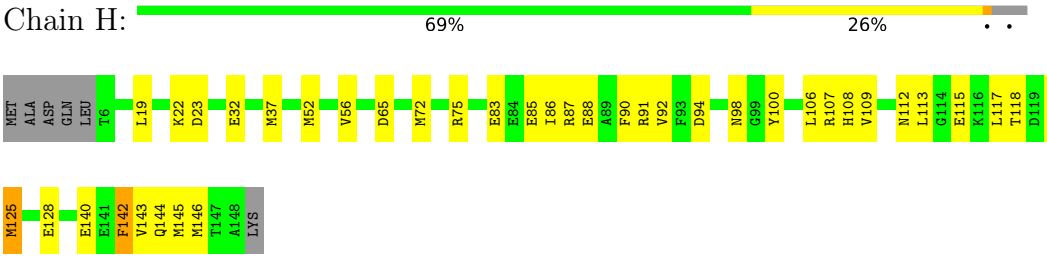
Chain D:

• Molecule 2: Calmodulin-1

Chain F:

• Molecule 2: Calmodulin-1

Chain H:


69%
26%
MET ALA ASP GLN LEU T6 L19 K22 D23 E32 M37 M52 V56 D65 M72 R75 E83 E84 E85 I86 R87 E88 A89 F90 R91 V92 F93 D94 N98 G99 Y100 L106 R107 H108 V109 N112 L113 G114 E115 K116 L117 T118 D119 E120 E121 V122
M125 E128 E140 E141 F142 V143 Q144 M145 M146 T147 A148 LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	151312	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	52	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 7Q0

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	0.32	0/2732	0.50	0/3688
1	C	0.32	0/2732	0.51	0/3688
1	E	0.32	0/2732	0.50	0/3688
1	G	0.32	0/2732	0.50	0/3688
2	B	0.26	0/1118	0.50	0/1502
2	D	0.25	0/1118	0.49	0/1502
2	F	0.25	0/1118	0.49	0/1502
2	H	0.25	0/1118	0.49	0/1502
All	All	0.30	0/15400	0.50	0/20760

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2666	2723	2722	58	0
1	C	2666	2723	2722	61	0
1	E	2666	2723	2722	62	0
1	G	2666	2723	2722	61	0
2	B	1106	1023	1023	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1106	1023	1023	34	0
2	F	1106	1023	1023	43	0
2	H	1106	1023	1023	36	0
3	A	23	15	0	2	0
3	C	23	15	0	2	0
3	E	23	15	0	2	0
3	G	23	15	0	2	0
All	All	15180	15044	14980	333	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 11.

