



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2025 – 12:10 PM EST

PDB ID : 9BB0
Title : D-Dopachrome Tautomerase with 4-Hydroxyphenylpyruvate Bound in Catalytic Site at Atomic (0.98 Angstrom) Resolution
Authors : Parkins, A.; Argueta, C.; Pantouris, G.
Deposited on : 2024-04-05
Resolution : 0.98 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 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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

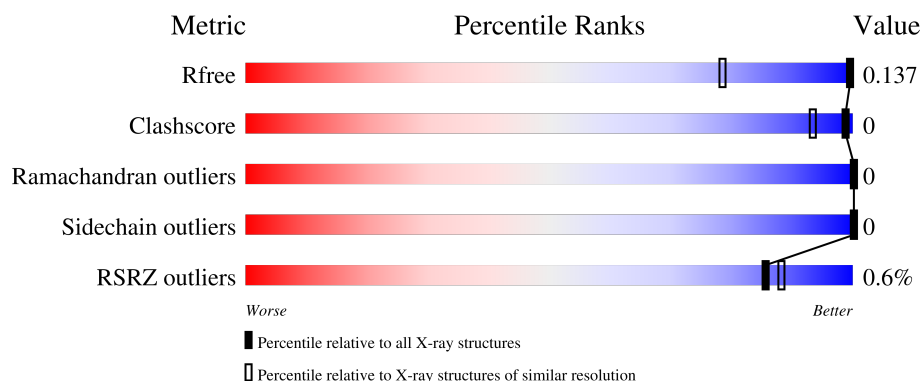
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


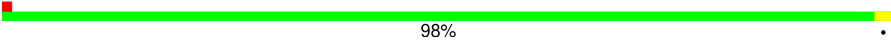
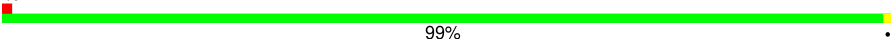
The reported resolution of this entry is 0.98 Å.

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}	164625	1026 (1.02-0.94)
Clashscore	180529	1154 (1.02-0.94)
Ramachandran outliers	177936	1094 (1.02-0.94)
Sidechain outliers	177891	1095 (1.02-0.94)
RSRZ outliers	164620	1025 (1.02-0.94)

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	117	 100%
1	BBB	117	 98%
1	CCC	117	 99%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3384 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.

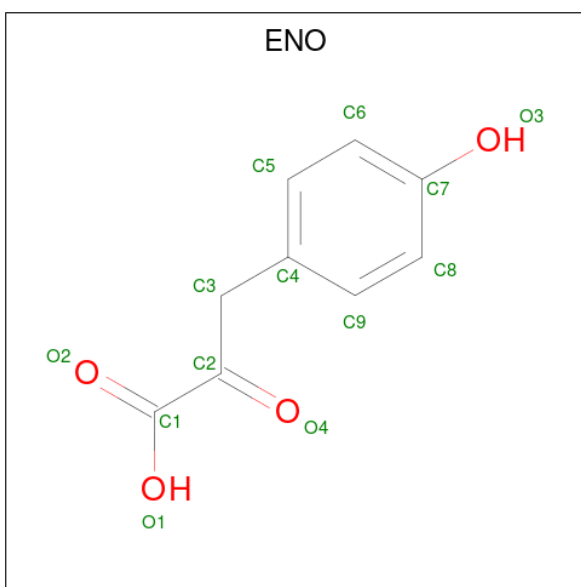
- Molecule 1 is a protein called D-dopachrome decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	117	Total	C	N	O	S	0	10	0
			952	606	161	181	4			
1	BBB	117	Total	C	N	O	S	0	9	0
			949	602	163	179	5			
1	CCC	117	Total	C	N	O	S	0	6	0
			929	593	157	175	4			

