



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 26, 2021 – 06:12 pm BST

PDB ID : 7OD0
Title : Mirolysin in complex with compound 9
Authors : Zak, K.M.; Bostock, M.J.; Ksiazek, M.
Deposited on : 2021-04-28
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.22
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.22

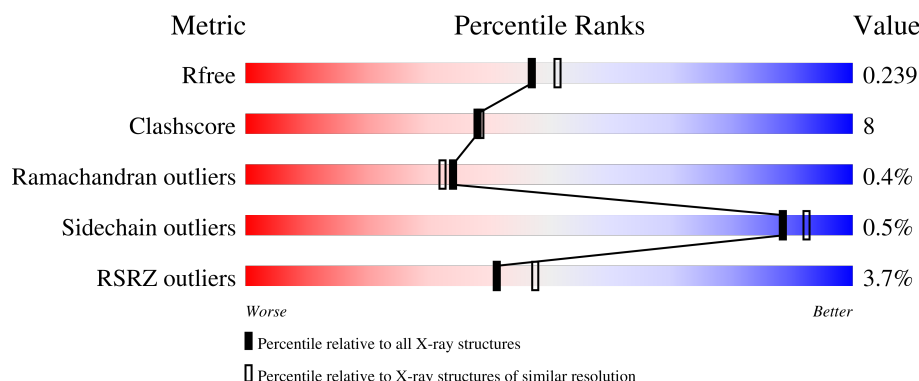
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AAA	277	<div> <div>4%</div> <div>85%</div> <div>12%</div> <div>.</div> </div>
1	BBB	277	<div> <div>4%</div> <div>89%</div> <div>7%</div> <div>.</div> </div>
1	CCC	277	<div> <div>3%</div> <div>86%</div> <div>10%</div> <div>..</div> </div>
1	DDD	277	<div> <div>4%</div> <div>86%</div> <div>11%</div> <div>.</div> </div>
1	EEE	277	<div> <div>4%</div> <div>90%</div> <div>6%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	FFF	277	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	AAA	402	-	-	X	-
4	ACT	AAA	403	-	-	X	-
4	ACT	BBB	403	-	-	X	-
4	ACT	CCC	402	-	-	X	-
4	ACT	DDD	402	-	-	X	-
4	ACT	DDD	403	-	-	X	-
4	ACT	EEE	404	-	-	X	-
4	ACT	FFF	404	-	-	X	-

2 Entry composition [i](#)

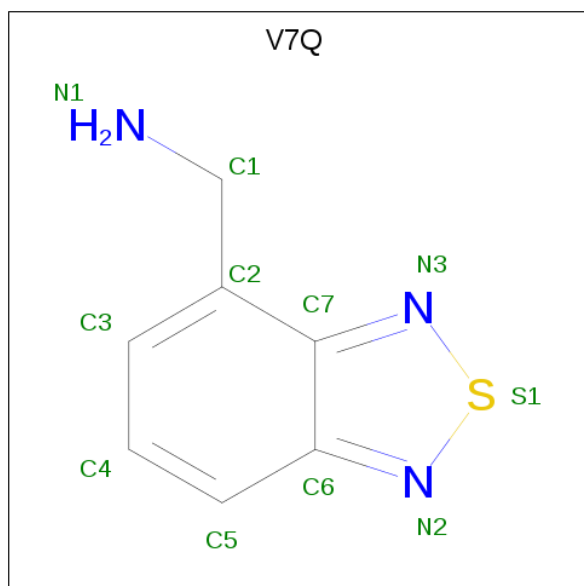
There are 8 unique types of molecules in this entry. The entry contains 26770 atoms, of which 12530 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Mirolysin.

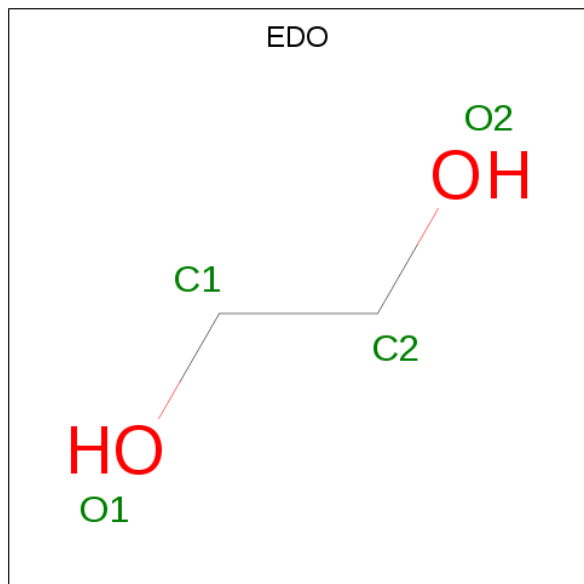
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	268	Total	C	H	N	O	S	71	13	0
			4234	1347	2066	377	425	19			
1	BBB	268	Total	C	H	N	O	S	71	14	0
			4252	1352	2076	379	425	20			
1	CCC	270	Total	C	H	N	O	S	71	11	0
			4237	1348	2066	378	426	19			
1	DDD	270	Total	C	H	N	O	S	71	14	0
			4280	1360	2089	382	429	20			
1	EEE	268	Total	C	H	N	O	S	71	11	0
			4215	1342	2057	376	422	18			
1	FFF	268	Total	C	H	N	O	S	71	12	0
			4226	1344	2065	377	421	19			