All (333) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:TYR:OH	1:A:140:GLU:OE1	1.97	0.83
1:C:95:TYR:OH	1:C:140:GLU:OE1	1.97	0.82
1:E:95:TYR:OH	1:E:140:GLU:OE1	1.97	0.82
1:G:95:TYR:OH	1:G:140:GLU:OE1	1.97	0.82
1:G:276:THR:O	1:G:277:THR:OG1	2.01	0.79
1:A:276:THR:O	1:A:277:THR:OG1	2.01	0.77
1:C:276:THR:O	1:C:277:THR:OG1	2.01	0.77
1:E:257:GLU:N	1:E:257:GLU:OE1	2.18	0.77
1:G:257:GLU:N	1:G:257:GLU:OE1	2.18	0.77
1:E:276:THR:O	1:E:277:THR:OG1	2.01	0.77
1:A:257:GLU:OE1	1:A:257:GLU:N	2.18	0.77
1:C:257:GLU:OE1	1:C:257:GLU:N	2.18	0.76
1:E:146:TRP:O	1:E:160:ARG:NH2	2.21	0.74
1:C:146:TRP:O	1:C:160:ARG:NH2	2.21	0.73
1:A:146:TRP:O	1:A:160:ARG:NH2	2.22	0.72
1:G:146:TRP:O	1:G:160:ARG:NH2	2.22	0.72
2:H:88:GLU:O	2:H:92:VAL:HG23	1.90	0.71
2:B:88:GLU:O	2:B:92:VAL:HG23	1.90	0.71
2:F:88:GLU:O	2:F:92:VAL:HG23	1.90	0.71
2:B:85:GLU:N	2:B:85:GLU:OE1	2.25	0.69
2:F:85:GLU:OE1	2:F:85:GLU:N	2.25	0.69
2:D:88:GLU:O	2:D:92:VAL:HG23	1.92	0.69
1:G:349:THR:OG1	1:G:544:CYS:SG	2.45	0.69
2:H:85:GLU:N	2:H:85:GLU:OE1	2.25	0.68
2:D:146:MET:N	2:D:146:MET:SD	2.67	0.68
2:D:85:GLU:OE1	2:D:85:GLU:N	2.25	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:GLY:HA2	1:A:176:LEU:HD21	1.74	0.68
2:F:117:LEU:HD12	2:F:118:THR:H	1.58	0.68
2:B:120:GLU:N	2:B:120:GLU:OE1	2.29	0.66
2:D:120:GLU:OE1	2:D:120:GLU:N	2.29	0.66
2:H:120:GLU:N	2:H:120:GLU:OE1	2.29	0.66
2:F:120:GLU:OE1	2:F:120:GLU:N	2.29	0.65
2:F:146:MET:SD	2:F:146:MET:N	2.69	0.65
2:H:22:LYS:N	2:H:32:GLU:OE1	2.30	0.65
2:F:110:MET:SD	2:F:111:THR:HG23	2.37	0.64
2:D:117:LEU:HD12	2:D:118:THR:H	1.62	0.63
2:H:109:VAL:HA	2:H:113:LEU:HD13	1.79	0.63
2:F:22:LYS:N	2:F:32:GLU:OE1	2.31	0.63
2:B:117:LEU:HD12	2:B:118:THR:H	1.62	0.63
2:B:90:PHE:O	2:B:94:ASP:N	2.32	0.62
1:E:303:SER:OG	3:E:801:7Q0:N2	2.33	0.62
2:H:112:ASN:C	2:H:113:LEU:HD12	2.20	0.61
1:C:303:SER:OG	3:C:801:7Q0:N2	2.33	0.61
1:A:341:GLN:NE2	2:B:110:MET:O	2.34	0.61
2:B:22:LYS:N	2:B:32:GLU:OE1	2.33	0.61
2:B:118:THR:OG1	2:B:121:GLU:OE1	2.19	0.61
2:D:90:PHE:O	2:D:94:ASP:N	2.32	0.61
1:G:303:SER:OG	3:G:801:7Q0:N2	2.33	0.61
1:A:303:SER:OG	3:A:801:7Q0:N2	2.33	0.60
1:C:341:GLN:NE2	2:D:110:MET:O	2.34	0.60
1:E:141:TYR:CE1	1:E:173:ILE:HD11	2.37	0.60
1:C:212:ASP:OD1	1:C:215:GLY:N	2.35	0.60
1:C:138:GLY:HA2	1:C:176:LEU:HD21	1.84	0.59
2:D:22:LYS:N	2:D:32:GLU:OE1	2.35	0.59
2:D:118:THR:OG1	2:D:121:GLU:OE1	2.21	0.59
1:G:141:TYR:CE1	1:G:173:ILE:HD11	2.38	0.59
2:H:90:PHE:O	2:H:94:ASP:N	2.35	0.59
1:A:141:TYR:CE1	1:A:173:ILE:HD11	2.38	0.58
1:E:341:GLN:NE2	2:F:110:MET:O	2.35	0.58
1:G:106:CYS:SG	1:G:129:LEU:HD23	2.44	0.58
1:C:106:CYS:SG	1:C:129:LEU:HD23	2.45	0.57
2:H:117:LEU:HD12	2:H:118:THR:H	1.70	0.57
1:A:106:CYS:SG	1:A:129:LEU:HD23	2.44	0.57
1:E:106:CYS:SG	1:E:129:LEU:HD23	2.45	0.56
1:E:141:TYR:CZ	1:E:173:ILE:HD11	2.41	0.56
2:F:90:PHE:O	2:F:94:ASP:N	2.39	0.56
1:C:292:LEU:O	1:C:296:THR:HG23	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:292:LEU:O	1:G:296:THR:HG23	2.06	0.56
1:A:292:LEU:O	1:A:296:THR:HG23	2.06	0.55
2:D:110:MET:SD	2:D:111:THR:HG23	2.46	0.55
1:E:292:LEU:O	1:E:296:THR:HG23	2.06	0.55
2:B:110:MET:SD	2:B:111:THR:HG23	2.47	0.55
2:F:56:VAL:HG23	2:F:72:MET:SD	2.47	0.54
1:A:141:TYR:CZ	1:A:173:ILE:HD11	2.42	0.54
1:A:581:ARG:O	1:A:585:LEU:HG	2.06	0.54
1:E:581:ARG:O	1:E:585:LEU:HG	2.07	0.54
2:H:128:GLU:N	2:H:128:GLU:OE1	2.41	0.54
1:A:345:ARG:CZ	2:B:117:LEU:HD13	2.38	0.54
1:C:345:ARG:CZ	2:D:117:LEU:HD13	2.38	0.54
2:B:128:GLU:OE1	2:B:128:GLU:N	2.41	0.54
1:C:581:ARG:O	1:C:585:LEU:HG	2.07	0.54
1:E:178:ALA:HB1	1:E:203:LEU:HD21	1.88	0.54
2:F:128:GLU:N	2:F:128:GLU:OE1	2.42	0.53
1:E:298:THR:O	1:E:302:VAL:HG22	2.08	0.53
2:H:87:ARG:NH2	2:H:144:GLN:OE1	2.42	0.53
2:D:87:ARG:NH2	2:D:144:GLN:OE1	2.42	0.53
1:G:212:ASP:OD2	1:G:215:GLY:N	2.41	0.53
1:G:543:VAL:HG13	2:H:37:MET:CE	2.39	0.53
1:A:577:ASP:O	1:A:580:SER:OG	2.24	0.53
2:F:101:ILE:HD11	2:F:105:GLU:HB2	1.91	0.53
1:G:141:TYR:CZ	1:G:173:ILE:HD11	2.43	0.53
2:F:23:ASP:N	2:F:32:GLU:OE1	2.39	0.52
1:E:349:THR:HG1	1:E:544:CYS:HG	0.57	0.52
1:A:114:THR:HG21	1:C:264:TYR:H	1.75	0.52
2:D:128:GLU:N	2:D:128:GLU:OE1	2.41	0.52
1:G:298:THR:O	1:G:302:VAL:HG22	2.08	0.52
1:A:282:ASP:OD1	1:A:283:LYS:N	2.42	0.52
2:F:118:THR:OG1	2:F:121:GLU:OE1	2.28	0.52
1:A:264:TYR:H	1:G:114:THR:HG21	1.74	0.52
1:C:141:TYR:CE1	1:C:173:ILE:HD11	2.44	0.52
1:C:298:THR:O	1:C:302:VAL:HG22	2.08	0.52
1:C:282:ASP:OD1	1:C:283:LYS:N	2.43	0.52
2:F:102:SER:N	2:F:136:GLN:OE1	2.43	0.52
1:A:585:LEU:HD13	1:G:585:LEU:HD11	1.92	0.52
1:A:298:THR:O	1:A:302:VAL:HG22	2.09	0.52
1:C:577:ASP:O	1:C:580:SER:OG	2.22	0.52
1:E:114:THR:HG21	1:G:264:TYR:H	1.75	0.52
1:A:579:LEU:HD11	1:G:577:ASP:OD1	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:282:ASP:OD1	1:E:283:LYS:N	2.43	0.52
1:G:282:ASP:OD1	1:G:283:LYS:N	2.43	0.52
1:G:575:HIS:O	1:G:579:LEU:HG	2.09	0.52
2:H:117:LEU:HD12	2:H:118:THR:N	2.25	0.51
1:C:114:THR:HG21	1:E:264:TYR:H	1.75	0.51
2:H:106:LEU:HD21	2:H:125:MET:CE	2.40	0.51
2:D:87:ARG:HE	2:D:143:VAL:HG21	1.75	0.51
1:E:294:ALA:O	1:E:298:THR:HG23	2.11	0.51
2:H:122:VAL:HG23	2:H:125:MET:CE	2.40	0.51
1:C:294:ALA:O	1:C:298:THR:HG23	2.11	0.51
