



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 17, 2020 – 07:56 PM BST

PDB ID : 6ZBA
Title : Crystal structure of PDE4D2 in complex with inhibitor LEO39652
Authors : Akutsu, M.; Hakansson, M.; Welin, M.; Svensson, A.; Logan, D.T.; Sorensen, M.D.
Deposited on : 2020-06-08
Resolution : 1.60 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 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	:	2.14.5
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)	:	2.14.5

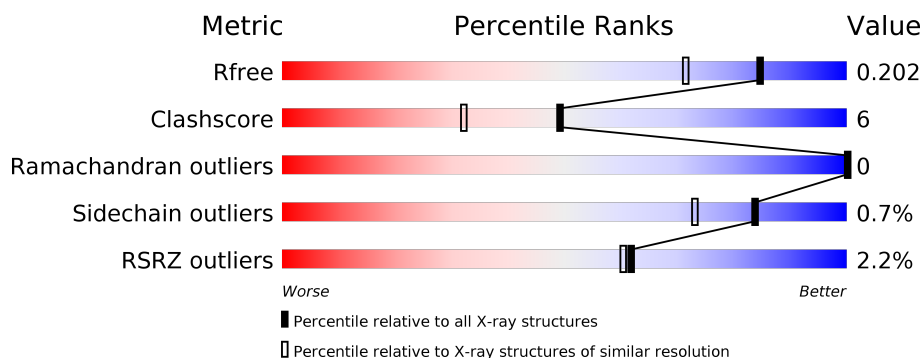
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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 on 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	360	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> % <div style="width: 100%; height: 10px; background-color: green;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 83% 7% 10% </div> </div>
1	BBB	360	<div> <div style="width: 4%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> 4% <div style="width: 100%; height: 10px; background-color: green;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 88% 5% 7% </div> </div>
1	CCC	360	<div> <div style="width: 4%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> 4% <div style="width: 100%; height: 10px; background-color: green;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 85% 7% 7% </div> </div>
1	DDD	360	<div> <div style="width: 100%; height: 10px; background-color: green;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> 84% 6% 10% </div> </div>

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	EDO	CCC	803	-	-	X	-
4	DMS	AAA	812	-	-	X	-
4	DMS	BBB	806	-	-	X	-
4	DMS	CCC	810[B]	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12640 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.

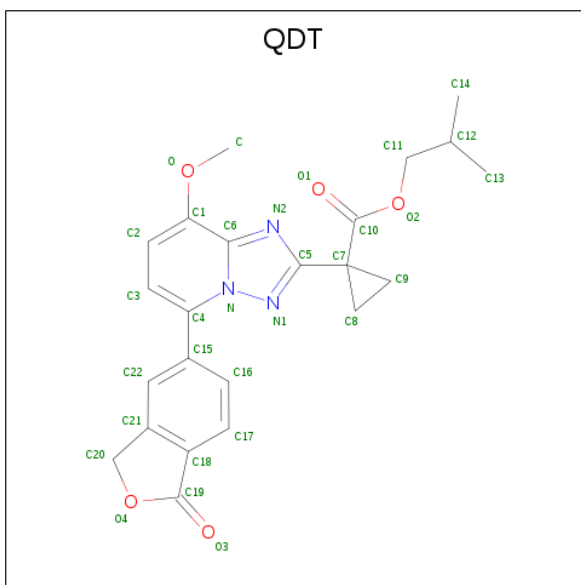
- Molecule 1 is a protein called cAMP-specific 3',5'-cyclic phosphodiesterase 4D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	324	Total	C	N	O	S	0	11	0
			2699	1709	459	515	16			
1	BBB	334	Total	C	N	O	S	0	11	0
			2783	1768	474	524	17			
1	CCC	334	Total	C	N	O	S	0	12	0
			2785	1767	472	527	19			
1	DDD	324	Total	C	N	O	S	0	10	0
			2695	1708	457	513	17			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	379	GLY	-	expression tag	UNP Q08499
AAA	380	MET	-	expression tag	UNP Q08499
BBB	379	GLY	-	expression tag	UNP Q08499
BBB	380	MET	-	expression tag	UNP Q08499
CCC	379	GLY	-	expression tag	UNP Q08499
CCC	380	MET	-	expression tag	UNP Q08499
DDD	379	GLY	-	expression tag	UNP Q08499
DDD	380	MET	-	expression tag	UNP Q08499

- Molecule 2 is 2-methylpropyl 1-[8-methoxy-5-(1-oxidanylidene-3 {H}-2-benzofuran-5-yl)-[1,2,4]triazolo[1,5-a]pyridin-2-yl]cyclopropane-1-carboxylate (three-letter code: QDT) (formula: C₂₃H₂₃N₃O₅) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	AAA	1	Total	C	N	O	0	0
			31	23	3	5		
2	BBB	1	Total	C	N	O	0	0
			31	23	3	5		
2	CCC	1	Total	C	N	O	0	0
			31	23	3	5		
2	DDD	1	Total	C	N	O	0	0
			31	23	3	5		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



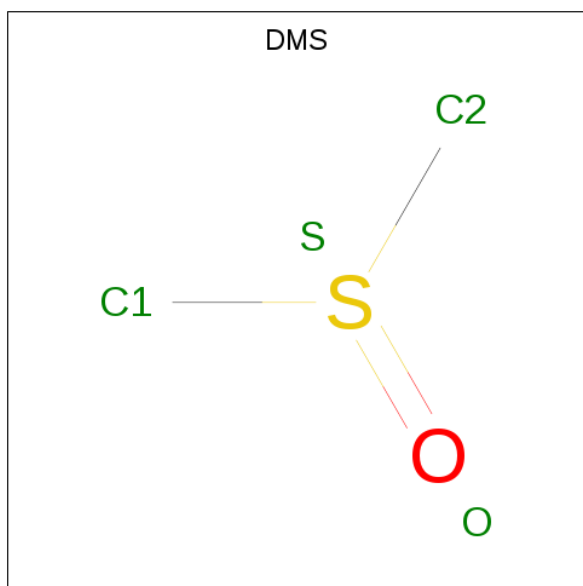
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total C O 4 2 2	0	0
3	AAA	1	Total C O 8 4 4	0	1
3	AAA	1	Total C O 4 2 2	0	0
3	AAA	1	Total C O 4 2 2	0	0
3	AAA	1	Total C O 4 2 2	0	0
3	AAA	1	Total C O 4 2 2	0	0
3	AAA	1	Total C O 4 2 2	0	0
3	AAA	1	Total C O 4 2 2	0	0
3	AAA	1	Total C O 4 2 2	0	0
3	AAA	1	Total C O 4 2 2	0	0
3	BBB	1	Total C O 4 2 2	0	0
3	BBB	1	Total C O 4 2 2	0	0
3	BBB	1	Total C O 4 2 2	0	0
3	BBB	1	Total C O 4 2 2	0	0
3	CCC	1	Total C O 4 2 2	0	0
3	CCC	1	Total C O 4 2 2	0	0
3	CCC	1	Total C O 4 2 2	0	0
3	CCC	1	Total C O 4 2 2	0	0
3	CCC	1	Total C O 4 2 2	0	0
3	CCC	1	Total C O 4 2 2	0	0
3	CCC	1	Total C O 4 2 2	0	0
3	CCC	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	DDD	1	Total	C	O	0	0
			4	2	2		
3	DDD	1	Total	C	O	0	0
			4	2	2		
3	DDD	1	Total	C	O	0	0
			4	2	2		
3	DDD	1	Total	C	O	0	0
			4	2	2		
3	DDD	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	AAA	1	Total	C	O	S	0	0
			4	2	1	1		
4	BBB	1	Total	C	O	S	0	0
			4	2	1	1		
4	CCC	1	Total	C	O	S	0	1
			8	4	2	2		
4	DDD	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	CCC	1	Total Mg 1 1	0	0
5	BBB	1	Total Mg 1 1	0	0
5	DDD	1	Total Mg 1 1	0	0
5	AAA	1	Total Mg 1 1	0	0