- Molecule 2 is 2,1,3-benzothiadiazol-4-ylmethanamine (three-letter code: V7Q) (formula: C₇H₇N₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	AAA	1	Total	C	H	N	S	0	0
			18	7	7	3	1		
2	BBB	1	Total	C	H	N	S	0	0
			18	7	7	3	1		
2	CCC	1	Total	C	H	N	S	0	0
			18	7	7	3	1		
2	DDD	1	Total	C	H	N	S	0	0
			18	7	7	3	1		
2	EEE	1	Total	C	H	N	S	0	0
			18	7	7	3	1		
2	FFF	1	Total	C	H	N	S	0	0
			18	7	7	3	1		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
3	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
3	DDD	1	Total	C	H	O	1	0
			10	2	6	2		
3	DDD	1	Total	C	H	O	1	0
			10	2	6	2		
3	EEE	1	Total	C	H	O	1	0
			10	2	6	2		
3	EEE	1	Total	C	H	O	1	0
			10	2	6	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	FFF	1	Total	C	H	O	1	0
			10	2	6	2		
3	FFF	1	Total	C	H	O	1	0
			10	2	6	2		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $\text{C}_2\text{H}_3\text{O}_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	AAA	1	Total	C	H	O	0	0
			7	2	3	2		
4	BBB	1	Total	C	H	O	0	0
			7	2	3	2		
4	CCC	1	Total	C	H	O	0	0
			7	2	3	2		
4	DDD	1	Total	C	H	O	0	0
			7	2	3	2		
4	DDD	1	Total	C	H	O	0	0
			7	2	3	2		
4	EEE	1	Total	C	H	O	0	0
			7	2	3	2		
4	FFF	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	1	Total 1	Zn 1	0	0
5	BBB	1	Total 1	Zn 1	0	0
5	CCC	1	Total 1	Zn 1	0	0
5	DDD	1	Total 1	Zn 1	0	0
5	EEE	1	Total 1	Zn 1	0	0
5	FFF	1	Total 1	Zn 1	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	AAA	2	Total 2	Ca 2	0	0
6	BBB	2	Total 2	Ca 2	0	0
6	CCC	3	Total 3	Ca 3	0	0
6	DDD	2	Total 2	Ca 2	0	0
6	EEE	2	Total 2	Ca 2	0	0
6	FFF	3	Total 3	Ca 3	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	CCC	1	Total 1	Cl 1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	AAA	183	Total 184	O 184	0	1
8	BBB	173	Total 173	O 173	0	0

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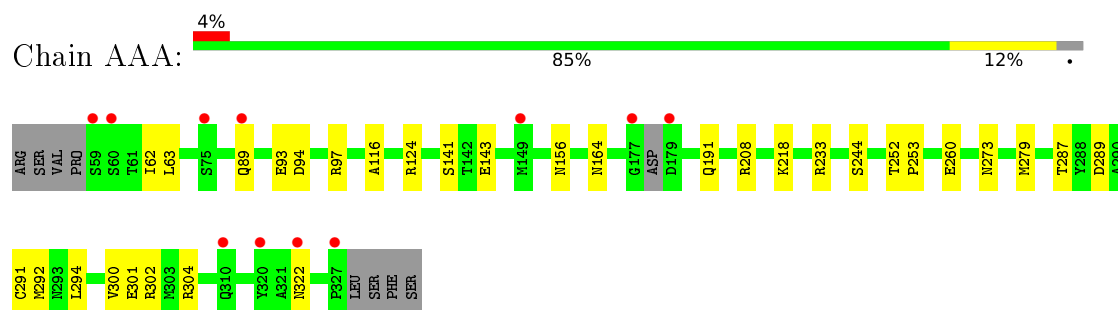
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	CCC	172	Total 172	O 172	0	0
8	DDD	182	Total 182	O 182	0	0
8	EEE	168	Total 168	O 168	0	0
8	FFF	189	Total 189	O 189	0	0

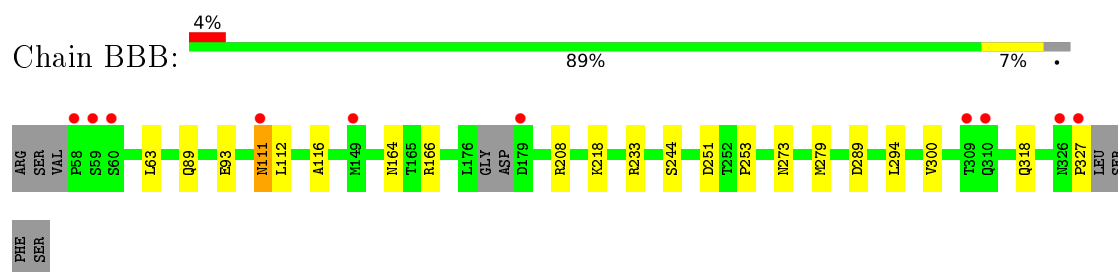
3 Residue-property plots [i](#)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

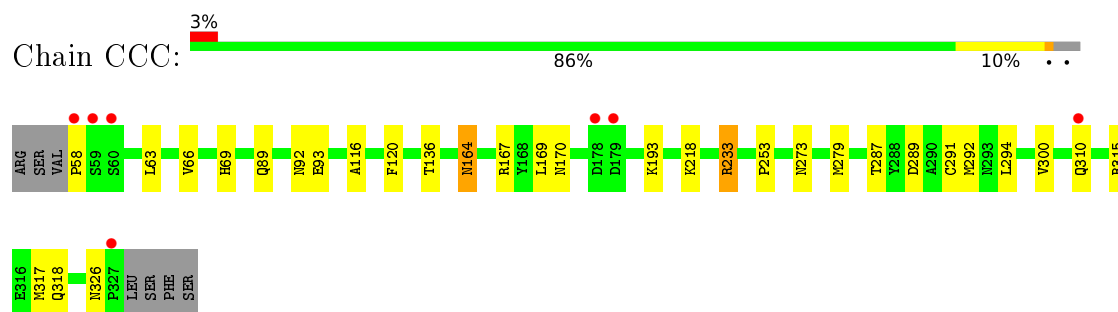
- Molecule 1: Mirolysin



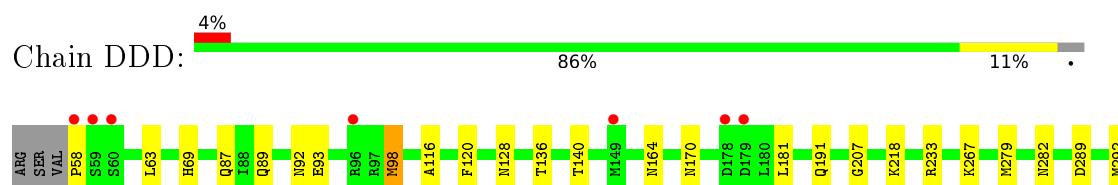
- Molecule 1: Mirolysin

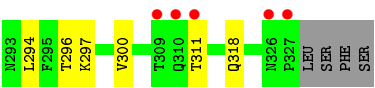


- Molecule 1: Mirolysin

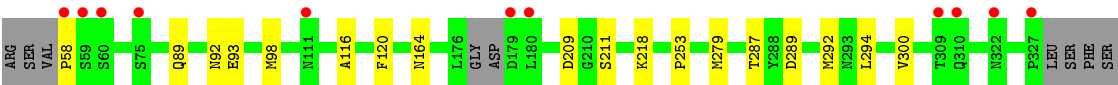
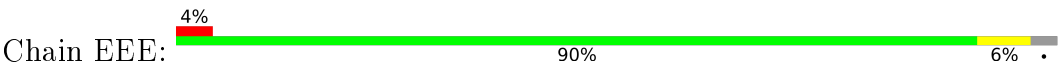