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

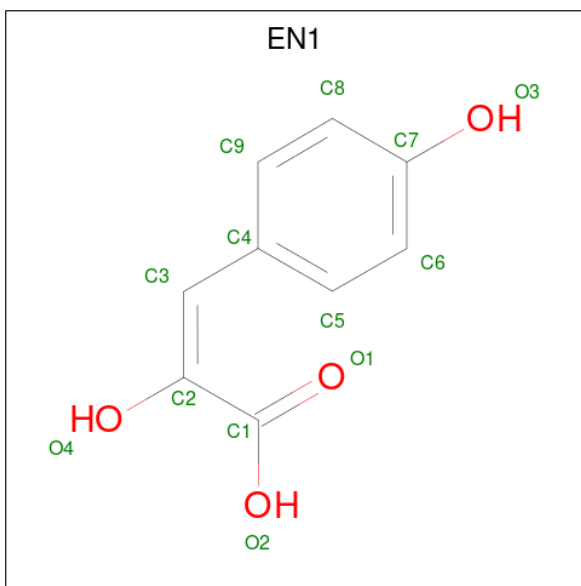
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	AAA	2	Total	Na	0	0
			2	2		
2	BBB	3	Total	Na	0	0
			3	3		
2	CCC	2	Total	Na	0	0
			2	2		

- Molecule 3 is 3-(4-HYDROXY-PHENYL)PYRUVIC ACID (three-letter code: ENO) (formula: C₉H₈O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	BBB	1	Total	C	O	0	1
			13	9	4		

- Molecule 4 is (2E)-2-hydroxy-3-(4-hydroxyphenyl)prop-2-enoic acid (three-letter code: EN1) (formula: $C_9H_8O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	BBB	1	Total	C	O	0	1
			13	9	4		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	173	Total 187	O 187	0	13
5	BBB	166	Total 181	O 181	0	14
5	CCC	147	Total 153	O 153	0	5

3 Residue-property plots

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

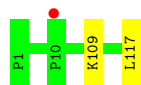
- Molecule 1: D-dopachrome decarboxylase

Chain AAA:  100%

There are no outlier residues recorded for this chain.

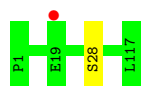
- Molecule 1: D-dopachrome decarboxylase

Chain BBB:  98%



- Molecule 1: D-dopachrome decarboxylase

Chain CCC:  99%



4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α , β , γ	83.77Å 83.77Å 40.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	72.54 – 0.98 72.54 – 0.98	Depositor EDS
% Data completeness (in resolution range)	99.1 (72.54-0.98) 62.3 (72.54-0.98)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	479.27 (at 0.99Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.132 , 0.147 0.127 , 0.137	Depositor DCC
R_{free} test set	10526 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	9.0	Xtriage
Anisotropy	1.068	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 36.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.046 for -h,-k,l 0.060 for h,-h-k,-l 0.058 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.99	EDS
Total number of atoms	3384	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.83 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.3189e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: ENO, EN1, NA

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	0.83	0/971	0.78	0/1316
1	BBB	0.82	0/968	0.77	0/1310
1	CCC	0.74	0/947	0.77	0/1283
All	All	0.80	0/2886	0.78	0/3909

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 [i](#)

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	AAA	952	0	941	0	0
1	BBB	949	0	945	2	0
1	CCC	929	0	933	1	0
2	AAA	2	0	0	0	0
2	BBB	3	0	0	0	0
2	CCC	2	0	0	0	0
3	BBB	13	0	6	0	0
4	BBB	13	0	5	1	0
5	AAA	187	0	0	0	0
5	BBB	181	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	CCC	153	0	0	0	0
All	All	3384	0	2830	2	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 0.

All (2) 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:BBB:117:LEU:HB3	1:CCC:28:SER:HB2	1.95	0.48
1:BBB:109:LYS:HD2	4:BBB:202[B]:EN1:O3	2.17	0.45

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 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	125/117 (107%)	121 (97%)	4 (3%)	0	100	100
1	BBB	124/117 (106%)	119 (96%)	5 (4%)	0	100	100
1	CCC	121/117 (103%)	118 (98%)	3 (2%)	0	100	100
All	All	370/351 (105%)	358 (97%)	12 (3%)	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 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	101/95 (106%)	101 (100%)	0	100	100
1	BBB	102/95 (107%)	102 (100%)	0	100	100
1	CCC	100/95 (105%)	100 (100%)	0	100	100
All	All	303/285 (106%)	303 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 7 are monoatomic - leaving 2 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$
3	ENO	BBB	201[A]	-	13,13,13	1.42	2 (15%)	16,17,17	2.06	6 (37%)
4	EN1	BBB	202[B]	-	13,13,13	5.83	3 (23%)	15,17,17	1.92	4 (26%)

