



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 17, 2022 – 06:16 pm GMT

PDB ID : 8B7R
Title : Bacterial chalcone isomerase with taxifolin chalcone
Authors : Hinrichs, W.; Palm, G.J.
Deposited on : 2022-10-02
Resolution : 2.15 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 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:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

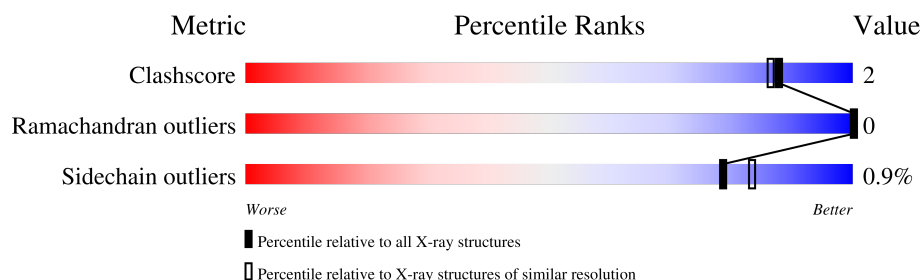
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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))
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)

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 $\leq 5\%$

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	283	86% 6% 8%
1	B	283	87% 5% 8%
1	C	283	86% 6% 8%
1	D	283	87% 5% 8%
1	E	283	88% . . 7%
1	F	283	87% 5% 8%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	B	308	-	-	X	-

2 Entry composition [i](#)

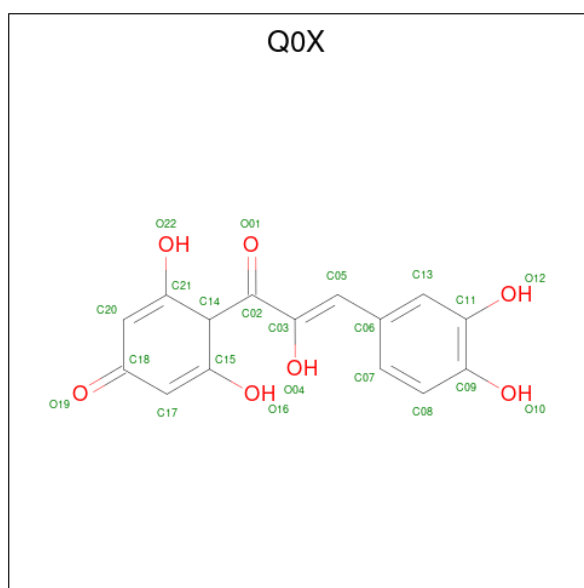
There are 5 unique types of molecules in this entry. The entry contains 14852 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Chalcone isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	259	Total	C	N	O	S	0	3	0
			2143	1400	347	381	15			
1	B	259	Total	C	N	O	S	0	3	0
			2145	1401	349	381	14			
1	C	260	Total	C	N	O	S	0	3	0
			2150	1404	350	382	14			
1	D	260	Total	C	N	O	S	0	2	0
			2140	1398	347	381	14			
1	E	262	Total	C	N	O	S	0	3	0
			2167	1414	354	385	14			
1	F	259	Total	C	N	O	S	0	3	0
			2145	1401	349	381	14			

- Molecule 2 is (2Z)-3-(3,4-dihydroxyphenyl)-2-(hydroxy)-1-(2,4,6-trihydroxyphenyl)prop-2-en-1-one (three-letter code: Q0X) (formula: C₁₅H₁₂O₇) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			22	15	7		
2	B	1	Total	C	O	0	0
			22	15	7		
2	C	1	Total	C	O	0	0
			22	15	7		
2	D	1	Total	C	O	0	0
			22	15	7		
2	E	1	Total	C	O	0	0
			22	15	7		
2	F	1	Total	C	O	0	0
			22	15	7		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Cl	0	0
			4	4		
3	B	7	Total	Cl	0	0
			7	7		
3	C	4	Total	Cl	0	0
			4	4		
3	D	3	Total	Cl	0	0
			3	3		
3	E	3	Total	Cl	0	0
			3	3		
3	F	5	Total	Cl	0	0
			5	5		

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	K	0	0
			1	1		
4	C	1	Total	K	0	0
			1	1		
4	E	1	Total	K	0	0
			1	1		

- Molecule 5 is water.