- Molecule 1: Mirolysin

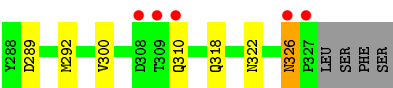
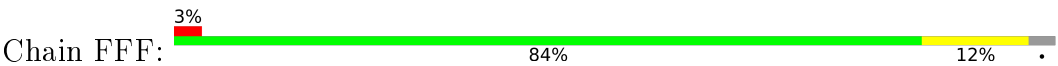




● Molecule 1: Mirolysin



● Molecule 1: Mirolysin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	77.59 Å 77.64 Å 82.00 Å 92.46° 90.00° 119.98°	Depositor
Resolution (Å)	38.80 – 2.10 38.80 – 2.10	Depositor EDS
% Data completeness (in resolution range)	92.2 (38.80-2.10) 92.2 (38.80-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.19 (at 2.10 Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.204 , 0.230 0.211 , 0.239	Depositor DCC
R_{free} test set	4127 reflections (4.64%)	wwPDB-VP
Wilson B-factor (Å ²)	12.6	Xtriage
Anisotropy	1.996	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.48 , 62.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.025 for -k,h+k,l 0.025 for h+k,-h,l 0.114 for -h-k,h,l 0.114 for k,-h-k,l 0.039 for h,-h-k,-l 0.028 for k,h,-l 0.025 for -h,-k,l 0.025 for -h-k,k,-l 0.185 for h+k,-k,-l 0.105 for -h,h+k,-l 0.177 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	26770	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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, EDO, ZN, V7Q, CL, ACT

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	AAA	0.69	0/2254	0.80	0/3055
1	BBB	0.67	0/2263	0.81	0/3068
1	CCC	0.69	0/2253	0.80	0/3056
1	DDD	0.69	0/2276	0.81	0/3086
1	EEE	0.69	0/2242	0.80	0/3039
1	FFF	0.69	0/2245	0.82	2/3043 (0.1%)
All	All	0.69	0/13533	0.80	2/18347 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	FFF	326	ASN	N-CA-CB	-5.28	101.10	110.60
1	FFF	124	ARG	CG-CD-NE	5.25	122.82	111.80

There are no chirality outliers.

There are no planarity outliers.

CLOSE-CONTACTS INFOmissingINFO

5.2 Torsion angles [i](#)

5.2.1 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 X-ray entries followed by that with respect to entries of similar resolution.

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	AAA	278/277 (100%)	271 (98%)	6 (2%)	1 (0%)	34	32
1	BBB	279/277 (101%)	271 (97%)	7 (2%)	1 (0%)	34	32
1	CCC	280/277 (101%)	272 (97%)	7 (2%)	1 (0%)	34	32
1	DDD	283/277 (102%)	276 (98%)	6 (2%)	1 (0%)	34	32
1	EEE	276/277 (100%)	269 (98%)	6 (2%)	1 (0%)	34	32
1	FFF	277/277 (100%)	270 (98%)	6 (2%)	1 (0%)	34	32
All	All	1673/1662 (101%)	1629 (97%)	38 (2%)	6 (0%)	34	32

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	164	ASN
1	BBB	164	ASN
1	CCC	164	ASN
1	DDD	164	ASN
1	EEE	164	ASN
1	FFF	164	ASN

5.2.2 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 X-ray entries followed by that with respect to entries of similar resolution.

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	AAA	244/239 (102%)	243 (100%)	1 (0%)	91	94
1	BBB	246/239 (103%)	245 (100%)	1 (0%)	91	94
1	CCC	244/239 (102%)	242 (99%)	2 (1%)	81	86
1	DDD	247/239 (103%)	243 (98%)	4 (2%)	62	69
1	EEE	243/239 (102%)	243 (100%)	0	100	100
1	FFF	243/239 (102%)	243 (100%)	0	100	100
All	All	1467/1434 (102%)	1459 (100%)	8 (0%)	88	92

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

Mol	Chain	Res	Type
1	AAA	301	GLU
1	BBB	111	ASN
1	CCC	233	ARG
1	CCC	326	ASN
1	DDD	98[A]	MET
1	DDD	98[B]	MET
1	DDD	191	GLN
1	DDD	292	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.2.3 RNA ⓘ

There are no RNA molecules in this entry.

5.3 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.4 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.5 Ligand geometry ⓘ