2:F:87:ARG:NH2	2:F:144:GLN:OE1	2.43	0.50
1:E:543:VAL:HG13	2:F:37:MET:CE	2.41	0.50
2:D:56:VAL:HG23	2:D:72:MET:SD	2.52	0.50
1:A:294:ALA:O	1:A:298:THR:HG23	2.11	0.50
1:E:345:ARG:CZ	2:F:117:LEU:HD13	2.41	0.50
1:G:294:ALA:O	1:G:298:THR:HG23	2.11	0.50
2:D:83:GLU:OE1	2:D:147:THR:OG1	2.23	0.50
1:C:141:TYR:CZ	1:C:173:ILE:HD11	2.47	0.50
1:C:542:ALA:HB2	2:D:73:MET:HE2	1.94	0.49
1:C:581:ARG:HG3	1:E:582:ILE:HD13	1.95	0.49
1:E:212:ASP:OD1	1:E:215:GLY:N	2.44	0.49
1:C:130:GLU:C	1:C:130:GLU:OE1	2.52	0.48
2:F:117:LEU:HD12	2:F:118:THR:N	2.26	0.48
2:B:122:VAL:HG23	2:B:125:MET:CE	2.43	0.48
1:G:577:ASP:O	1:G:580:SER:OG	2.25	0.48
1:A:543:VAL:HG13	2:B:37:MET:CE	2.43	0.48
2:H:106:LEU:HD21	2:H:125:MET:HE2	1.96	0.48
2:B:91:ARG:O	2:B:91:ARG:NH1	2.38	0.48
1:C:280:TYR:HH	1:E:270:TRP:HE1	1.61	0.48
1:C:539:SER:OG	2:D:19:LEU:HD23	2.13	0.48
1:G:577:ASP:O	1:G:581:ARG:HG2	2.14	0.48
1:A:105:SER:HB3	1:A:129:LEU:HD21	1.96	0.48
1:A:543:VAL:HG13	2:B:37:MET:HE1	1.94	0.48
1:C:118:TYR:HH	1:G:288:TRP:HD1	1.62	0.48
1:E:539:SER:OG	2:F:19:LEU:HD23	2.13	0.48
1:E:577:ASP:O	1:E:580:SER:OG	2.24	0.48
2:B:142:PHE:O	2:B:146:MET:HG2	2.14	0.48
1:A:288:TRP:HD1	1:E:118:TYR:HH	1.62	0.47
1:E:577:ASP:O	1:E:581:ARG:HG2	2.14	0.47
1:G:105:SER:HB3	1:G:129:LEU:HD21	1.96	0.47
2:H:91:ARG:O	2:H:91:ARG:NH1	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:ASP:OD2	1:A:215:GLY:N	2.41	0.47
1:G:172:ASP:OD1	1:G:176:LEU:HD12	2.14	0.47
1:G:276:THR:C	1:G:277:THR:HG1	2.08	0.47
1:C:577:ASP:O	1:C:581:ARG:HG2	2.15	0.47
1:G:341:GLN:NE2	2:H:115:GLU:O	2.48	0.47
2:D:122:VAL:HG23	2:D:125:MET:CE	2.45	0.47
1:E:105:SER:HB3	1:E:129:LEU:HD21	1.97	0.47
1:E:581:ARG:HG3	1:G:582:ILE:HD13	1.97	0.47
1:C:575:HIS:O	1:C:579:LEU:HD22	2.14	0.46
1:E:341:GLN:NE2	2:F:115:GLU:O	2.48	0.46
2:H:142:PHE:O	2:H:146:MET:HG2	2.16	0.46
2:F:28:ILE:HG23	2:F:28:ILE:O	2.15	0.46
1:G:345:ARG:CZ	2:H:117:LEU:HD13	2.45	0.46
1:A:577:ASP:O	1:A:581:ARG:HG2	2.15	0.46
1:C:238:ILE:HG21	1:C:304:PHE:CZ	2.51	0.46
2:F:98:ASN:OD1	2:F:100:TYR:N	2.48	0.46
1:G:172:ASP:OD1	1:G:172:ASP:C	2.53	0.46
1:C:105:SER:HB3	1:C:129:LEU:HD21	1.96	0.46
1:C:549:LEU:HD11	2:D:75:ARG:NH2	2.30	0.46
1:G:238:ILE:HG21	1:G:304:PHE:CZ	2.51	0.46
1:E:238:ILE:HG21	1:E:304:PHE:CZ	2.51	0.46
1:C:270:TRP:O	1:C:274:THR:HG22	2.16	0.46
1:E:138:GLY:CA	1:E:176:LEU:HD21	2.46	0.46
1:A:206:LEU:HD13	1:A:206:LEU:C	2.35	0.46
1:C:299:LEU:O	3:C:801:7Q0:N1	2.49	0.46
1:G:275:LEU:HD22	1:G:301:GLY:HA3	1.98	0.46
1:A:270:TRP:O	1:A:274:THR:HG22	2.16	0.45
2:D:110:MET:SD	2:D:122:VAL:HB	2.56	0.45
1:E:138:GLY:HA2	1:E:176:LEU:HD21	1.98	0.45
1:E:172:ASP:C	1:E:172:ASP:OD1	2.54	0.45
1:E:299:LEU:O	3:E:801:7Q0:N1	2.49	0.45
1:E:575:HIS:O	1:E:579:LEU:HD22	2.15	0.45
1:A:275:LEU:HD22	1:A:301:GLY:HA3	1.98	0.45
1:A:582:ILE:HD13	1:G:581:ARG:HG3	1.98	0.45
1:A:238:ILE:HG21	1:A:304:PHE:CZ	2.50	0.45
1:A:539:SER:OG	2:B:19:LEU:HD23	2.16	0.45
1:G:206:LEU:C	1:G:206:LEU:HD13	2.36	0.45
1:A:549:LEU:HD11	2:B:75:ARG:NH2	2.31	0.45
1:A:581:ARG:HG3	1:C:582:ILE:HD13	1.98	0.45
2:H:56:VAL:HG23	2:H:72:MET:SD	2.56	0.45
1:A:118:TYR:HH	1:E:288:TRP:HD1	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:THR:HG1	1:A:544:CYS:HG	0.48	0.45
1:E:270:TRP:O	1:E:274:THR:HG22	2.16	0.45
2:F:69:PHE:O	2:F:72:MET:HG2	2.17	0.45
2:D:83:GLU:OE2	2:D:143:VAL:HG23	2.16	0.45
1:A:172:ASP:OD1	1:A:172:ASP:C	2.55	0.45
1:A:299:LEU:O	3:A:801:7Q0:N1	2.50	0.45
2:B:110:MET:SD	2:B:122:VAL:HB	2.57	0.45
2:F:140:GLU:O	2:F:143:VAL:HG22	2.17	0.45
1:G:270:TRP:O	1:G:274:THR:HG22	2.16	0.45
2:B:65:ASP:OD1	2:B:65:ASP:C	2.55	0.44
2:B:83:GLU:OE2	2:B:143:VAL:HG23	2.17	0.44
1:C:275:LEU:HD22	1:C:301:GLY:HA3	1.98	0.44
1:E:172:ASP:OD1	1:E:176:LEU:HD12	2.17	0.44
1:G:299:LEU:O	3:G:801:7Q0:N1	2.50	0.44
2:H:65:ASP:C	2:H:65:ASP:OD1	2.56	0.44
1:A:232:LEU:HD11	1:A:312:LEU:HD21	1.99	0.44
1:C:288:TRP:HD1	1:G:118:TYR:HH	1.64	0.44
1:E:232:LEU:HD11	1:E:312:LEU:HD21	1.99	0.44
1:E:275:LEU:HD22	1:E:301:GLY:HA3	1.98	0.44
2:F:52:MET:O	2:F:56:VAL:HG12	2.18	0.44
1:C:232:LEU:HD11	1:C:312:LEU:HD21	1.99	0.44
2:F:122:VAL:HG23	2:F:125:MET:CE	2.48	0.44
1:G:543:VAL:HG13	2:H:37:MET:HE2	2.00	0.44
1:A:270:TRP:HE1	1:G:280:TYR:HH	1.64	0.44
2:D:98:ASN:OD1	2:D:100:TYR:N	2.51	0.44
1:A:544:CYS:O	1:A:547:ARG:NH2	2.49	0.43
2:B:56:VAL:HG23	2:B:72:MET:SD	2.58	0.43
1:C:77:LEU:O	1:C:81:LEU:HG	2.17	0.43
2:F:142:PHE:O	2:F:146:MET:SD	2.76	0.43
1:C:206:LEU:C	1:C:206:LEU:HD13	2.39	0.43
1:G:588:ARG:O	1:G:591:GLN:HG2	2.19	0.43
1:E:102:LEU:HD13	1:E:102:LEU:C	2.39	0.43
1:A:100:PHE:O	1:A:103:VAL:HG12	2.19	0.43
1:G:102:LEU:HD13	1:G:102:LEU:C	2.38	0.43
1:C:178:ALA:HB1	1:C:203:LEU:HD21	2.01	0.43
1:E:588:ARG:O	1:E:591:GLN:HG2	2.19	0.43
1:G:100:PHE:O	1:G:103:VAL:HG12	2.18	0.43
1:A:102:LEU:HD13	1:A:102:LEU:C	2.39	0.43
1:A:172:ASP:OD1	1:A:176:LEU:HD13	2.19	0.43
1:C:100:PHE:O	1:C:103:VAL:HG12	2.19	0.43
2:H:83:GLU:OE2	2:H:143:VAL:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:ASP:OD1	2:B:67:PRO:HD2	2.19	0.43
2:F:83:GLU:OE1	2:F:147:THR:OG1	2.17	0.43
1:G:178:ALA:HB1	1:G:203:LEU:HD21	2.00	0.43
1:G:337:ALA:O	1:G:340:ILE:HG13	2.18	0.43