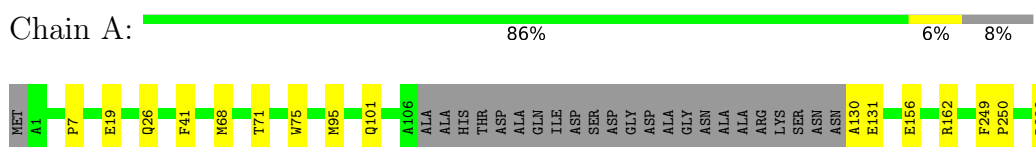
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	294	Total 294	O 294	0	0
5	B	321	Total 322	O 322	0	1
5	C	305	Total 306	O 306	0	1
5	D	317	Total 317	O 317	0	0
5	E	278	Total 278	O 278	0	0
5	F	283	Total 284	O 284	0	1

3 Residue-property plots [i](#)

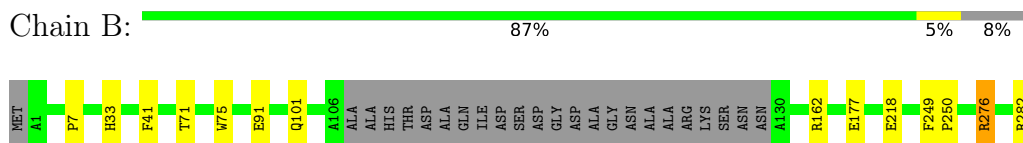
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

Note EDS failed to run properly.