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	CCC	1	Total Zn 1 1	0	0
6	BBB	1	Total Zn 1 1	0	0
6	DDD	1	Total Zn 1 1	0	0
6	AAA	1	Total Zn 1 1	0	0

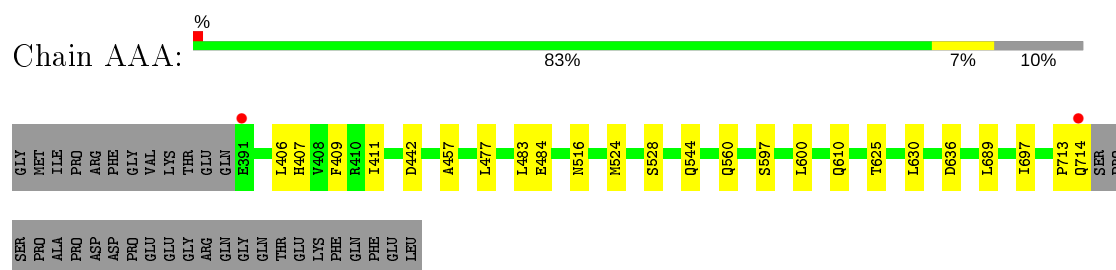
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	AAA	363	Total O 382 382	0	19
7	BBB	333	Total O 347 347	0	14
7	CCC	284	Total O 299 299	0	15
7	DDD	364	Total O 382 382	0	20

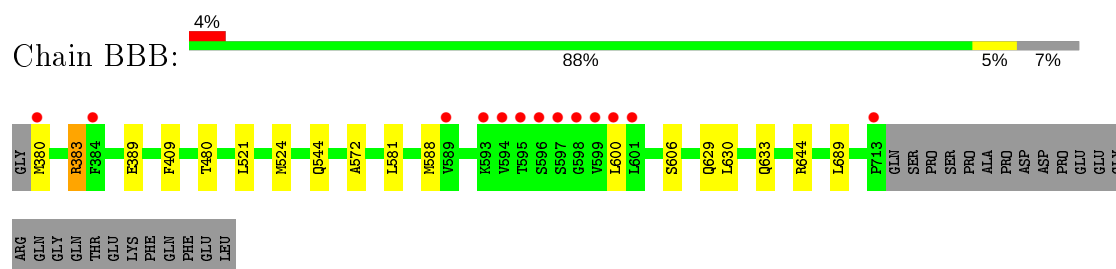
3 Residue-property plots [i](#)

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.

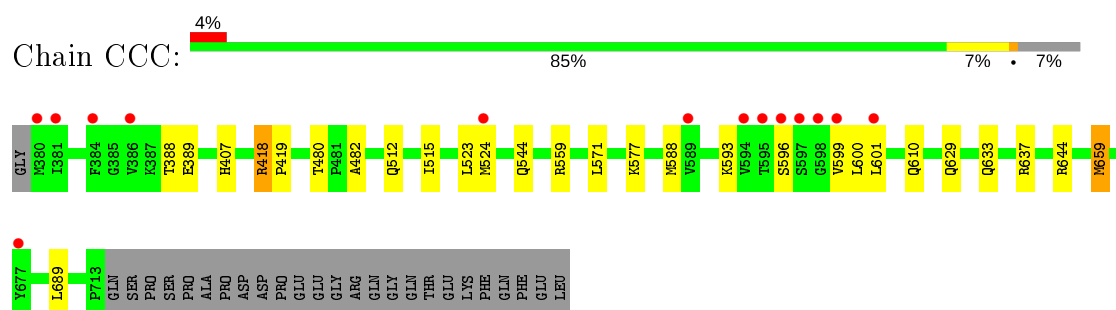
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



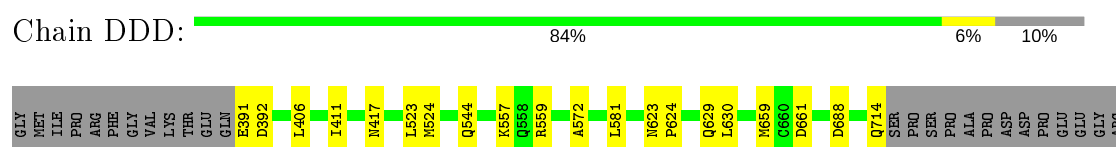
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



GLN
GLY
GLN
THR
GLU
LYS
PHE
GLN
PHE
GLU
LEU

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.03Å 111.87Å 159.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	79.94 – 1.60 79.81 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (79.94-1.60) 99.9 (79.81-1.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.162 , 0.192 0.174 , 0.202	Depositor DCC
R_{free} test set	11947 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	23.4	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 53.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12640	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: QDT, MG, DMS, ZN, EDO

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	0.73	0/2762	0.79	0/3750
1	BBB	0.72	1/2848 (0.0%)	0.76	0/3863
1	CCC	0.72	0/2853	0.79	3/3870 (0.1%)
1	DDD	0.76	0/2755	0.78	2/3741 (0.1%)
All	All	0.73	1/11218 (0.0%)	0.78	5/15224 (0.0%)