1:A:206:LEU:HA	1:A:209:ILE:HG22	2.01	0.43
1:C:544:CYS:O	1:C:547:ARG:NH2	2.52	0.43
1:G:232:LEU:HD11	1:G:312:LEU:HD21	1.99	0.43
1:A:341:GLN:NE2	2:B:115:GLU:O	2.52	0.43
1:E:552:LYS:O	1:E:556:LYS:HG2	2.19	0.43
2:F:106:LEU:C	2:F:106:LEU:HD23	2.39	0.43
1:A:173:ILE:HD13	1:A:173:ILE:HA	1.90	0.42
1:C:102:LEU:HD13	1:C:102:LEU:C	2.38	0.42
1:E:100:PHE:O	1:E:103:VAL:HG12	2.19	0.42
1:E:331:LYS:O	1:E:331:LYS:CG	2.67	0.42
2:H:113:LEU:HD12	2:H:113:LEU:N	2.34	0.42
1:E:549:LEU:HD11	2:F:75:ARG:NH2	2.34	0.42
2:H:52:MET:O	2:H:56:VAL:HG12	2.19	0.42
1:A:178:ALA:HB1	1:A:203:LEU:HD21	2.01	0.42
1:A:276:THR:C	1:A:277:THR:HG1	2.11	0.42
1:A:337:ALA:O	1:A:340:ILE:HG13	2.20	0.42
1:C:138:GLY:CA	1:C:176:LEU:HD21	2.46	0.42
1:G:543:VAL:HG13	2:H:37:MET:HE1	2.01	0.42
1:G:560:ARG:HB2	1:G:561:PRO:HD3	2.01	0.42
2:B:98:ASN:OD1	2:B:100:TYR:N	2.52	0.42
1:C:109:LEU:HB3	1:C:126:LEU:HD13	2.02	0.42
1:C:349:THR:HG1	1:C:544:CYS:HG	0.49	0.42
1:E:331:LYS:O	1:E:331:LYS:HG2	2.19	0.42
1:E:544:CYS:O	1:E:547:ARG:NH2	2.53	0.42
1:C:130:GLU:OE1	1:C:131:ILE:N	2.52	0.42
1:C:206:LEU:HA	1:C:209:ILE:HG22	2.02	0.42
1:E:206:LEU:HA	1:E:209:ILE:HG22	2.02	0.42
1:E:337:ALA:O	1:E:340:ILE:HG13	2.20	0.42
1:E:560:ARG:HB2	1:E:561:PRO:HD3	2.02	0.42
2:F:119:ASP:O	2:F:122:VAL:HG12	2.20	0.42
1:C:588:ARG:O	1:C:591:GLN:HG2	2.19	0.42
1:E:109:LEU:HB3	1:E:126:LEU:HD13	2.02	0.42
2:H:108:HIS:NE2	2:H:113:LEU:HD11	2.35	0.42
1:C:337:ALA:O	1:C:340:ILE:HG13	2.19	0.42
1:C:546:MET:CE	2:D:52:MET:O	2.68	0.42
1:E:543:VAL:HG13	2:F:37:MET:HE2	2.01	0.42
2:F:110:MET:SD	2:F:111:THR:N	2.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:581:ARG:O	1:G:585:LEU:HG	2.20	0.42
2:D:142:PHE:O	2:D:146:MET:SD	2.78	0.42
2:H:106:LEU:HD23	2:H:107:ARG:N	2.34	0.42
1:C:86:GLU:O	1:C:87:ARG:C	2.59	0.41
2:D:69:PHE:O	2:D:72:MET:HG2	2.20	0.41
1:E:178:ALA:CB	1:E:203:LEU:HD21	2.50	0.41
1:E:206:LEU:C	1:E:206:LEU:HD13	2.40	0.41
2:F:91:ARG:O	2:F:91:ARG:NH1	2.40	0.41
1:G:206:LEU:HA	1:G:209:ILE:HG22	2.02	0.41
1:G:552:LYS:O	1:G:556:LYS:HG2	2.20	0.41
1:C:173:ILE:HD13	1:C:173:ILE:HA	1.91	0.41
2:D:23:ASP:N	2:D:32:GLU:OE1	2.41	0.41
2:F:101:ILE:HD12	2:F:102:SER:H	1.85	0.41
1:G:546:MET:HE2	2:H:52:MET:O	2.20	0.41
1:A:109:LEU:HB3	1:A:126:LEU:HD13	2.02	0.41
2:B:59:ASP:OD1	2:B:60:GLY:N	2.53	0.41
2:B:125:MET:SD	2:B:126:ILE:N	2.93	0.41
1:C:552:LYS:O	1:C:556:LYS:HG2	2.21	0.41
1:E:343:ALA:HB2	2:F:86:ILE:HD11	2.01	0.41
1:G:109:LEU:HB3	1:G:126:LEU:HD13	2.02	0.41
1:G:549:LEU:HD11	2:H:75:ARG:NH2	2.35	0.41
1:A:254:GLU:OE2	1:A:287:THR:N	2.51	0.41
2:D:59:ASP:OD1	2:D:60:GLY:N	2.54	0.41
2:F:90:PHE:CZ	2:F:101:ILE:HG21	2.54	0.41
1:A:86:GLU:O	1:A:87:ARG:C	2.59	0.41
1:C:341:GLN:NE2	2:D:115:GLU:O	2.53	0.41
1:C:560:ARG:HB2	1:C:561:PRO:CD	2.51	0.41
1:G:581:ARG:HA	1:G:581:ARG:CZ	2.51	0.41
1:C:87:ARG:HG2	1:C:87:ARG:O	2.21	0.41
2:H:98:ASN:OD1	2:H:100:TYR:N	2.54	0.41
1:G:539:SER:OG	2:H:19:LEU:HD23	2.21	0.41
1:G:565:MET:O	1:G:565:MET:SD	2.79	0.41
2:B:110:MET:SD	2:B:110:MET:C	2.99	0.41
1:C:142:PHE:O	1:C:145:ILE:HG22	2.21	0.41
2:D:87:ARG:O	2:D:91:ARG:HG3	2.21	0.41
1:E:581:ARG:HA	1:E:581:ARG:CZ	2.51	0.41
2:F:110:MET:SD	2:F:122:VAL:HB	2.60	0.41
1:G:142:PHE:O	1:G:145:ILE:HG22	2.21	0.41
1:G:343:ALA:HB2	2:H:86:ILE:HD11	2.02	0.41
1:G:344:TRP:CE2	2:H:125:MET:HB2	2.56	0.41
1:A:581:ARG:CZ	1:A:581:ARG:HA	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:581:ARG:CZ	1:C:581:ARG:HA	2.51	0.41
2:F:65:ASP:C	2:F:65:ASP:OD1	2.60	0.41
2:F:145:MET:HE2	2:F:145:MET:HB3	1.99	0.41
1:C:577:ASP:OD1	1:E:579:LEU:HD11	2.21	0.40
1:A:560:ARG:HB2	1:A:561:PRO:CD	2.51	0.40
2:D:125:MET:SD	2:D:126:ILE:N	2.94	0.40
1:E:86:GLU:O	1:E:87:ARG:C	2.59	0.40
1:E:344:TRP:CE2	2:F:125:MET:HB2	2.57	0.40
1:G:173:ILE:HD13	1:G:173:ILE:HA	1.90	0.40
2:H:140:GLU:O	2:H:143:VAL:HG22	2.21	0.40
2:B:110:MET:SD	2:B:111:THR:N	2.95	0.40
2:D:52:MET:O	2:D:56:VAL:HG12	2.20	0.40
1:A:87:ARG:O	1:A:87:ARG:HG2	2.21	0.40
1:A:577:ASP:OD1	1:C:579:LEU:HD11	2.21	0.40
1:E:87:ARG:HG2	1:E:87:ARG:O	2.21	0.40
2:F:59:ASP:OD1	2:F:60:GLY:N	2.54	0.40
1:G:87:ARG:HG2	1:G:87:ARG:O	2.21	0.40
2:H:23:ASP:N	2:H:32:GLU:OE1	2.43	0.40
2:D:110:MET:SD	2:D:110:MET:C	2.99	0.40
2:D:110:MET:SD	2:D:111:THR:N	2.95	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	321/656 (49%)	306 (95%)	15 (5%)	0	100	100
1	C	321/656 (49%)	305 (95%)	16 (5%)	0	100	100
1	E	321/656 (49%)	307 (96%)	14 (4%)	0	100	100
1	G	321/656 (49%)	307 (96%)	14 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	141/149 (95%)	138 (98%)	3 (2%)	0	100	100
2	D	141/149 (95%)	139 (99%)	2 (1%)	0	100	100
2	F	141/149 (95%)	138 (98%)	3 (2%)	0	100	100
2	H	141/149 (95%)	138 (98%)	3 (2%)	0	100	100
All	All	1848/3220 (57%)	1778 (96%)	70 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	278/558 (50%)	269 (97%)	9 (3%)	39	74
1	C	278/558 (50%)	267 (96%)	11 (4%)	31	68
1	E	278/558 (50%)	267 (96%)	11 (4%)	31	68
1	G	278/558 (50%)	268 (96%)	10 (4%)	35	70
2	B	118/127 (93%)	114 (97%)	4 (3%)	37	72
2	D	118/127 (93%)	114 (97%)	4 (3%)	37	72
2	F	118/127 (93%)	115 (98%)	3 (2%)	47	79
2	H	118/127 (93%)	115 (98%)	3 (2%)	47	79
All	All	1584/2740 (58%)	1529 (96%)	55 (4%)	39	71