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	ENO	BBB	201[A]	-	-	0/8/8/8	0/1/1/1
4	EN1	BBB	202[B]	-	-	2/8/8/8	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	BBB	202[B]	EN1	C3-C2	20.32	1.54	1.34
4	BBB	202[B]	EN1	C4-C3	-4.04	1.39	1.46
3	BBB	201[A]	ENO	C3-C4	-3.08	1.46	1.51
4	BBB	202[B]	EN1	O2-C1	-2.67	1.23	1.30
3	BBB	201[A]	ENO	C6-C7	2.39	1.43	1.39

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	BBB	202[B]	EN1	O4-C2-C3	-4.62	119.80	123.01
4	BBB	202[B]	EN1	O2-C1-C2	3.74	119.95	115.78
3	BBB	201[A]	ENO	C8-C9-C4	3.65	125.80	121.00
3	BBB	201[A]	ENO	C5-C6-C7	3.55	123.63	119.88
3	BBB	201[A]	ENO	C9-C8-C7	-3.05	116.65	119.88
3	BBB	201[A]	ENO	O1-C1-C2	2.85	121.48	113.59
3	BBB	201[A]	ENO	O2-C1-C2	-2.66	118.50	121.81
3	BBB	201[A]	ENO	C6-C5-C4	-2.43	117.80	121.00
4	BBB	202[B]	EN1	O4-C2-C1	2.21	116.26	114.17
4	BBB	202[B]	EN1	O2-C1-O1	-2.19	118.69	123.90

There are no chirality outliers.

All (2) torsion outliers are listed below:

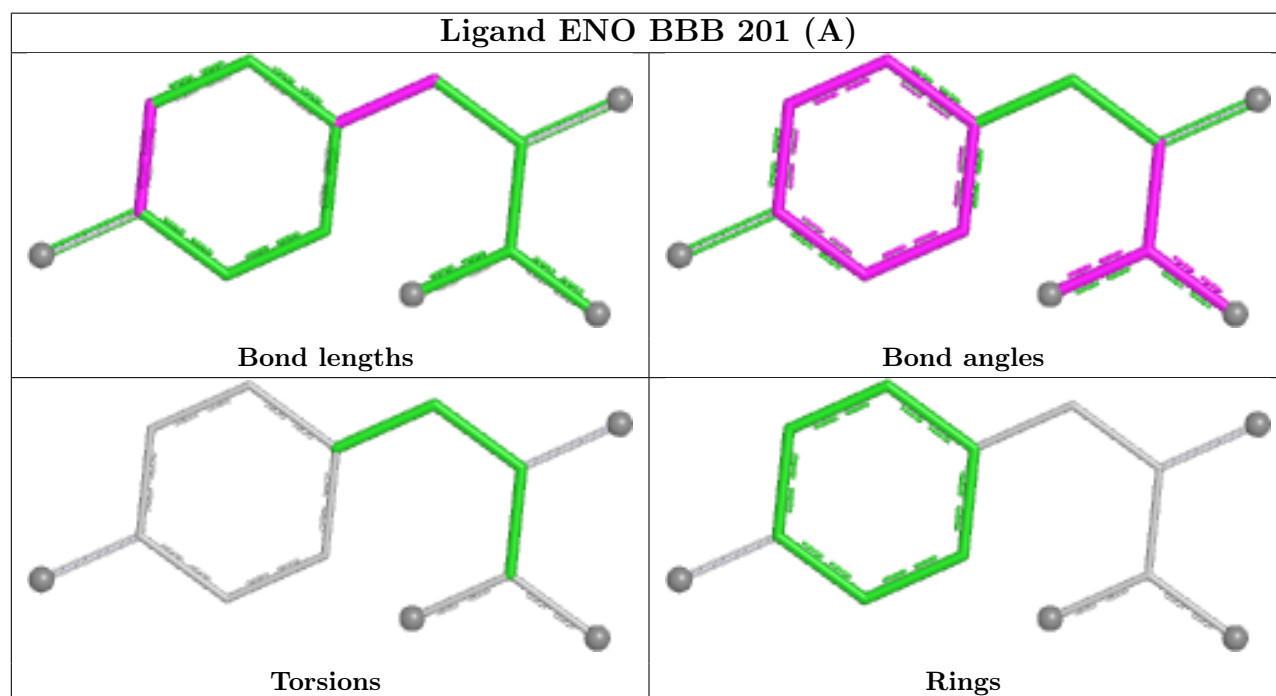
Mol	Chain	Res	Type	Atoms
4	BBB	202[B]	EN1	C2-C3-C4-C5
4	BBB	202[B]	EN1	C2-C3-C4-C9