Of 42 ligands modelled in this entry, 21 are monoatomic - leaving 21 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	ACT	CCC	402	5	1,3,3	3.30	1 (100%)	0,3,3	0.00	-
4	ACT	DDD	403	-	1,3,3	5.17	1 (100%)	0,3,3	0.00	-
2	V7Q	CCC	401	-	12,12,12	0.87	1 (8%)	9,16,16	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ACT	DDD	402	5	1,3,3	6.07	1 (100%)	0,3,3	0.00	-
4	ACT	FFF	404	5	1,3,3	5.21	1 (100%)	0,3,3	0.00	-
2	V7Q	AAA	401	-	12,12,12	0.84	1 (8%)	9,16,16	0.99	0
4	ACT	BBB	403	5	1,3,3	4.54	1 (100%)	0,3,3	0.00	-
3	EDO	FFF	403	-	3,3,3	0.19	0	2,2,2	0.05	0
3	EDO	FFF	402	-	3,3,3	0.16	0	2,2,2	0.14	0
3	EDO	BBB	402	-	3,3,3	0.15	0	2,2,2	0.11	0
2	V7Q	EEE	401	-	12,12,12	0.75	0	9,16,16	0.98	0
3	EDO	EEE	402	-	3,3,3	0.14	0	2,2,2	0.49	0
3	EDO	DDD	405	-	3,3,3	0.09	0	2,2,2	0.19	0
3	EDO	AAA	402	-	3,3,3	0.65	0	2,2,2	0.60	0
2	V7Q	FFF	401	-	12,12,12	0.71	0	9,16,16	1.06	0
4	ACT	AAA	403	5	1,3,3	4.46	1 (100%)	0,3,3	0.00	-
4	ACT	EEE	404	5	1,3,3	4.64	1 (100%)	0,3,3	0.00	-
3	EDO	DDD	404	-	3,3,3	0.14	0	2,2,2	0.06	0
2	V7Q	BBB	401	-	12,12,12	0.71	0	9,16,16	0.94	0
3	EDO	EEE	403	-	3,3,3	0.11	0	2,2,2	0.19	0
2	V7Q	DDD	401	-	12,12,12	0.83	1 (8%)	9,16,16	0.93	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	V7Q	FFF	401	-	-	1/2/2/2	0/2/2/2
2	V7Q	AAA	401	-	-	1/2/2/2	0/2/2/2
2	V7Q	DDD	401	-	-	1/2/2/2	0/2/2/2
2	V7Q	CCC	401	-	-	1/2/2/2	0/2/2/2
3	EDO	DDD	404	-	-	0/1/1/1	-
3	EDO	AAA	402	-	-	0/1/1/1	-
3	EDO	FFF	403	-	-	1/1/1/1	-
2	V7Q	BBB	401	-	-	0/2/2/2	0/2/2/2
3	EDO	FFF	402	-	-	1/1/1/1	-
3	EDO	DDD	405	-	-	0/1/1/1	-
3	EDO	BBB	402	-	-	0/1/1/1	-
3	EDO	EEE	403	-	-	0/1/1/1	-
2	V7Q	EEE	401	-	-	1/2/2/2	0/2/2/2
3	EDO	EEE	402	-	-	1/1/1/1	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	DDD	402	ACT	CH3-C	6.07	1.56	1.48
4	FFF	404	ACT	CH3-C	5.21	1.55	1.48
4	DDD	403	ACT	CH3-C	5.17	1.55	1.48
4	EEE	404	ACT	CH3-C	4.64	1.54	1.48
4	BBB	403	ACT	CH3-C	4.54	1.54	1.48
4	AAA	403	ACT	CH3-C	4.46	1.54	1.48
4	CCC	402	ACT	CH3-C	3.30	1.52	1.48
2	CCC	401	V7Q	C2-C7	-2.48	1.38	1.43
2	DDD	401	V7Q	C2-C7	-2.16	1.38	1.43
2	AAA	401	V7Q	C2-C7	-2.15	1.38	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AAA	401	V7Q	N1-C1-C2-C7
2	CCC	401	V7Q	N1-C1-C2-C7
2	DDD	401	V7Q	N1-C1-C2-C7
2	EEE	401	V7Q	N1-C1-C2-C7
2	FFF	401	V7Q	N1-C1-C2-C7
3	EEE	402	EDO	O1-C1-C2-O2
3	FFF	403	EDO	O1-C1-C2-O2
3	FFF	402	EDO	O1-C1-C2-O2

There are no ring outliers.

15 monomers are involved in 39 short contacts:

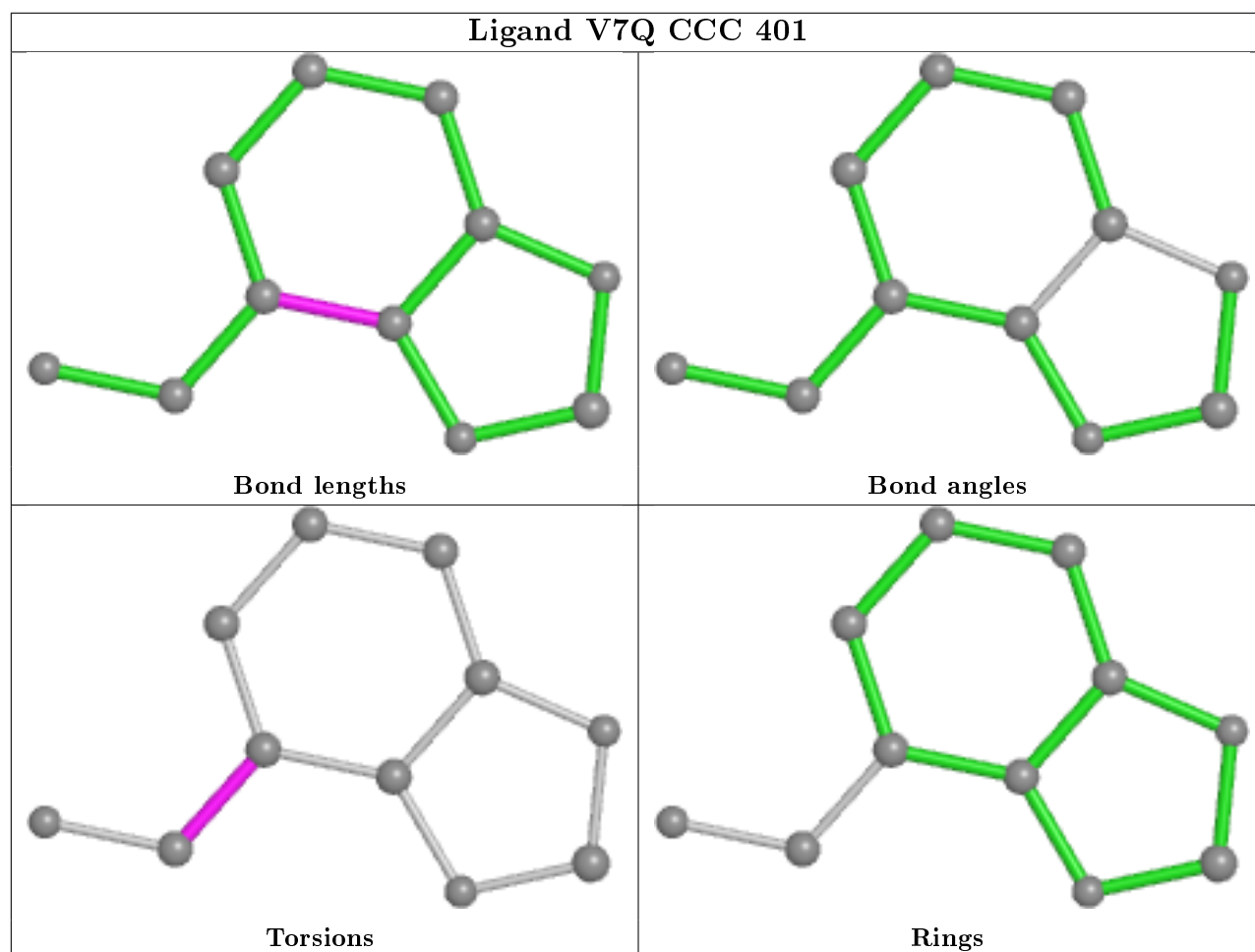
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	CCC	402	ACT	3	0
4	DDD	403	ACT	2	0
2	CCC	401	V7Q	1	0
4	DDD	402	ACT	2	0
4	FFF	404	ACT	4	0
2	AAA	401	V7Q	1	0
4	BBB	403	ACT	2	0
3	FFF	402	EDO	3	0
2	EEE	401	V7Q	1	0
3	AAA	402	EDO	9	0
4	AAA	403	ACT	5	0
4	EEE	404	ACT	2	0
3	DDD	404	EDO	2	0