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	ARG
1	A	161	LEU
1	A	210	ARG
1	A	229	SER
1	A	322	GLU
1	A	327	LYS

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Mol	Chain	Res	Type
1	A	342	SER
1	A	544	CYS
1	A	547	ARG
2	B	52	MET
2	B	65	ASP
2	B	110	MET
2	B	142	PHE
1	C	87	ARG
1	C	158	ARG
1	C	202	PHE
1	C	210	ARG
1	C	229	SER
1	C	327	LYS
1	C	342	SER
1	C	346	PHE
1	C	544	CYS
1	C	547	ARG
1	C	562	TYR
2	D	37	MET
2	D	79	ASP
2	D	110	MET
2	D	142	PHE
1	E	87	ARG
1	E	107	LEU
1	E	161	LEU
1	E	176	LEU
1	E	202	PHE
1	E	210	ARG
1	E	327	LYS
1	E	331	LYS
1	E	342	SER
1	E	544	CYS
1	E	562	TYR
2	F	110	MET
2	F	125	MET
2	F	142	PHE
1	G	87	ARG
1	G	176	LEU
1	G	202	PHE
1	G	210	ARG
1	G	322	GLU
1	G	327	LYS

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Mol	Chain	Res	Type
1	G	342	SER
1	G	544	CYS
1	G	562	TYR
1	G	569	GLU
2	H	125	MET
2	H	142	PHE
2	H	145	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	575	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