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	AAA	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	389	GLU	CD-OE2	5.18	1.31	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CCC	637	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	DDD	559	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	CCC	637	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	DDD	559	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	CCC	559	ARG	NE-CZ-NH1	5.23	122.92	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AAA	713	PRO	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	AAA	2699	0	2662	32	0
1	BBB	2783	0	2769	18	0
1	CCC	2785	0	2762	46	0
1	DDD	2695	0	2659	38	0
2	AAA	31	0	0	0	0
2	BBB	31	0	0	0	0
2	CCC	31	0	0	2	0
2	DDD	31	0	0	8	0
3	AAA	44	0	66	8	0
3	BBB	16	0	24	2	0
3	CCC	32	0	48	6	0
3	DDD	24	0	36	2	0
4	AAA	4	0	6	4	0
4	BBB	4	0	6	5	0
4	CCC	8	0	12	9	0
4	DDD	4	0	6	2	0
5	AAA	1	0	0	0	0
5	BBB	1	0	0	0	0
5	CCC	1	0	0	0	0
5	DDD	1	0	0	0	0
6	AAA	1	0	0	0	0
6	BBB	1	0	0	0	0
6	CCC	1	0	0	0	0
6	DDD	1	0	0	0	0
7	AAA	382	0	0	17	0
7	BBB	347	0	0	8	0
7	CCC	299	0	0	14	0
7	DDD	382	0	0	13	0
All	All	12640	0	11056	131	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 6.

The worst 5 of 131 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:AAA:524[A]:MET:HE3	1:CCC:524[A]:MET:CE	1.48	1.43
1:AAA:524[A]:MET:CE	1:CCC:524[A]:MET:HE3	1.50	1.41
1:AAA:516[A]:ASN:ND2	7:AAA:901:HOH:O	1.66	1.28
1:AAA:544:GLN:NE2	1:BBB:544:GLN:OE1	1.81	1.13
1:AAA:524[A]:MET:CE	1:CCC:524[A]:MET:CE	2.12	1.09

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	333/360 (92%)	326 (98%)	7 (2%)	0	100	100
1	BBB	343/360 (95%)	334 (97%)	9 (3%)	0	100	100
1	CCC	344/360 (96%)	337 (98%)	7 (2%)	0	100	100
1	DDD	332/360 (92%)	327 (98%)	5 (2%)	0	100	100
All	All	1352/1440 (94%)	1324 (98%)	28 (2%)	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	307/327 (94%)	307 (100%)	0	100	100
1	BBB	316/327 (97%)	314 (99%)	2 (1%)	86	77
1	CCC	317/327 (97%)	311 (98%)	6 (2%)	57	34
1	DDD	306/327 (94%)	305 (100%)	1 (0%)	92	87
All	All	1246/1308 (95%)	1237 (99%)	9 (1%)	84	73

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	CCC	596	SER
1	DDD	629	GLN
1	CCC	659[A]	MET
1	CCC	418	ARG
1	CCC	601	LEU

Some 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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 46 ligands modelled in this entry, 8 are monoatomic - leaving 38 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	EDO	BBB	802	-	3,3,3	0.47	0	2,2,2	0.15	0
3	EDO	BBB	803	-	3,3,3	0.44	0	2,2,2	0.26	0
3	EDO	AAA	807	-	3,3,3	0.31	0	2,2,2	0.42	0
3	EDO	DDD	806	-	3,3,3	0.29	0	2,2,2	0.53	0
2	QDT	BBB	801	-	32,35,35	0.73	1 (3%)	40,53,53	1.33	3 (7%)
3	EDO	AAA	811	-	3,3,3	0.08	0	2,2,2	0.06	0
3	EDO	AAA	803[B]	-	3,3,3	0.14	0	2,2,2	0.40	0
3	EDO	DDD	807	-	3,3,3	0.35	0	2,2,2	0.34	0
3	EDO	DDD	803	-	3,3,3	0.23	0	2,2,2	0.69	0
3	EDO	CCC	806	-	3,3,3	0.15	0	2,2,2	0.43	0
3	EDO	DDD	805	-	3,3,3	0.11	0	2,2,2	0.43	0
3	EDO	CCC	808	-	3,3,3	0.39	0	2,2,2	0.33	0
2	QDT	DDD	801	-	32,35,35	0.77	1 (3%)	40,53,53	1.48	4 (10%)
3	EDO	BBB	804	-	3,3,3	0.25	0	2,2,2	0.26	0
3	EDO	BBB	805	-	3,3,3	0.17	0	2,2,2	0.43	0
4	DMS	CCC	810[A]	-	3,3,3	0.28	0	3,3,3	0.30	0
4	DMS	CCC	810[B]	-	3,3,3	0.13	0	3,3,3	0.31	0
3	EDO	DDD	804	-	3,3,3	0.36	0	2,2,2	0.12	0
3	EDO	CCC	809	-	3,3,3	0.26	0	2,2,2	0.14	0
3	EDO	CCC	802	-	3,3,3	0.38	0	2,2,2	0.32	0
2	QDT	CCC	801	-	32,35,35	0.72	2 (6%)	40,53,53	1.44	2 (5%)
2	QDT	AAA	801	-	32,35,35	0.93	2 (6%)	40,53,53	1.42	4 (10%)
3	EDO	DDD	802	-	3,3,3	0.13	0	2,2,2	0.30	0
3	EDO	AAA	810	-	3,3,3	0.28	0	2,2,2	0.76	0
3	EDO	AAA	808	-	3,3,3	0.20	0	2,2,2	0.29	0
3	EDO	CCC	807	-	3,3,3	0.34	0	2,2,2	0.25	0
3	EDO	AAA	802	-	3,3,3	0.17	0	2,2,2	0.17	0
3	EDO	CCC	803	-	3,3,3	0.13	0	2,2,2	0.30	0
3	EDO	CCC	805	-	3,3,3	0.25	0	2,2,2	0.42	0
3	EDO	AAA	804	-	3,3,3	0.41	0	2,2,2	0.42	0
3	EDO	AAA	809	-	3,3,3	0.24	0	2,2,2	0.19	0
3	EDO	CCC	804	-	3,3,3	0.40	0	2,2,2	0.28	0
4	DMS	AAA	812	-	3,3,3	0.26	0	3,3,3	0.68	0
3	EDO	AAA	806	-	3,3,3	0.40	0	2,2,2	0.42	0
4	DMS	DDD	808	-	3,3,3	0.09	0	3,3,3	0.49	0
4	DMS	BBB	806	-	3,3,3	0.56	0	3,3,3	0.65	0
3	EDO	AAA	805	-	3,3,3	0.23	0	2,2,2	0.26	0
3	EDO	AAA	803[A]	-	3,3,3	0.41	0	2,2,2	0.14	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
3	EDO	BBB	802	-	-	0/1/1/1	-
3	EDO	BBB	803	-	-	0/1/1/1	-
3	EDO	AAA	807	-	-	1/1/1/1	-
3	EDO	DDD	806	-	-	0/1/1/1	-
2	QDT	BBB	801	-	-	3/17/36/36	0/5/5/5
3	EDO	AAA	811	-	-	0/1/1/1	-
3	EDO	AAA	803[B]	-	-	0/1/1/1	-
3	EDO	DDD	807	-	-	0/1/1/1	-
3	EDO	DDD	803	-	-	1/1/1/1	-
3	EDO	CCC	806	-	-	1/1/1/1	-
3	EDO	DDD	805	-	-	1/1/1/1	-
3	EDO	CCC	808	-	-	1/1/1/1	-
2	QDT	DDD	801	-	-	4/17/36/36	0/5/5/5
3	EDO	BBB	804	-	-	0/1/1/1	-
3	EDO	BBB	805	-	-	1/1/1/1	-
3	EDO	DDD	804	-	-	0/1/1/1	-
3	EDO	CCC	809	-	-	0/1/1/1	-
3	EDO	CCC	802	-	-	0/1/1/1	-
2	QDT	CCC	801	-	-	7/17/36/36	0/5/5/5
2	QDT	AAA	801	-	-	4/17/36/36	0/5/5/5
3	EDO	DDD	802	-	-	0/1/1/1	-
3	EDO	AAA	810	-	-	1/1/1/1	-
3	EDO	AAA	808	-	-	1/1/1/1	-
3	EDO	CCC	807	-	-	0/1/1/1	-
3	EDO	AAA	802	-	-	0/1/1/1	-
3	EDO	CCC	803	-	-	1/1/1/1	-
3	EDO	CCC	805	-	-	1/1/1/1	-
3	EDO	AAA	804	-	-	0/1/1/1	-
3	EDO	AAA	809	-	-	0/1/1/1	-
3	EDO	CCC	804	-	-	0/1/1/1	-
3	EDO	AAA	806	-	-	0/1/1/1	-
3	EDO	AAA	805	-	-	0/1/1/1	-
3	EDO	AAA	803[A]	-	-	1/1/1/1	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	801	QDT	C3-C2	3.01	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	BBB	801	QDT	C3-C2	2.40	1.43	1.38
2	AAA	801	QDT	C6-N2	2.35	1.35	1.33
2	DDD	801	QDT	C3-C2	2.32	1.43	1.38
2	CCC	801	QDT	C3-C2	2.16	1.42	1.38