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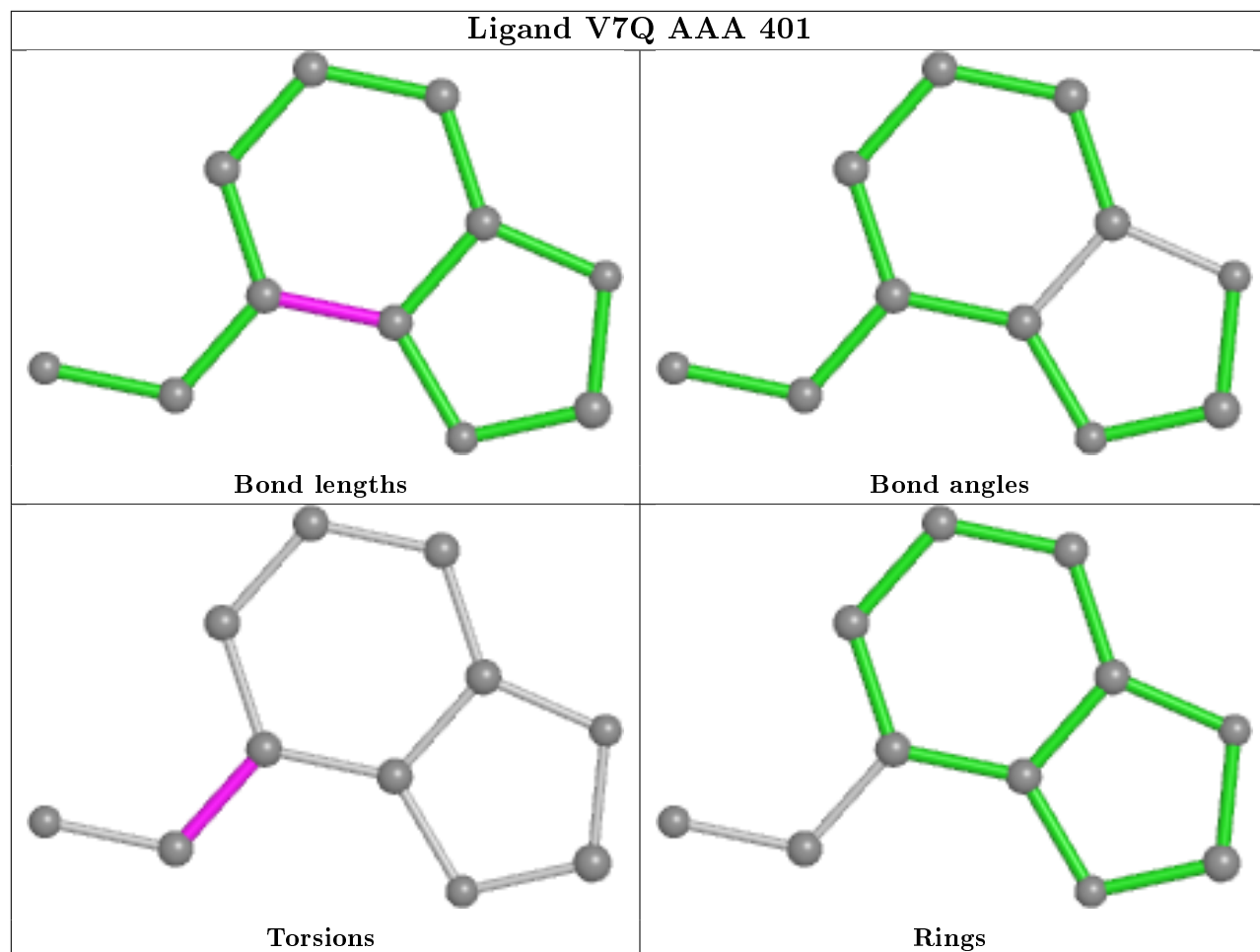
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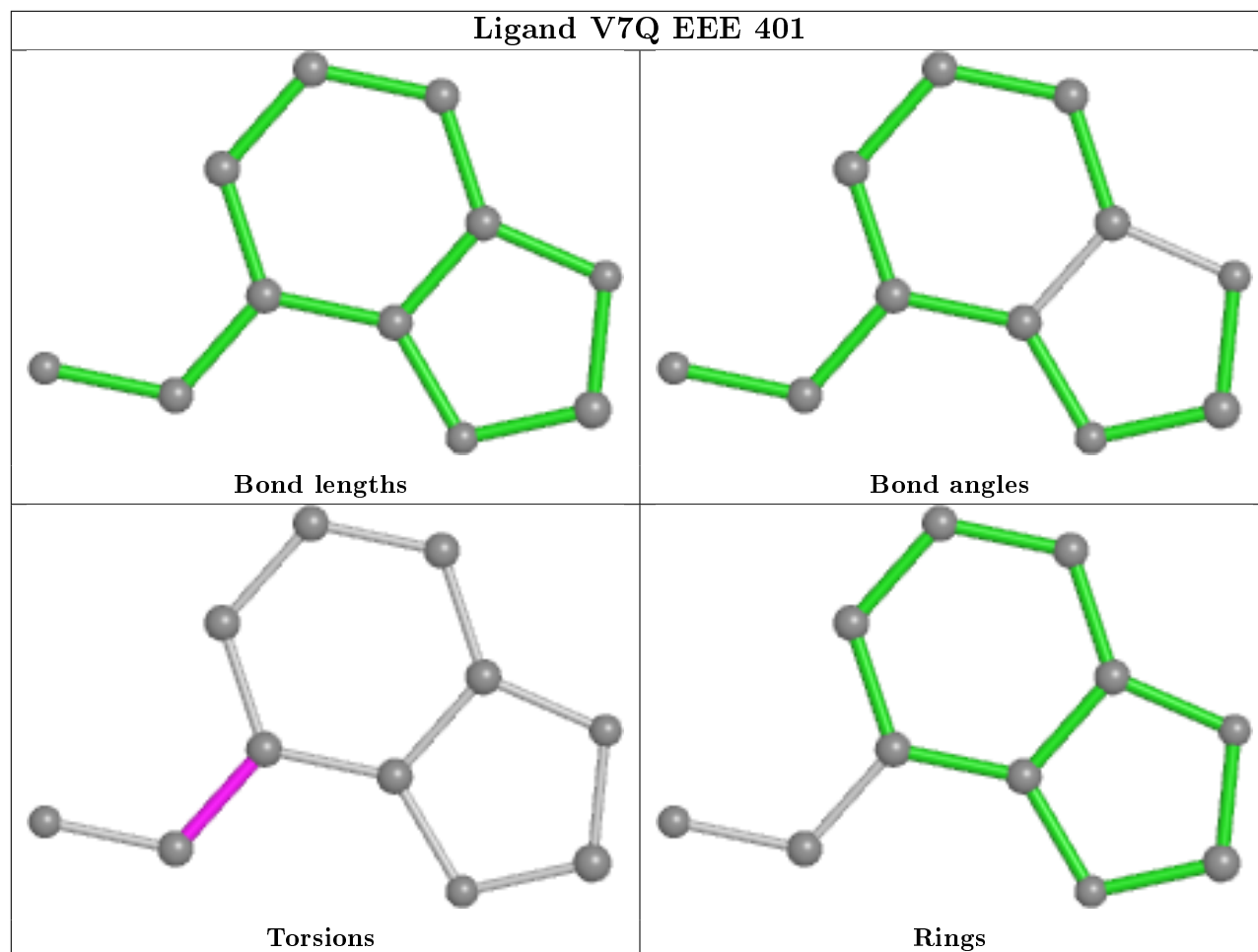
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	BBB	401	V7Q	1	0
2	DDD	401	V7Q	2	0