4 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	7Q0	C	801	-	26,26,26	1.54	5 (19%)	33,38,38	1.26	3 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	7Q0	A	801	-	26,26,26	1.54	5 (19%)	33,38,38	1.24	2 (6%)
3	7Q0	E	801	-	26,26,26	1.53	5 (19%)	33,38,38	1.25	2 (6%)
3	7Q0	G	801	-	26,26,26	1.53	5 (19%)	33,38,38	1.26	2 (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
3	7Q0	C	801	-	-	4/8/13/13	0/4/4/4
3	7Q0	A	801	-	-	4/8/13/13	0/4/4/4
3	7Q0	E	801	-	-	4/8/13/13	0/4/4/4
3	7Q0	G	801	-	-	4/8/13/13	0/4/4/4

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	7Q0	C12-C11	-3.49	1.49	1.55
3	C	801	7Q0	C12-C11	-3.49	1.49	1.55
3	G	801	7Q0	C12-C11	-3.47	1.49	1.55
3	E	801	7Q0	C12-C11	-3.47	1.49	1.55
3	C	801	7Q0	C13-N1	3.38	1.44	1.35
3	E	801	7Q0	C13-N1	3.37	1.44	1.35
3	G	801	7Q0	C13-N1	3.36	1.44	1.35
3	A	801	7Q0	C13-N1	3.35	1.44	1.35
3	C	801	7Q0	C3-C4	-3.16	1.36	1.42
3	A	801	7Q0	C3-C4	-3.16	1.36	1.42
3	E	801	7Q0	C3-C4	-3.11	1.36	1.42
3	G	801	7Q0	C3-C4	-3.08	1.36	1.42
3	C	801	7Q0	O1-C13	-2.45	1.18	1.23
3	A	801	7Q0	O1-C13	-2.43	1.18	1.23
3	G	801	7Q0	O1-C13	-2.42	1.18	1.23
3	E	801	7Q0	O1-C13	-2.41	1.18	1.23
3	A	801	7Q0	C8-N2	2.17	1.45	1.37
3	G	801	7Q0	C8-N2	2.17	1.45	1.37
3	C	801	7Q0	C8-N2	2.16	1.45	1.37
3	E	801	7Q0	C8-N2	2.14	1.45	1.37

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	801	7Q0	C12-C10-C4	-2.14	105.94	108.73
3	E	801	7Q0	C12-C10-C4	-2.11	105.98	108.73
3	G	801	7Q0	C12-C10-C4	-2.08	106.02	108.73
3	C	801	7Q0	C11-C12-C10	2.07	106.58	105.04
3	A	801	7Q0	C12-C10-C4	-2.06	106.05	108.73
3	E	801	7Q0	C7-N1-C13	-2.03	118.44	123.41
3	C	801	7Q0	C7-N1-C13	-2.02	118.45	123.41
3	A	801	7Q0	C7-N1-C13	-2.00	118.49	123.41
3	G	801	7Q0	C7-N1-C13	-2.00	118.49	123.41

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	801	7Q0	O1-C13-C14-C19
3	A	801	7Q0	O1-C13-C14-C19
3	C	801	7Q0	O1-C13-C14-C19
3	G	801	7Q0	O1-C13-C14-C19
3	E	801	7Q0	N1-C13-C14-C19
3	G	801	7Q0	N1-C13-C14-C19
3	C	801	7Q0	N1-C13-C14-C19
3	A	801	7Q0	N1-C13-C14-C19
3	C	801	7Q0	O1-C13-C14-C15
3	E	801	7Q0	O1-C13-C14-C15
3	A	801	7Q0	O1-C13-C14-C15
3	G	801	7Q0	O1-C13-C14-C15
3	E	801	7Q0	N1-C13-C14-C15
3	C	801	7Q0	N1-C13-C14-C15
3	G	801	7Q0	N1-C13-C14-C15
3	A	801	7Q0	N1-C13-C14-C15

There are no ring outliers.