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	CCC	801	QDT	C7-C5-N2	-6.35	117.14	122.93
2	BBB	801	QDT	C2-C3-C4	5.23	123.03	118.53
2	AAA	801	QDT	C7-C5-N2	-5.23	118.16	122.93
2	DDD	801	QDT	C2-C3-C4	4.95	122.79	118.53
2	CCC	801	QDT	C2-C3-C4	4.63	122.50	118.53

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	DDD	801	QDT	O1-C10-C7-C5
2	CCC	801	QDT	C7-C10-O2-C11
3	AAA	807	EDO	O1-C1-C2-O2
3	BBB	805	EDO	O1-C1-C2-O2
3	DDD	803	EDO	O1-C1-C2-O2

There are no ring outliers.

17 monomers are involved in 48 short contacts:

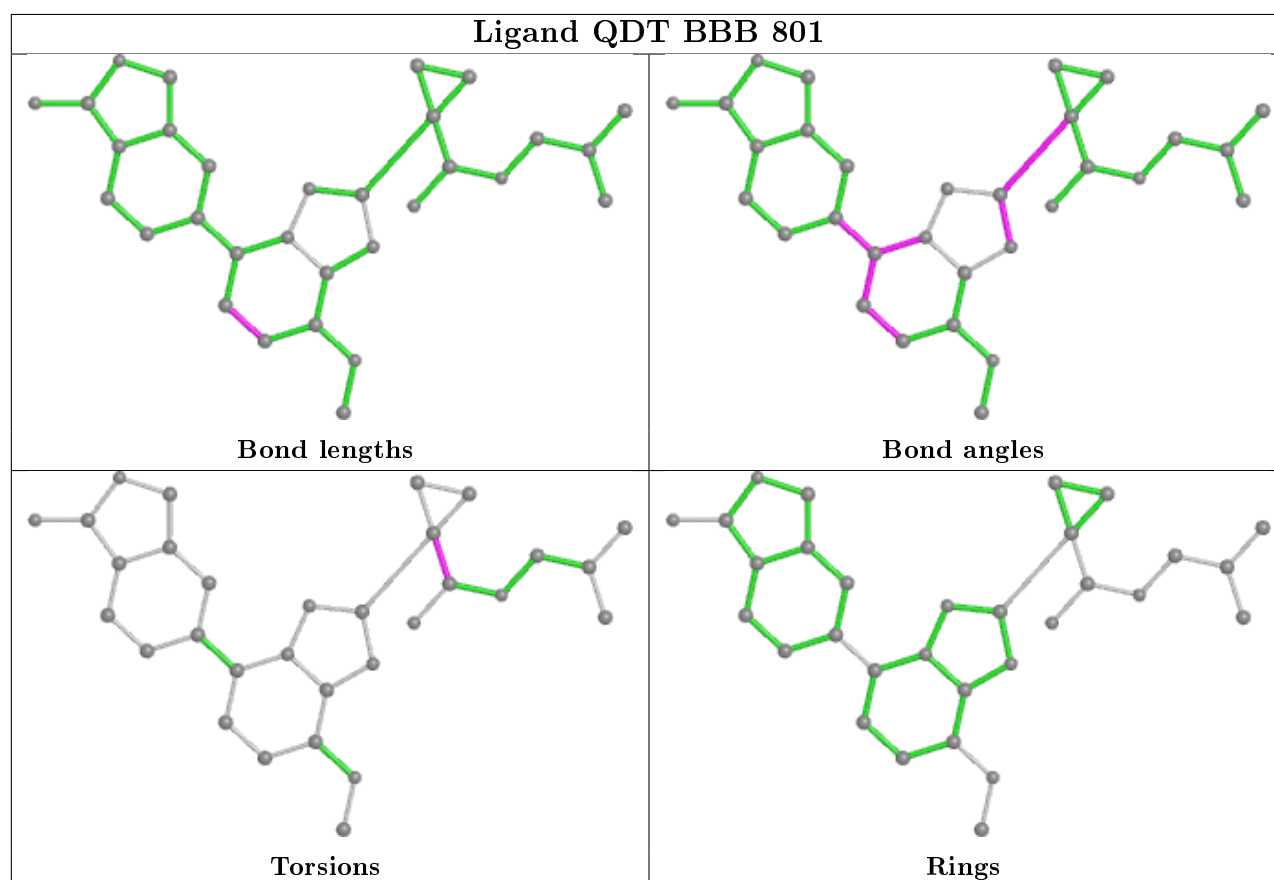
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AAA	807	EDO	1	0
3	AAA	803[B]	EDO	3	0
3	DDD	803	EDO	2	0
3	CCC	806	EDO	1	0
2	DDD	801	QDT	8	0
3	BBB	805	EDO	2	0
4	CCC	810[A]	DMS	3	0
4	CCC	810[B]	DMS	6	0
2	CCC	801	QDT	2	0
3	AAA	810	EDO	1	0
3	CCC	803	EDO	4	0
3	CCC	805	EDO	1	0
4	AAA	812	DMS	4	0