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 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.

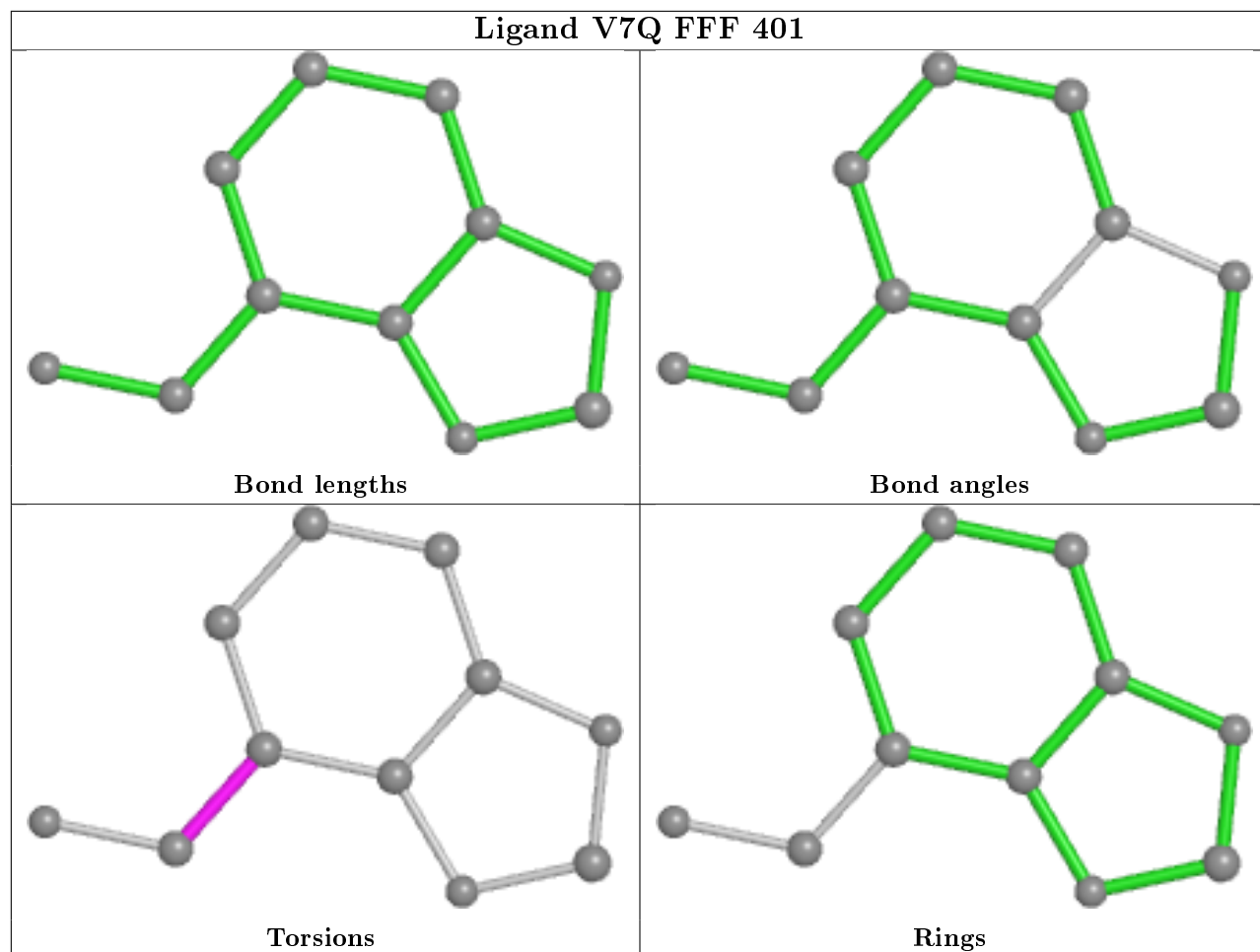


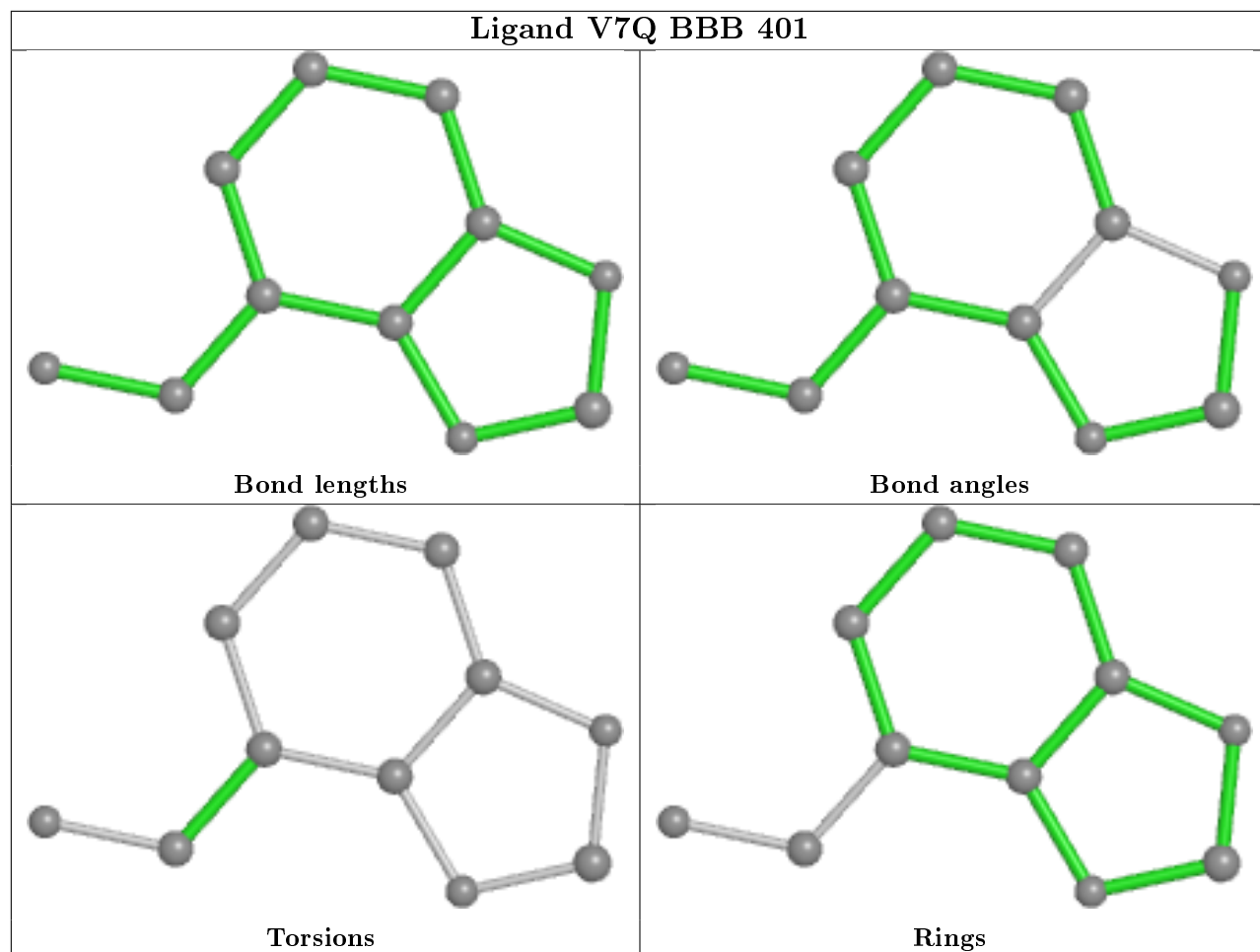