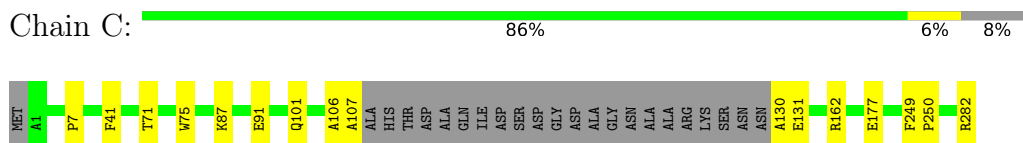
- Molecule 1: Chalcone isomerase



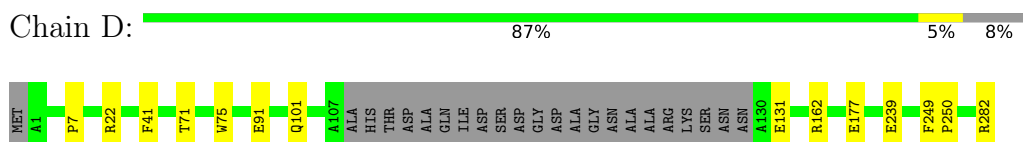
- Molecule 1: Chalcone isomerase



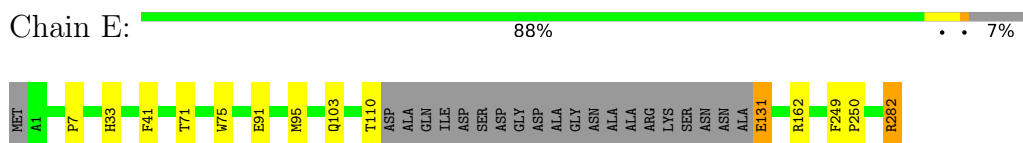
- Molecule 1: Chalcone isomerase



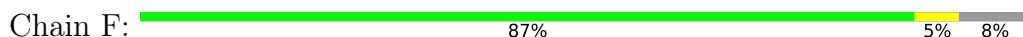
- Molecule 1: Chalcone isomerase

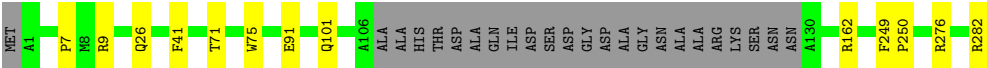


- Molecule 1: Chalcone isomerase



- Molecule 1: Chalcone isomerase





4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	173.82Å 193.15Å 205.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.29 – 2.15	Depositor
% Data completeness (in resolution range)	99.7 (48.29-2.15)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 2.12Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.163 , 0.190	Depositor
Wilson B-factor (Å ²)	33.2	Xtriage
Anisotropy	0.255	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14852	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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: Q0X, K, CL

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	0.56	2/2220 (0.1%)	0.78	1/3016 (0.0%)
1	B	0.51	2/2223 (0.1%)	0.77	2/3021 (0.1%)
1	C	0.48	0/2228	0.79	2/3028 (0.1%)
1	D	0.54	1/2217 (0.0%)	0.80	3/3013 (0.1%)
1	E	0.46	0/2246	0.80	2/3053 (0.1%)
1	F	0.51	0/2223	0.79	3/3021 (0.1%)
All	All	0.51	5/13357 (0.0%)	0.79	13/18152 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	2
1	E	0	2
All	All	0	6

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	156	GLU	CD-OE1	7.19	1.33	1.25
1	B	177	GLU	CD-OE1	6.19	1.32	1.25
1	A	19	GLU	CD-OE2	6.06	1.32	1.25
1	D	177	GLU	CD-OE2	5.28	1.31	1.25
1	B	218	GLU	CD-OE1	5.27	1.31	1.25

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	162	ARG	NE-CZ-NH2	-8.47	116.07	120.30
1	C	162	ARG	NE-CZ-NH2	-8.11	116.25	120.30
1	D	162	ARG	NE-CZ-NH2	-7.79	116.40	120.30
1	F	162	ARG	NE-CZ-NH2	-7.74	116.43	120.30
1	D	282	ARG	NE-CZ-NH2	-7.16	116.72	120.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	130	ALA	Peptide
1	A	282	ARG	Sidechain
1	C	130	ALA	Peptide
1	C	131	GLU	Peptide
1	E	131	GLU	Peptide

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	2143	0	2079	7	0
1	B	2145	0	2077	8	0
1	C	2150	0	2082	9	0
1	D	2140	0	2076	7	0
1	E	2167	0	2096	12	0
1	F	2145	0	2077	7	0
2	A	22	0	0	2	0
2	B	22	0	0	2	0
2	C	22	0	0	2	0
2	D	22	0	0	3	0
2	E	22	0	0	5	0
2	F	22	0	0	2	0
3	A	4	0	0	0	0
3	B	7	0	0	2	0
3	C	4	0	0	0	0
3	D	3	0	0	0	0
3	E	3	0	0	0	0
3	F	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
5	A	294	0	0	3	0
5	B	322	0	0	3	1
5	C	306	0	0	4	1
5	D	317	0	0	3	0
5	E	278	0	0	5	0
5	F	284	0	0	2	0
All	All	14852	0	12487	51	1

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 2.

The worst 5 of 51 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:E:33[B]:HIS:CD2	5:E:401:HOH:O	1.76	1.27
1:E:33[B]:HIS:HD2	5:E:401:HOH:O	1.28	0.87
1:E:33[A]:HIS:NE2	2:E:301:Q0X:O16	2.23	0.70
1:B:91:GLU:HG2	5:B:540:HOH:O	1.94	0.67
1:D:71:THR:HG21	2:D:301:Q0X:O01	1.95	0.67

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:566:HOH:O	5:C:468:HOH:O[8_565]	2.18	0.02