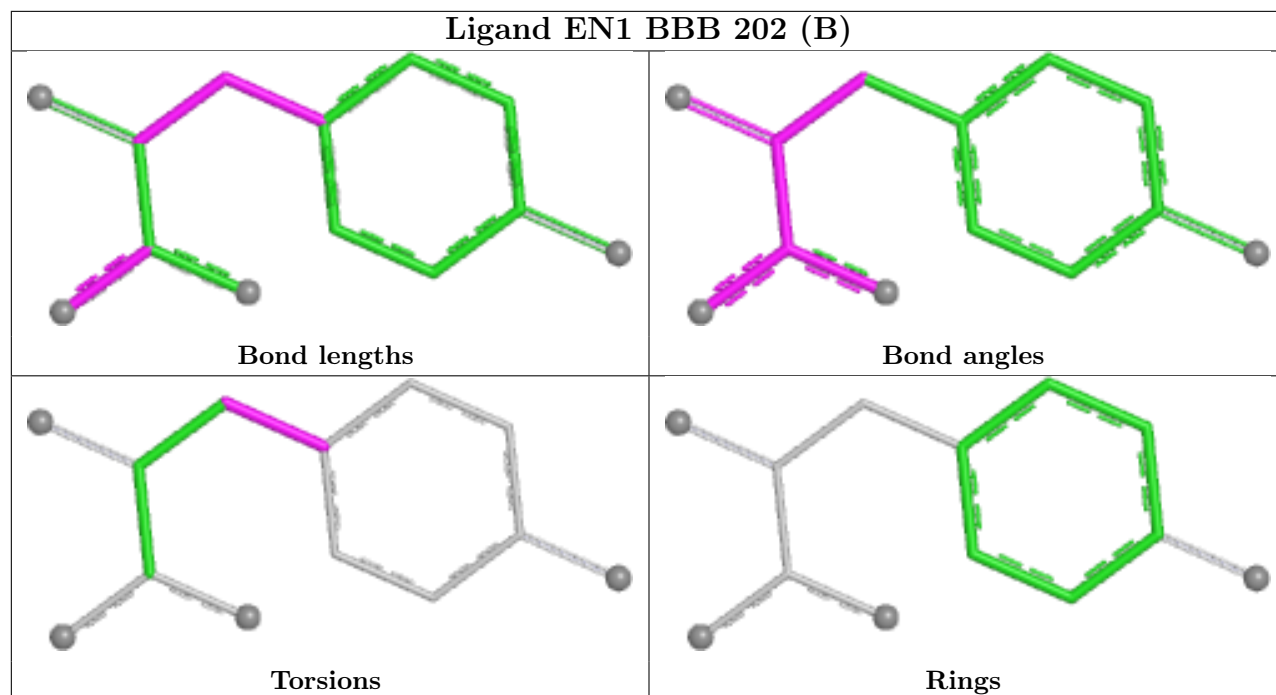
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	BBB	202[B]	EN1	1	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	117/117 (100%)	-0.15	0 100 100	4, 9, 16, 65	10 (8%)
1	BBB	117/117 (100%)	-0.05	1 (0%) 81 84	5, 10, 17, 111	9 (7%)
1	CCC	117/117 (100%)	-0.01	1 (0%) 81 84	5, 11, 23, 101	6 (5%)
All	All	351/351 (100%)	-0.07	2 (0%) 85 88	4, 10, 20, 111	25 (7%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	10[A]	PRO	3.2
1	CCC	19	GLU	2.4

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.