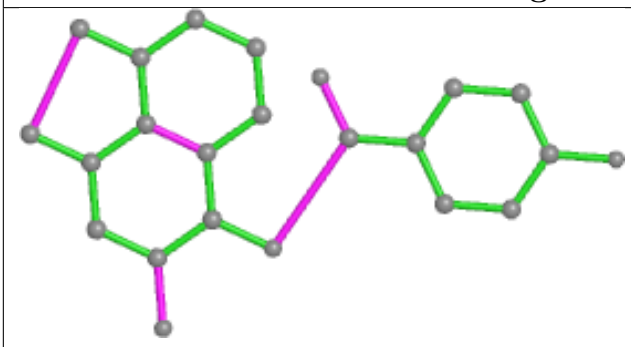
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	801	7Q0	2	0
3	A	801	7Q0	2	0
3	E	801	7Q0	2	0
3	G	801	7Q0	2	0

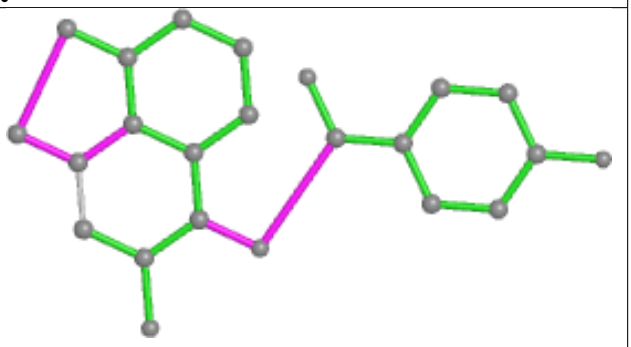
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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

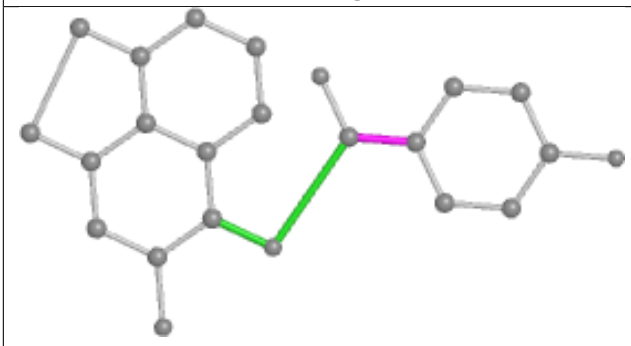
Ligand 7Q0 C 801



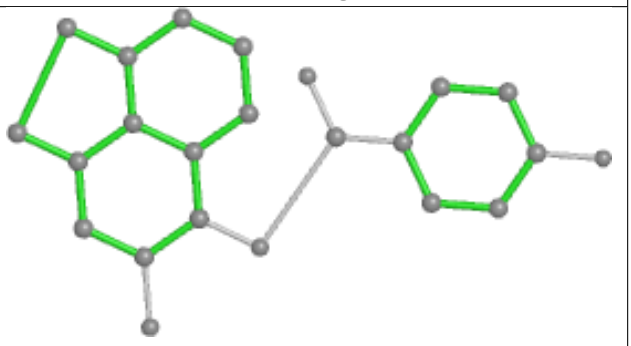
Bond lengths



Bond angles

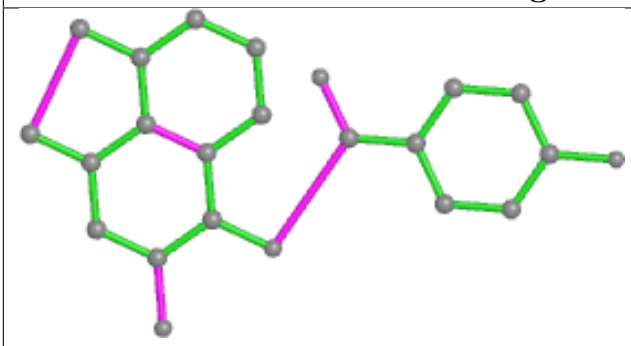


Torsions

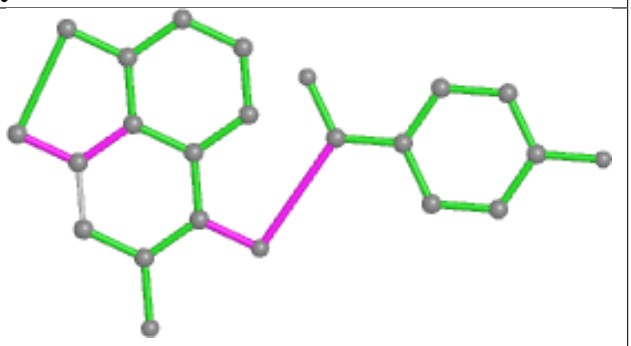


Rings

Ligand 7Q0 A 801



Bond lengths



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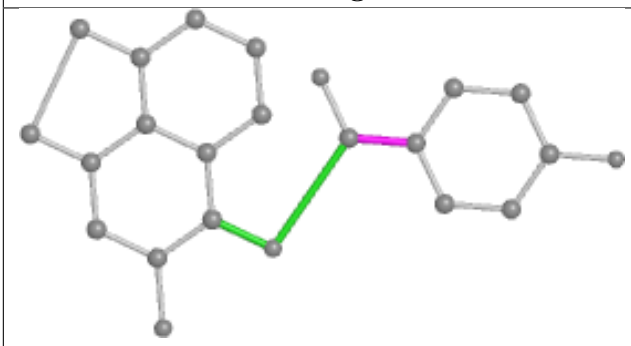