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 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	A	258/283 (91%)	253 (98%)	5 (2%)	0	100	100
1	B	258/283 (91%)	254 (98%)	4 (2%)	0	100	100
1	C	259/283 (92%)	255 (98%)	4 (2%)	0	100	100
1	D	258/283 (91%)	253 (98%)	5 (2%)	0	100	100
1	E	261/283 (92%)	257 (98%)	4 (2%)	0	100	100
1	F	258/283 (91%)	253 (98%)	5 (2%)	0	100	100
All	All	1552/1698 (91%)	1525 (98%)	27 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	A	228/241 (95%)	225 (99%)	3 (1%)	69	74
1	B	228/241 (95%)	226 (99%)	2 (1%)	78	83
1	C	228/241 (95%)	227 (100%)	1 (0%)	91	93
1	D	227/241 (94%)	225 (99%)	2 (1%)	78	83
1	E	230/241 (95%)	226 (98%)	4 (2%)	60	65
1	F	228/241 (95%)	227 (100%)	1 (0%)	91	93
All	All	1369/1446 (95%)	1356 (99%)	13 (1%)	78	83

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	131	GLU
1	E	41	PHE
1	F	41	PHE
1	E	110	THR
1	E	131	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	101	GLN
1	F	103	GLN
1	B	101	GLN
1	B	103	GLN
1	D	101	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 35 ligands modelled in this entry, 29 are monoatomic - leaving 6 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	$\# Z > 2$
2	Q0X	B	301	-	23,23,23	1.78	5 (21%)	24,33,33	2.72	7 (29%)
2	Q0X	F	301	-	23,23,23	1.84	7 (30%)	24,33,33	2.70	7 (29%)
2	Q0X	C	301	-	23,23,23	2.12	7 (30%)	24,33,33	2.09	6 (25%)
2	Q0X	D	301	-	23,23,23	1.90	7 (30%)	24,33,33	2.85	7 (29%)
2	Q0X	A	301	-	23,23,23	1.81	5 (21%)	24,33,33	2.89	7 (29%)
2	Q0X	E	301	-	23,23,23	1.88	6 (26%)	24,33,33	2.28	7 (29%)

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	Q0X	B	301	-	-	6/9/28/28	0/2/2/2
2	Q0X	F	301	-	-	5/9/28/28	0/2/2/2
2	Q0X	C	301	-	-	4/9/28/28	0/2/2/2
2	Q0X	D	301	-	-	6/9/28/28	0/2/2/2
2	Q0X	A	301	-	-	7/9/28/28	0/2/2/2
2	Q0X	E	301	-	-	5/9/28/28	0/2/2/2

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	Q0X	C14-C15	-4.62	1.40	1.53
2	C	301	Q0X	C14-C21	-4.59	1.40	1.53
2	E	301	Q0X	C14-C15	-4.48	1.40	1.53
2	E	301	Q0X	C14-C21	-4.25	1.41	1.53
2	A	301	Q0X	C14-C21	-4.09	1.41	1.53

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	Q0X	O04-C03-C05	-9.97	117.59	122.87
2	D	301	Q0X	O04-C03-C05	-9.92	117.61	122.87
2	B	301	Q0X	O04-C03-C05	-9.79	117.68	122.87
2	F	301	Q0X	O04-C03-C05	-8.70	118.26	122.87
2	E	301	Q0X	O04-C03-C05	-7.07	119.12	122.87