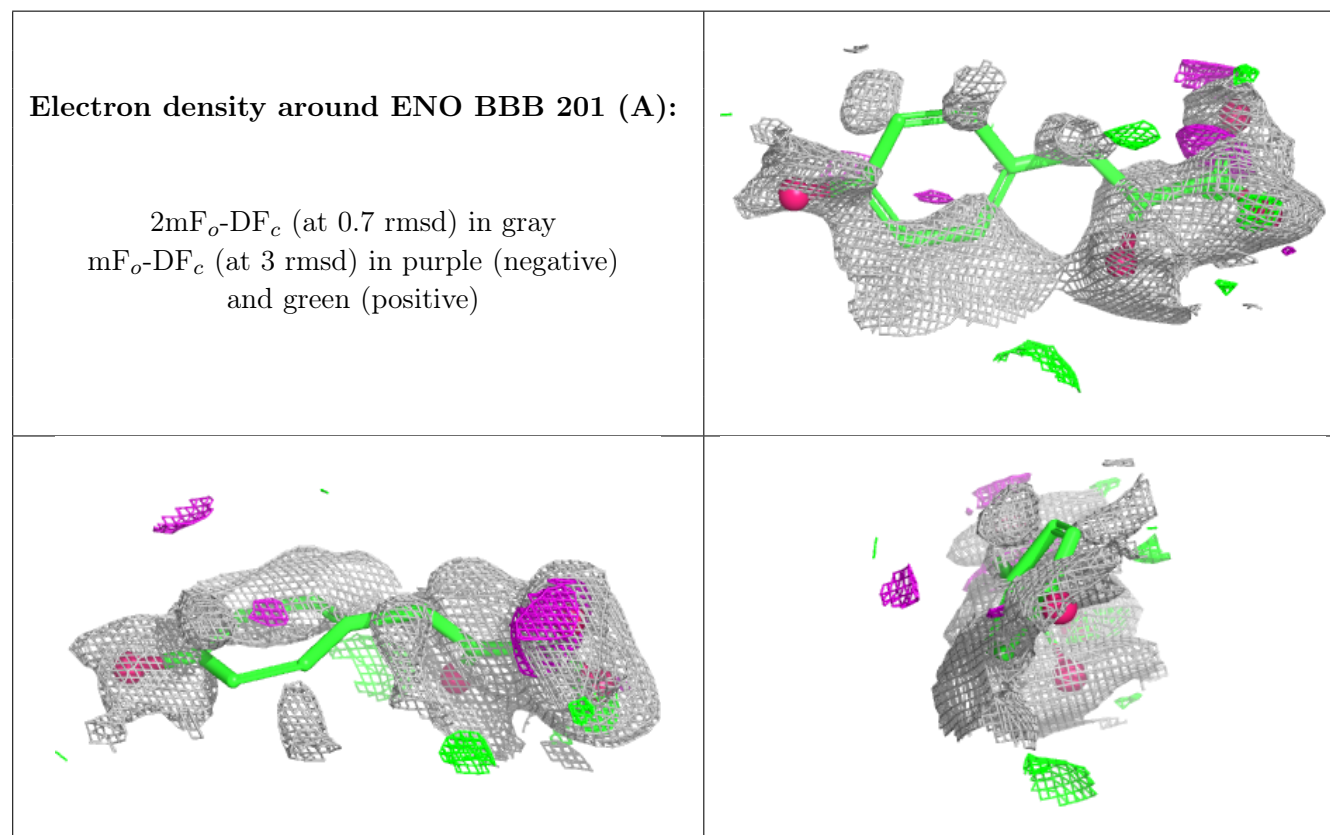
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NA	BBB	205	1/1	0.67	0.21	29,29,29,29	0