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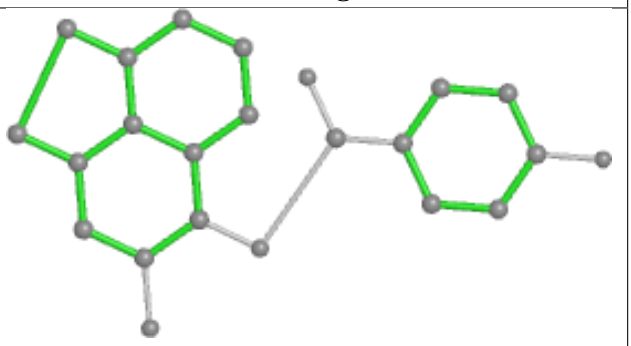
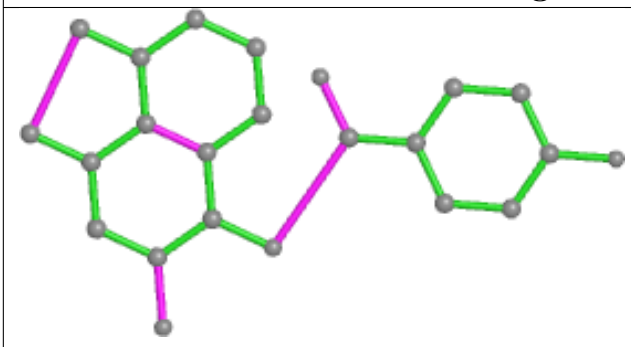
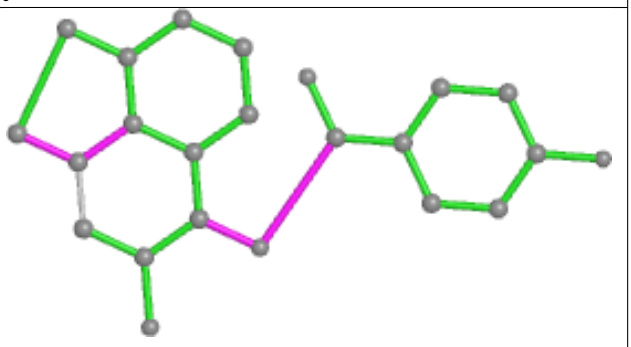


Rings

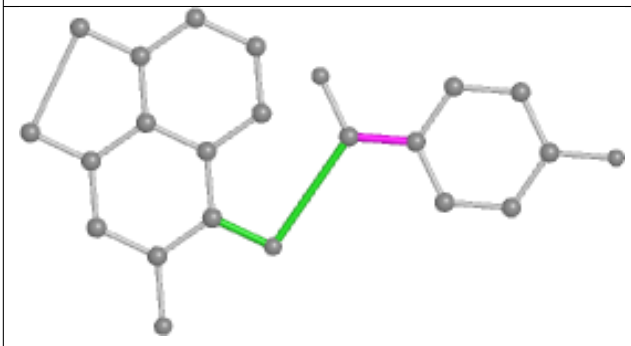
Ligand 7Q0 E 801



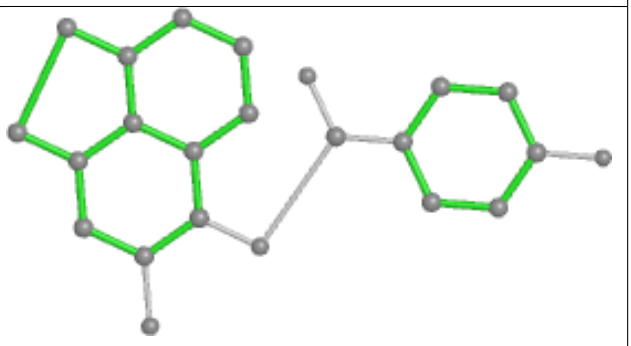
Bond lengths



Bond angles

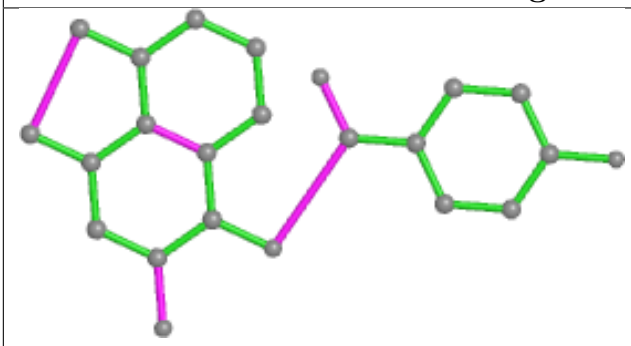


Torsions

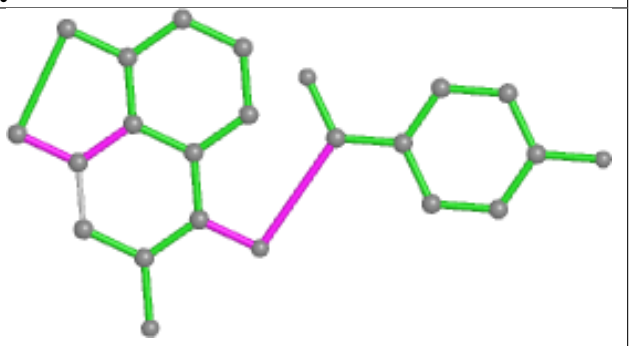


Rings

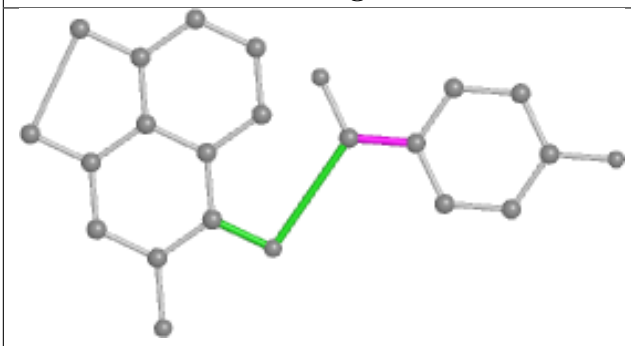
Ligand 7Q0 G 801



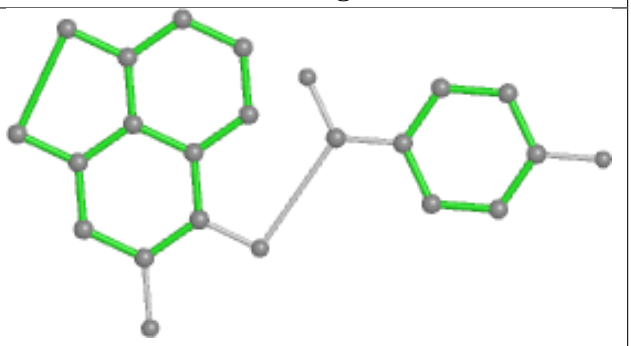
Bond lengths



Bond angles



Torsions



Rings

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.