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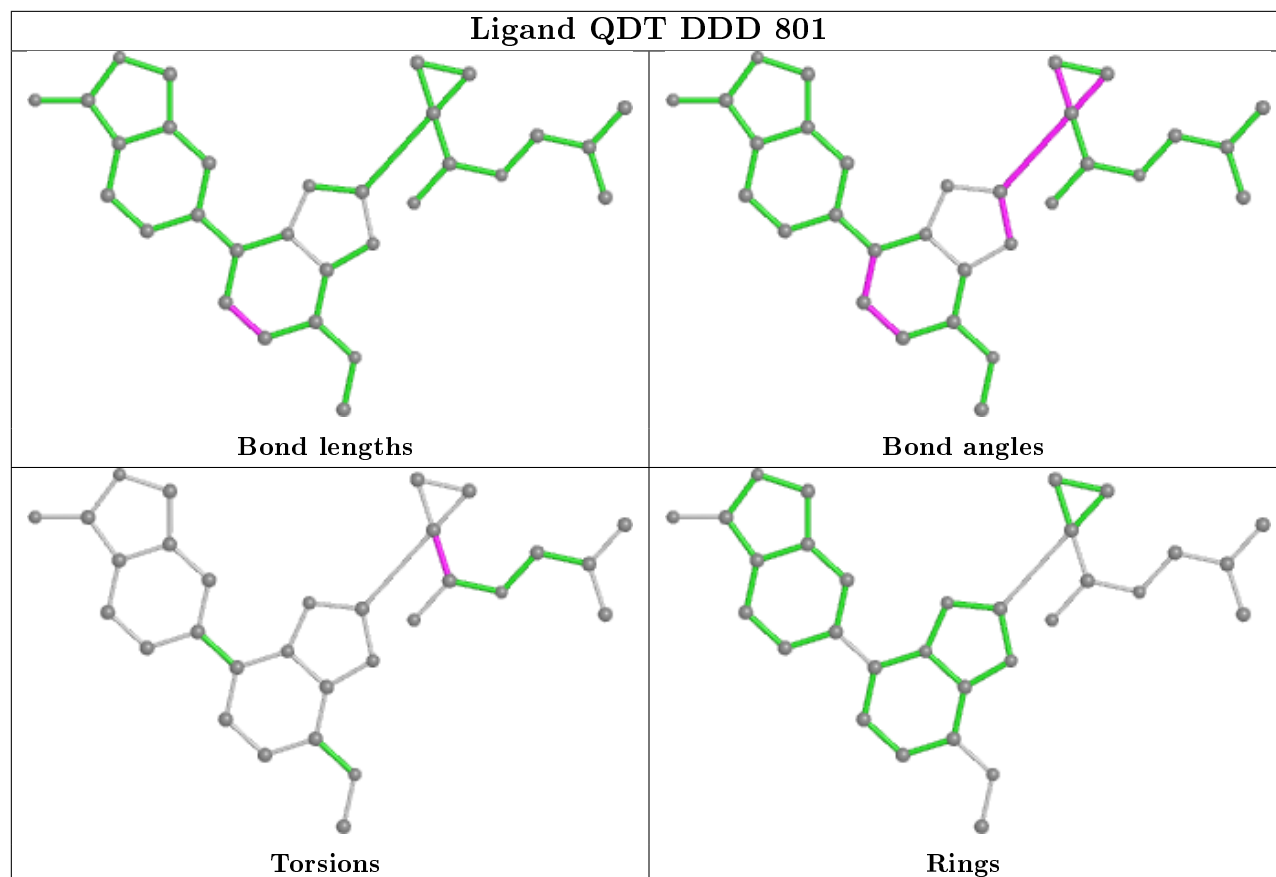
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	DDD	808	DMS	2	0
4	BBB	806	DMS	5	0
3	AAA	805	EDO	2	0
3	AAA	803[A]	EDO	1	0