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

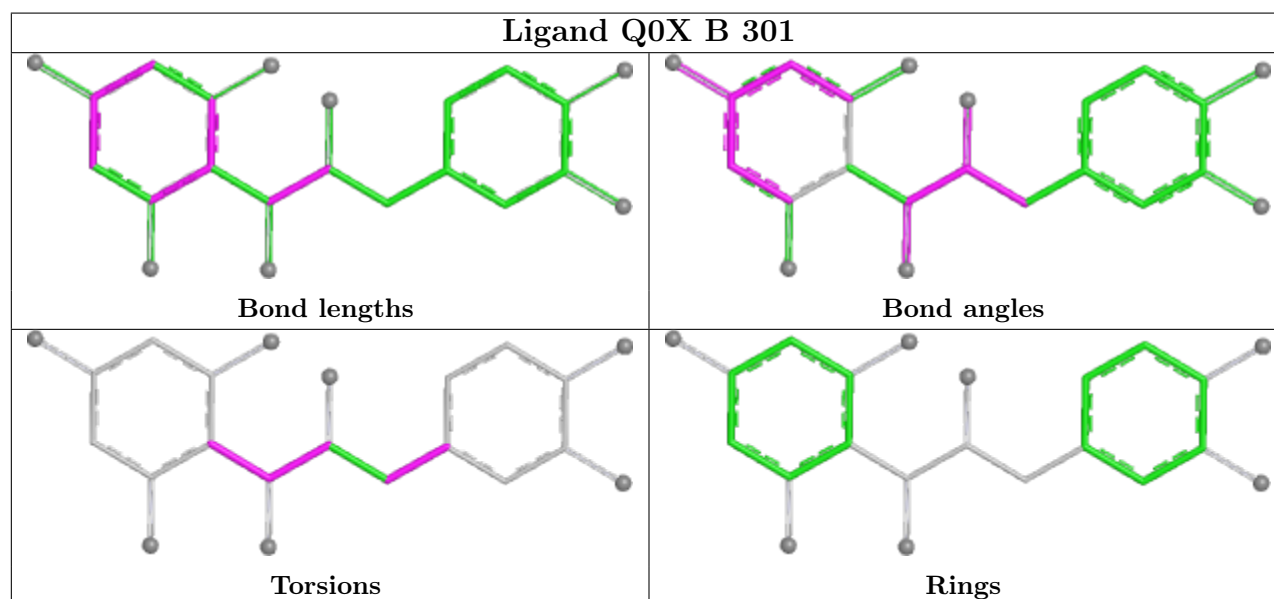
Mol	Chain	Res	Type	Atoms
2	A	301	Q0X	O01-C02-C03-C05
2	A	301	Q0X	O01-C02-C14-C15
2	A	301	Q0X	O01-C02-C14-C21
2	A	301	Q0X	C03-C02-C14-C21
2	A	301	Q0X	C03-C05-C06-C07

There are no ring outliers.

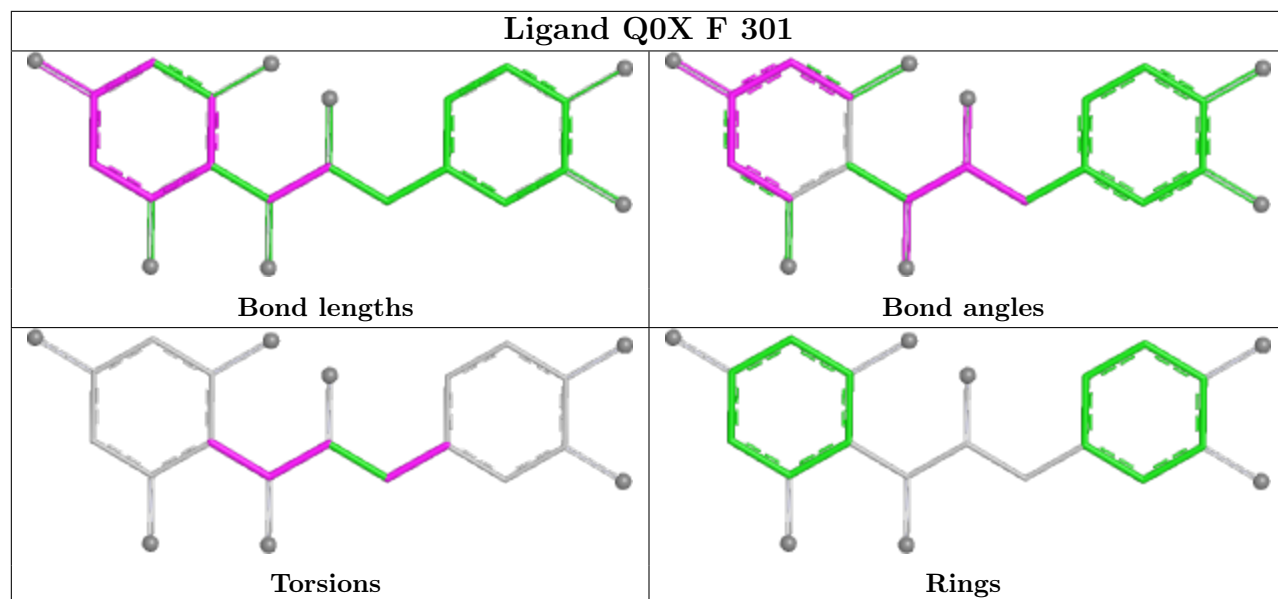
6 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	Q0X	2	0
2	F	301	Q0X	2	0
2	C	301	Q0X	2	0
2	D	301	Q0X	3	0
2	A	301	Q0X	2	0
2	E	301	Q0X	5	0