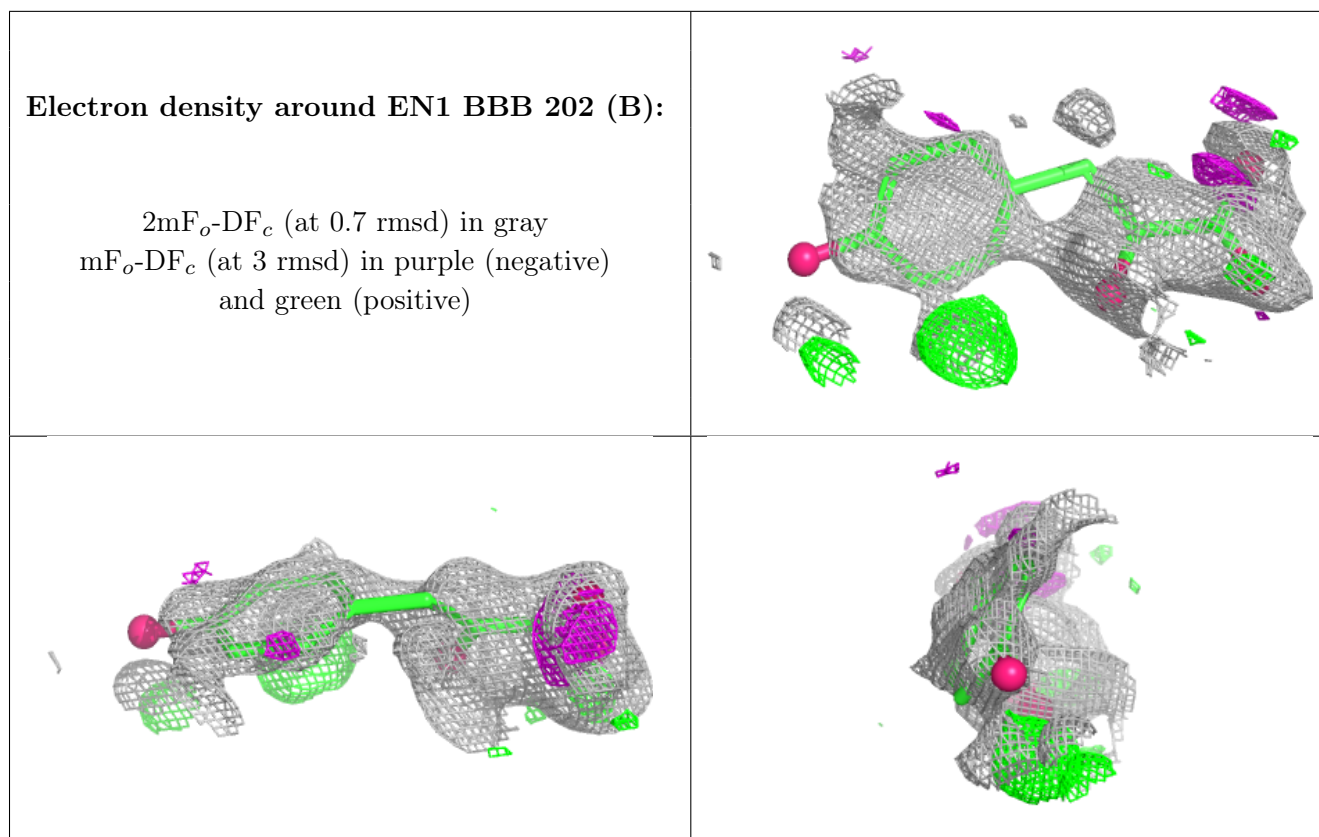
Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NA	CCC	202	1/1	0.89	0.08	25,25,25,25	0
3	ENO	BBB	201[A]	13/13	0.90	0.12	17,21,32,40	13
4	EN1	BBB	202[B]	13/13	0.90	0.14	24,38,44,55	13
2	NA	CCC	201	1/1	0.99	0.04	23,23,23,23	0
2	NA	BBB	203	1/1	0.99	0.05	18,18,18,18	0
2	NA	BBB	204	1/1	0.99	0.04	15,15,15,15	0
2	NA	AAA	201	1/1	0.99	0.07	17,17,17,17	0
2	NA	AAA	202	1/1	1.00	0.07	13,13,13,13	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





6.5 Other polymers [i](#)

There are no such residues in this entry.