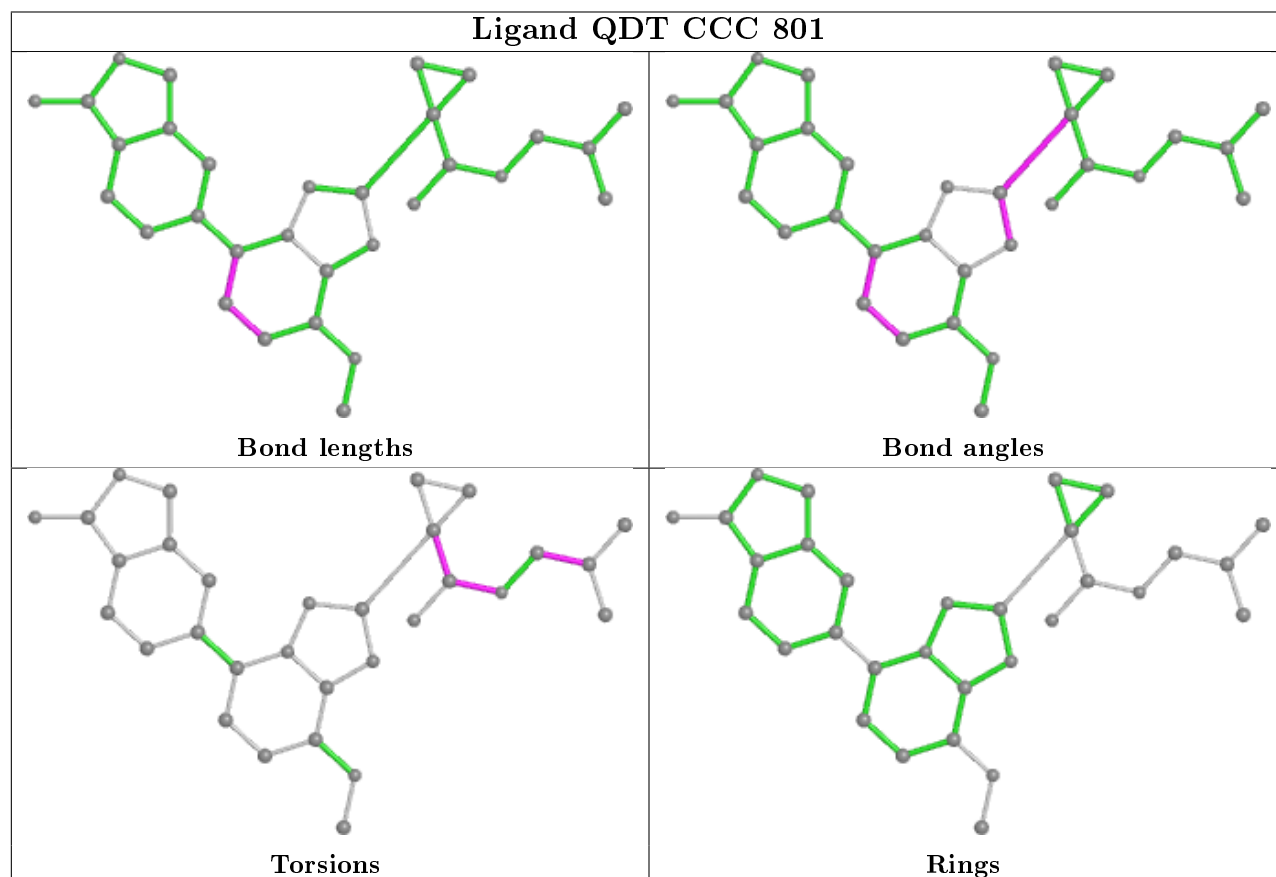
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

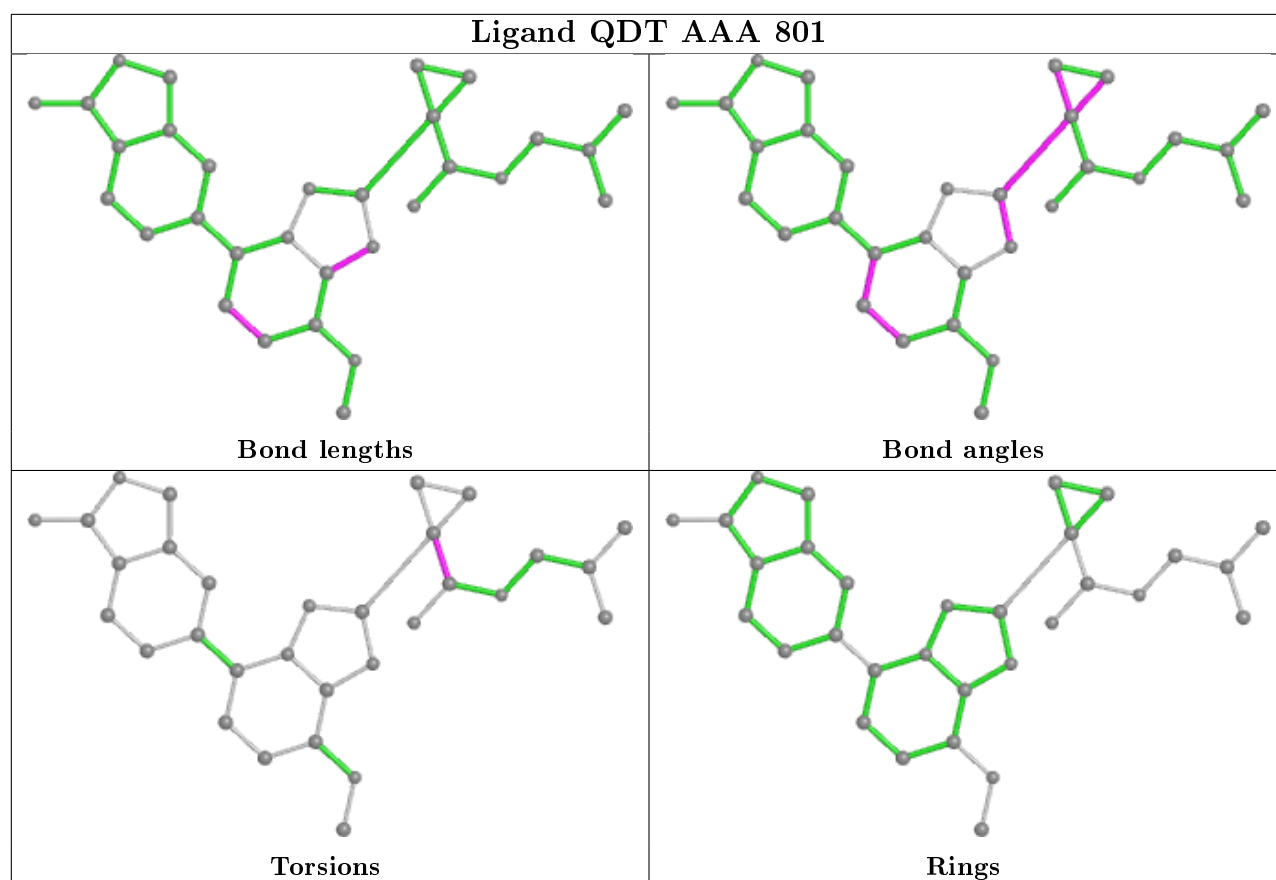


Ligand QDT DDD 801



Ligand QDT CCC 801





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	324/360 (90%)	-0.46	2 (0%) 89 89	16, 24, 41, 71	0
1	BBB	334/360 (92%)	-0.20	13 (3%) 39 36	16, 25, 53, 84	0
1	CCC	334/360 (92%)	-0.10	14 (4%) 36 33	16, 28, 59, 86	0
1	DDD	324/360 (90%)	-0.44	0 100 100	16, 25, 41, 73	1 (0%)
All	All	1316/1440 (91%)	-0.30	29 (2%) 62 60	16, 25, 49, 86	1 (0%)