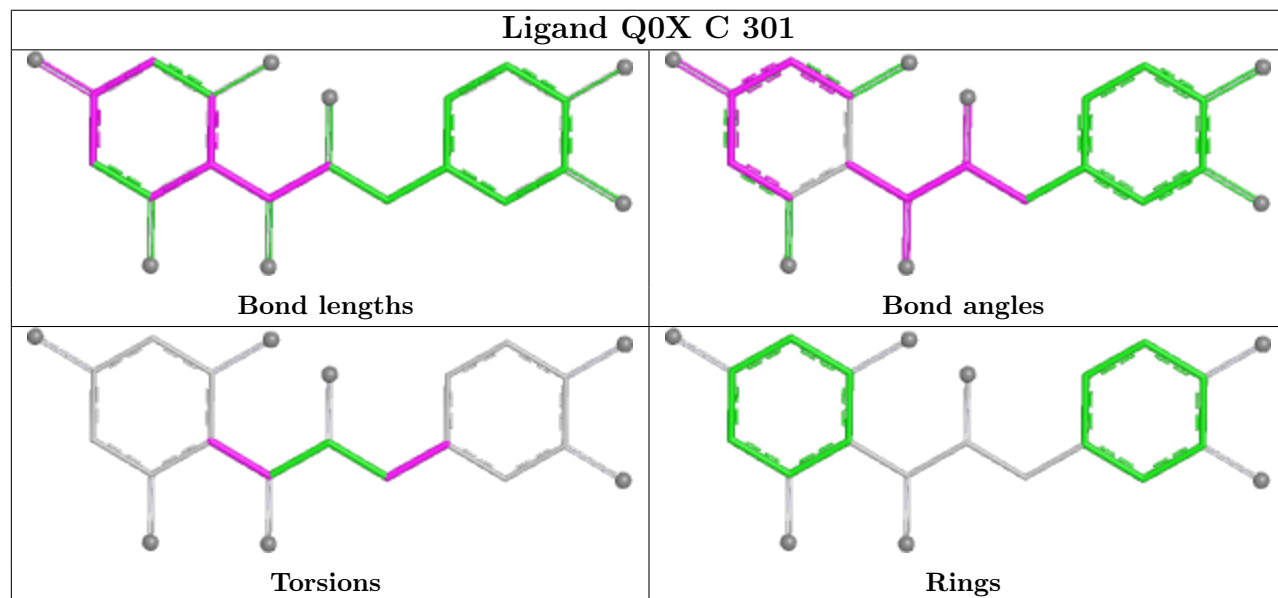
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