Ligand V7Q AAA 401

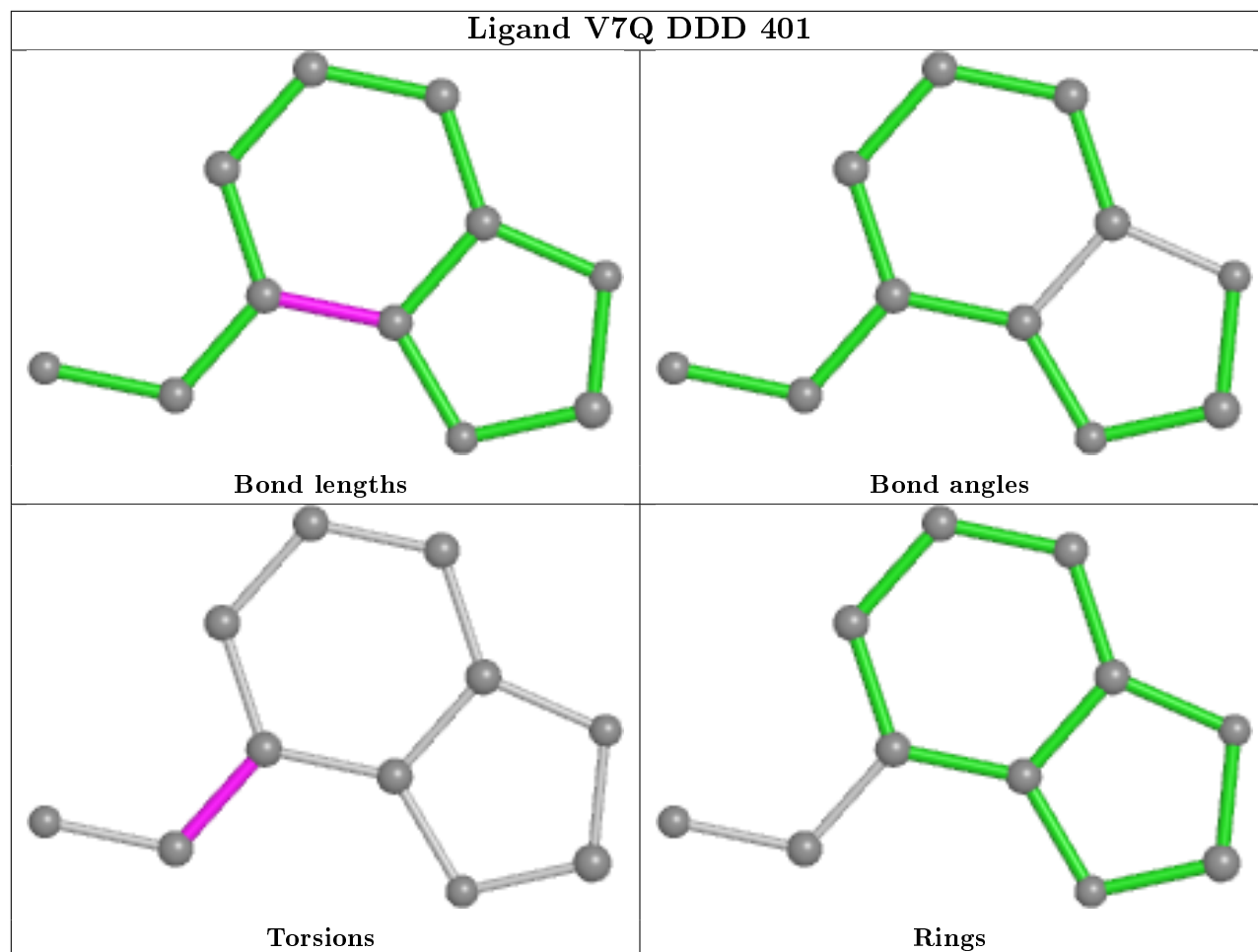




Ligand V7Q FFF 401







5.6 Other polymers [i](#)

There are no such residues in this entry.