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	598	GLY	7.5
1	BBB	597	SER	4.9
1	CCC	596	SER	4.9
1	BBB	599	VAL	4.1
1	CCC	599	VAL	4.0

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	DDD	803	4/4	0.74	0.18	41,47,48,50	0
2	QDT	BBB	801	31/31	0.82	0.16	27,34,45,48	31
3	EDO	CCC	808	4/4	0.83	0.10	45,45,46,50	0
2	QDT	CCC	801	31/31	0.83	0.14	32,37,50,53	31
3	EDO	AAA	805	4/4	0.84	0.17	41,48,50,51	0
3	EDO	AAA	806	4/4	0.85	0.11	42,42,44,47	0
2	QDT	AAA	801	31/31	0.85	0.13	26,32,43,44	31
3	EDO	DDD	806	4/4	0.88	0.11	42,43,44,48	0
3	EDO	CCC	803	4/4	0.89	0.33	43,45,48,54	0
2	QDT	DDD	801	31/31	0.89	0.13	27,32,47,49	31
3	EDO	CCC	807	4/4	0.89	0.15	49,50,51,51	0
3	EDO	DDD	805	4/4	0.90	0.11	50,53,56,66	0
3	EDO	AAA	808	4/4	0.90	0.13	56,56,57,62	0
3	EDO	AAA	809	4/4	0.91	0.11	36,37,37,40	0
3	EDO	CCC	804	4/4	0.91	0.09	31,33,33,34	0
3	EDO	DDD	807	4/4	0.91	0.10	32,34,36,37	0
3	EDO	BBB	805	4/4	0.91	0.09	37,41,46,51	0
3	EDO	BBB	804	4/4	0.93	0.10	32,36,36,38	0
3	EDO	CCC	805	4/4	0.93	0.09	28,31,33,41	0
3	EDO	CCC	802	4/4	0.93	0.14	41,41,42,45	0
3	EDO	CCC	809	4/4	0.94	0.07	30,30,32,36	0
3	EDO	CCC	806	4/4	0.94	0.08	44,49,50,50	0
3	EDO	DDD	804	4/4	0.94	0.08	39,39,40,43	0
3	EDO	AAA	804	4/4	0.95	0.10	25,28,31,33	0
3	EDO	AAA	807	4/4	0.95	0.10	32,41,44,59	0
3	EDO	BBB	802	4/4	0.95	0.07	28,32,33,41	0
3	EDO	BBB	803	4/4	0.95	0.08	26,28,28,31	0
3	EDO	AAA	810	4/4	0.95	0.09	29,34,40,43	0
3	EDO	AAA	811	4/4	0.96	0.14	39,45,48,49	0
3	EDO	DDD	802	4/4	0.96	0.08	29,30,31,41	0
3	EDO	AAA	803[A]	4/4	0.97	0.10	24,25,25,26	4
3	EDO	AAA	802	4/4	0.97	0.07	25,25,26,28	0
3	EDO	AAA	803[B]	4/4	0.97	0.10	23,23,23,26	4
5	MG	AAA	813	1/1	0.98	0.07	29,29,29,29	0
5	MG	CCC	811	1/1	0.98	0.08	31,31,31,31	0
4	DMS	CCC	810[A]	4/4	0.99	0.10	26,31,32,35	4
4	DMS	AAA	812	4/4	0.99	0.10	26,37,39,40	0
5	MG	BBB	807	1/1	0.99	0.06	27,27,27,27	0
5	MG	DDD	809	1/1	0.99	0.09	31,31,31,31	0
4	DMS	DDD	808	4/4	0.99	0.11	30,39,43,47	0
4	DMS	BBB	806	4/4	0.99	0.13	27,34,40,40	0
4	DMS	CCC	810[B]	4/4	0.99	0.10	24,27,27,33	4
6	ZN	BBB	808	1/1	1.00	0.08	19,19,19,19	1

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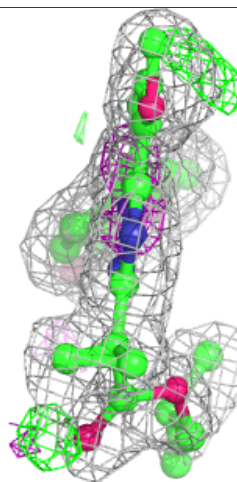
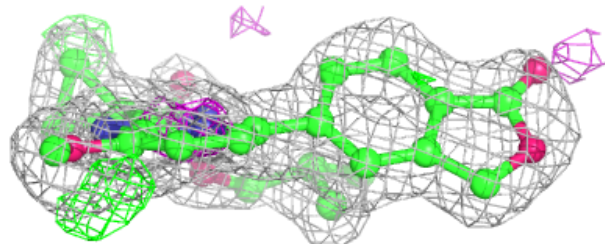
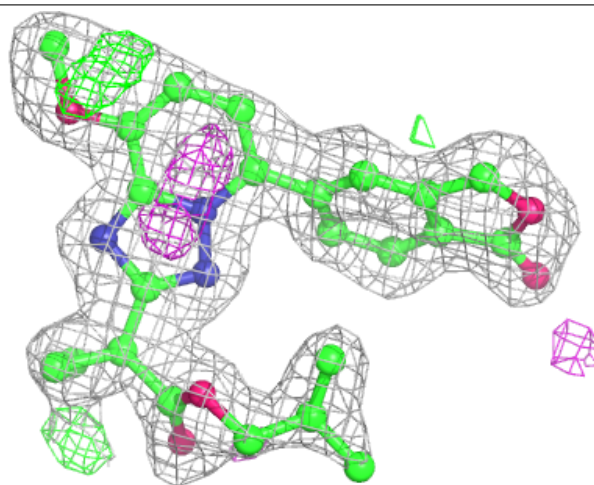
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	ZN	CCC	812	1/1	1.00	0.07	21,21,21,21	1
6	ZN	DDD	810	1/1	1.00	0.05	20,20,20,20	1
6	ZN	AAA	814	1/1	1.00	0.08	19,19,19,19	1

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.