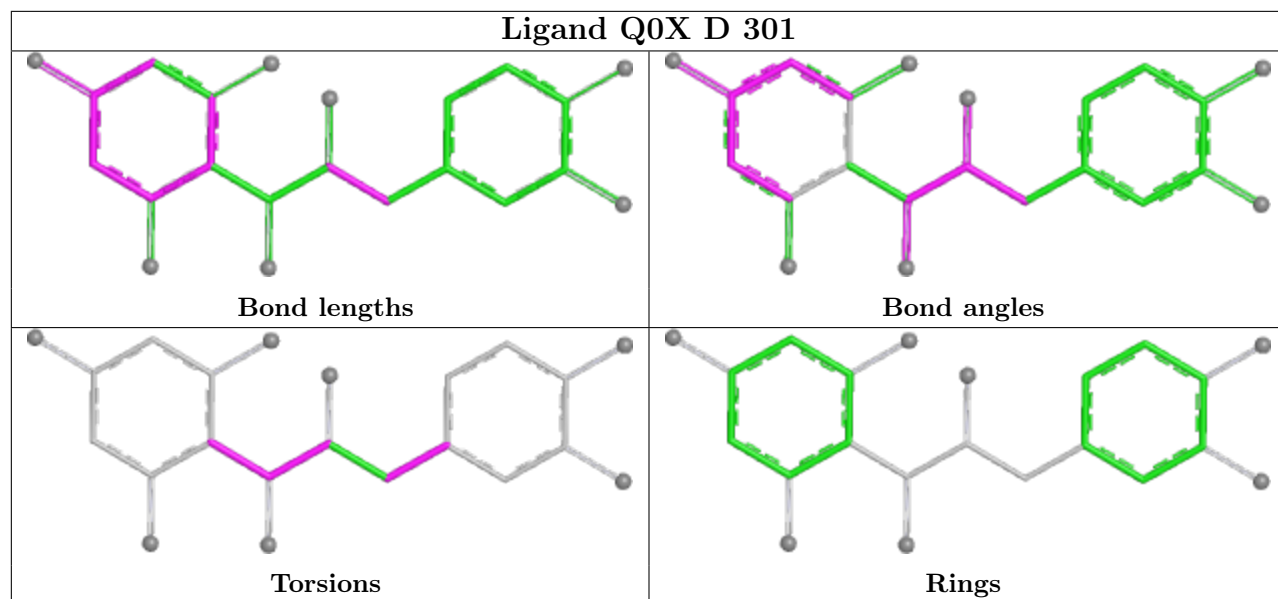
Ligand Q0X F 301



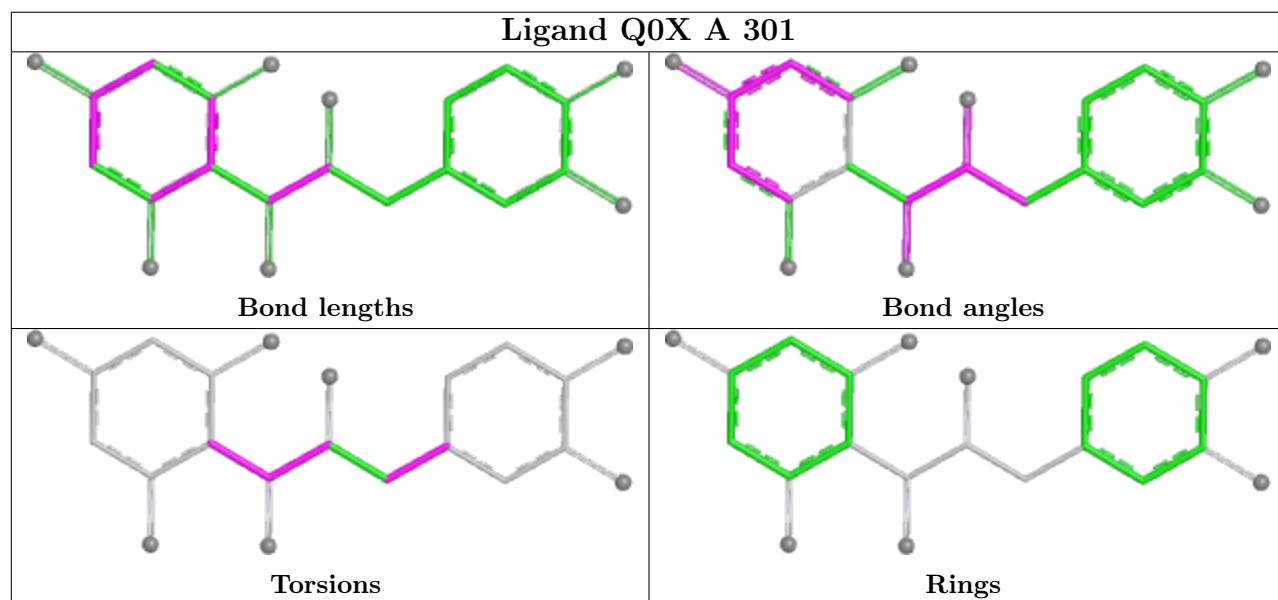
Ligand Q0X C 301

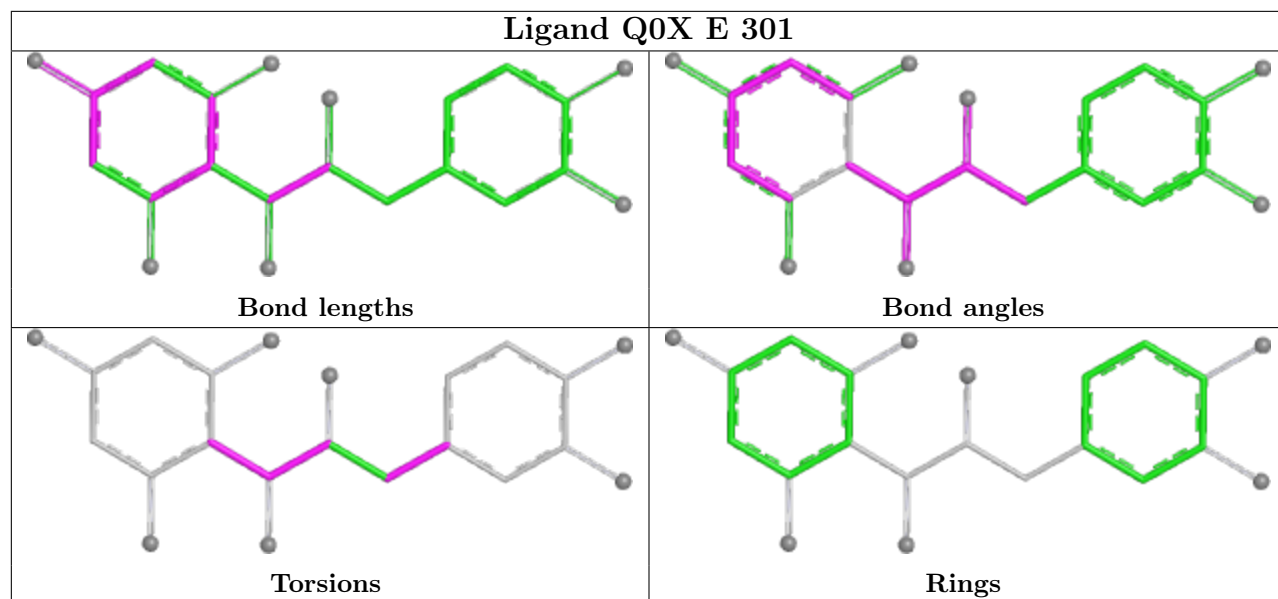


Ligand Q0X D 301



Ligand Q0X A 301





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.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.