5.7 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AAA	268/277 (96%)	0.21	11 (4%) 37 43	7, 13, 29, 56	0
1	BBB	268/277 (96%)	0.21	10 (3%) 41 48	7, 14, 29, 90	0
1	CCC	270/277 (97%)	0.21	7 (2%) 56 61	7, 14, 33, 57	0
1	DDD	270/277 (97%)	0.25	12 (4%) 34 40	6, 13, 31, 85	0
1	EEE	268/277 (96%)	0.26	11 (4%) 37 43	7, 14, 32, 87	0
1	FFF	268/277 (96%)	0.23	9 (3%) 45 51	6, 14, 30, 87	0
All	All	1612/1662 (96%)	0.23	60 (3%) 41 48	6, 14, 31, 90	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	DDD	58	PRO	12.2
1	EEE	58	PRO	11.9
1	FFF	58	PRO	10.9
1	BBB	58	PRO	10.3
1	EEE	59	SER	8.5
1	DDD	59	SER	7.8
1	BBB	59	SER	7.1
1	CCC	58	PRO	6.7
1	CCC	59	SER	6.0
1	BBB	327	PRO	5.8
1	FFF	310	GLN	5.8
1	FFF	59	SER	5.8
1	AAA	327	PRO	5.6
1	AAA	179	ASP	5.3
1	AAA	59	SER	5.2
1	FFF	327	PRO	5.1
1	AAA	177	GLY	5.0
1	FFF	60	SER	4.9
1	EEE	60	SER	4.6

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Mol	Chain	Res	Type	RSRZ
1	BBB	179	ASP	4.5
1	DDD	310	GLN	4.3
1	DDD	327	PRO	4.3
1	BBB	60	SER	4.3
1	CCC	310	GLN	4.1
1	CCC	60	SER	4.1
1	DDD	179	ASP	4.0
1	DDD	309	THR	3.8
1	FFF	326	ASN	3.7
1	CCC	327	PRO	3.7
1	DDD	60	SER	3.6
1	BBB	326	ASN	3.6
1	DDD	326	ASN	3.5
1	EEE	327	PRO	3.5
1	AAA	60	SER	3.3
1	AAA	310	GLN	3.2
1	EEE	310	GLN	3.1
1	AAA	322	ASN	3.0
1	EEE	179	ASP	3.0
1	DDD	149	MET	2.9
1	EEE	309	THR	2.9
1	FFF	308	ASP	2.8
1	DDD	96	ARG	2.8
1	EEE	322	ASN	2.8
1	BBB	309	THR	2.6
1	CCC	178	ASP	2.6
1	BBB	310	GLN	2.5
1	EEE	75[A]	SER	2.5
1	DDD	311	THR	2.4
1	BBB	149	MET	2.3
1	BBB	111	ASN	2.3
1	EEE	180	LEU	2.2
1	FFF	96	ARG	2.2
1	CCC	179	ASP	2.2
1	EEE	111	ASN	2.2
1	AAA	75[A]	SER	2.1
1	FFF	309	THR	2.1
1	AAA	149	MET	2.1
1	AAA	89[A]	GLN	2.1
1	AAA	320	TYR	2.0
1	DDD	178	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	EDO	EEE	402	4/4	0.73	0.20	33,34,34,35	1
2	V7Q	BBB	401	11/11	0.78	0.18	22,24,26,27	0
2	V7Q	FFF	401	11/11	0.80	0.17	15,17,18,20	0
3	EDO	DDD	404	4/4	0.83	0.15	29,32,34,35	1
2	V7Q	AAA	401	11/11	0.84	0.16	20,22,23,27	0
4	ACT	DDD	403	4/4	0.84	0.13	21,23,23,24	0
3	EDO	FFF	403	4/4	0.85	0.12	35,36,39,41	1
2	V7Q	CCC	401	11/11	0.86	0.14	16,17,19,21	0
3	EDO	EEE	403	4/4	0.86	0.14	22,23,24,25	1
4	ACT	CCC	402	4/4	0.88	0.11	8,11,11,11	0
2	V7Q	EEE	401	11/11	0.88	0.13	19,20,22,23	0
4	ACT	DDD	402	4/4	0.89	0.15	15,18,18,20	0
4	ACT	EEE	404	4/4	0.89	0.15	13,16,16,18	0
2	V7Q	DDD	401	11/11	0.90	0.13	16,18,20,20	0
3	EDO	DDD	405	4/4	0.91	0.11	20,23,23,23	1
3	EDO	BBB	402	4/4	0.91	0.16	22,22,24,25	1
3	EDO	FFF	402	4/4	0.92	0.15	22,23,25,29	1
3	EDO	AAA	402	4/4	0.94	0.13	13,14,14,16	1
4	ACT	BBB	403	4/4	0.94	0.10	10,13,13,13	0
4	ACT	AAA	403	4/4	0.95	0.11	8,9,9,10	0
4	ACT	FFF	404	4/4	0.96	0.11	8,11,11,12	0
6	CA	FFF	408	1/1	0.96	0.07	35,35,35,35	0
7	CL	CCC	407	1/1	0.96	0.09	31,31,31,31	0
6	CA	BBB	406	1/1	0.98	0.06	15,15,15,15	0
6	CA	FFF	407	1/1	0.98	0.06	16,16,16,16	0
6	CA	CCC	405	1/1	0.99	0.06	14,14,14,14	0
6	CA	CCC	406	1/1	0.99	0.04	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	CA	DDD	407	1/1	0.99	0.05	10,10,10,10	0
6	CA	DDD	408	1/1	0.99	0.05	15,15,15,15	0
6	CA	EEE	406	1/1	0.99	0.08	11,11,11,11	0
6	CA	EEE	407	1/1	0.99	0.05	12,12,12,12	0
6	CA	BBB	405	1/1	0.99	0.05	10,10,10,10	0
6	CA	AAA	406	1/1	0.99	0.05	18,18,18,18	0
6	CA	CCC	404	1/1	0.99	0.08	10,10,10,10	0
6	CA	AAA	405	1/1	1.00	0.04	9,9,9,9	0
5	ZN	AAA	404	1/1	1.00	0.08	8,8,8,8	0
5	ZN	BBB	404	1/1	1.00	0.08	8,8,8,8	0
5	ZN	CCC	403	1/1	1.00	0.08	7,7,7,7	0
6	CA	FFF	406	1/1	1.00	0.07	9,9,9,9	0
5	ZN	DDD	406	1/1	1.00	0.06	8,8,8,8	0
5	ZN	EEE	405	1/1	1.00	0.06	8,8,8,8	0
5	ZN	FFF	405	1/1	1.00	0.06	7,7,7,7	0

6.5 Other polymers [i](#)

There are no such residues in this entry.