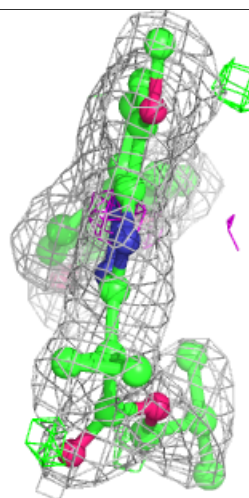
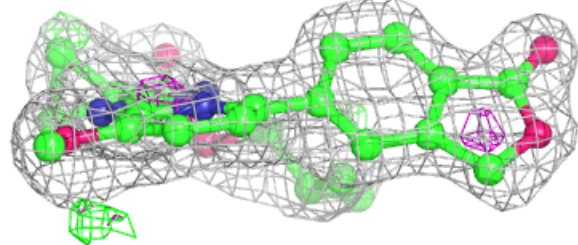
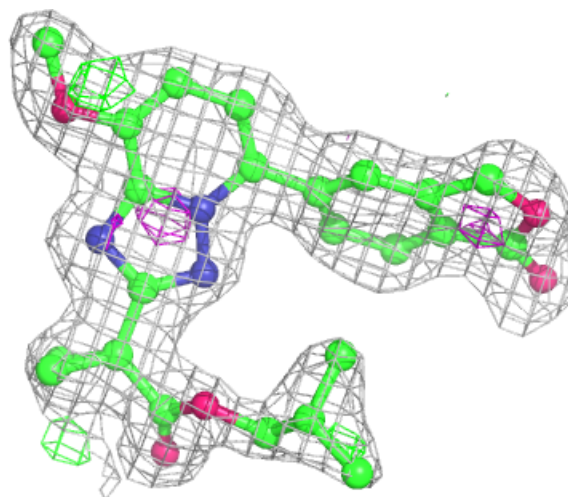
Electron density around QDT BBB 801:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



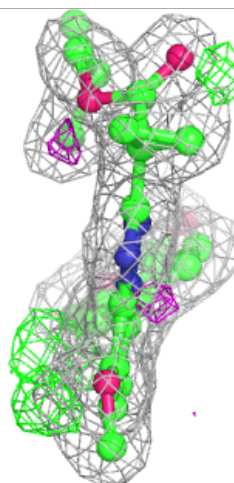
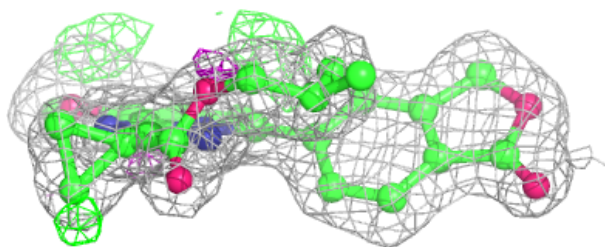
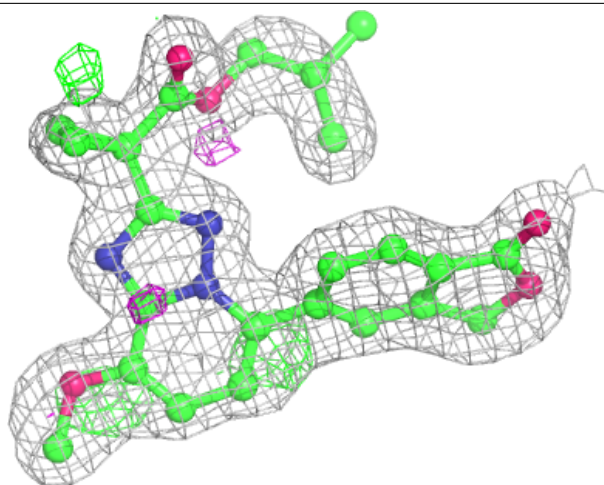
Electron density around QDT CCC 801:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



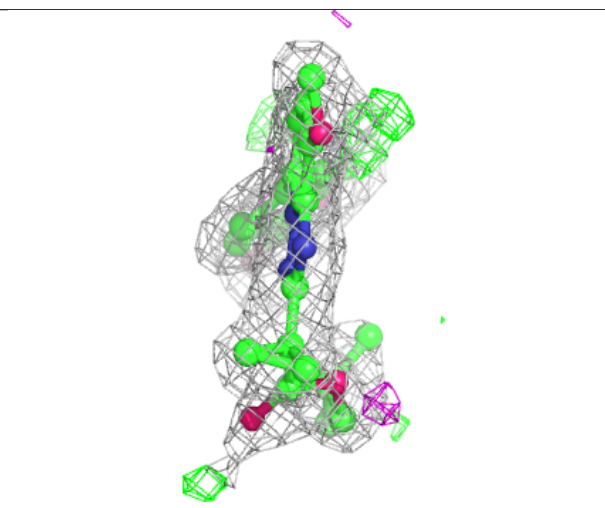
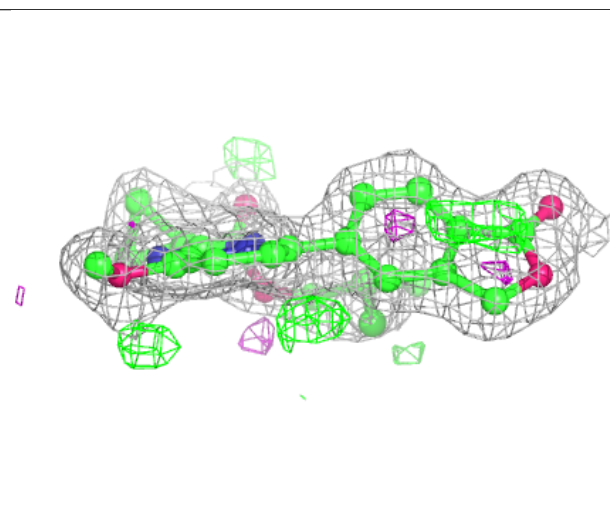
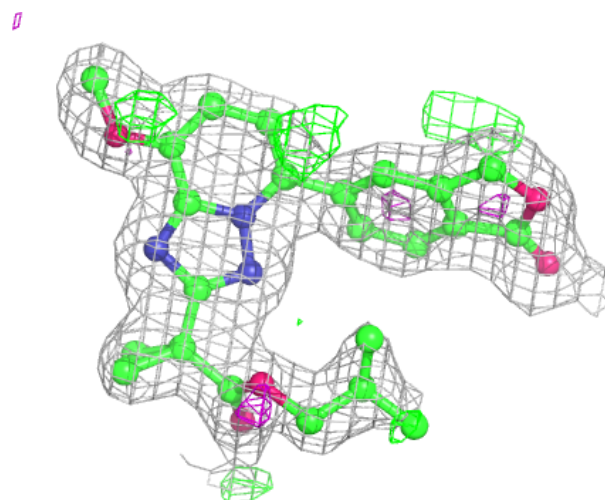
Electron density around QDT AAA 801:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around QDT DDD 801:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.