



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 3, 2025 – 05:33 PM JST

PDB ID : 8ZQ2  
Title : The crystal structure of PDE4D with isoaurostatin derivatives 2-1  
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Deposited on : 2024-05-31  
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](mailto: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>.

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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)	:	1.21
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)	:	2.40

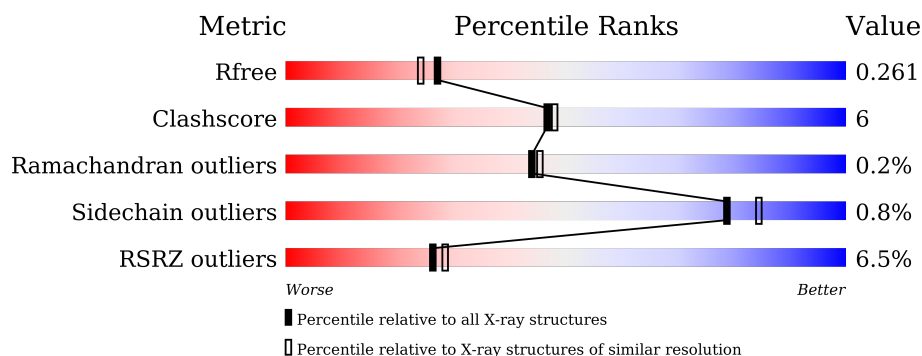
# 1 Overall quality at a glance

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))
$R_{free}$	164625	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (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  $\geq 3$ , 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	A	506	<div> <div>2%</div> <div>58%</div> <div>5%</div> <div>36%</div> </div>
1	B	506	<div> <div>7%</div> <div>55%</div> <div>9%</div> <div>36%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5507 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 3',5'-cyclic-AMP phosphodiesterase 4D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	0	0
			2624	1659	448	503	14			
1	B	324	Total	C	N	O	S	0	0	0
			2624	1659	448	503	14			

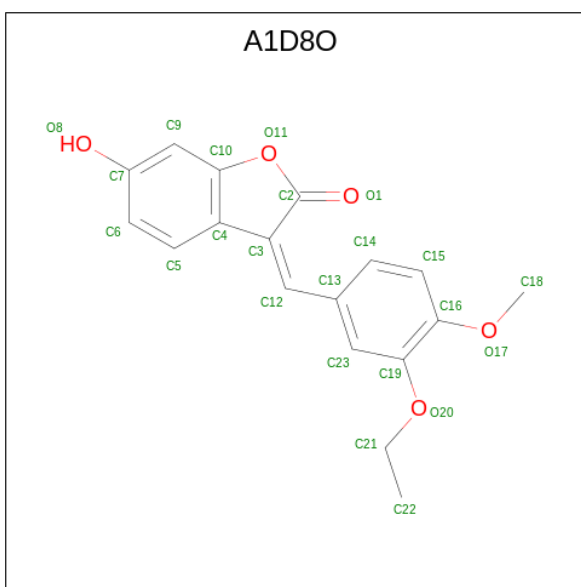
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is (3 {Z})-3-[(3-ethoxy-4-methoxy-phenyl)methylidene]-6-oxidanyl-1-benzofuran-2-one (three-letter code: A1D8O) (formula: C<sub>18</sub>H<sub>16</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			23	18	5		
4	B	1	Total	C	O	0	0
			23	18	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	127	Total	O	0	0
			127	127		
5	B	82	Total	O	0	0
			82	82		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.19Å 80.17Å 162.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.67 – 2.10 23.67 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.6 (23.67-2.10) 99.5 (23.67-2.10)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.60 (at 2.10Å)	Xtriage
Refinement program	REFMAC V8, PHENIX 1.10_2155	Depositor
R, $R_{free}$	0.210 , 0.251 0.219 , 0.261	Depositor DCC
$R_{free}$ test set	2277 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.0	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 41.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	5507	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: ZN, MG, A1D8O

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	0.28	0/2677	0.46	2/3636 (0.1%)
1	B	0.26	0/2677	0.45	0/3636
All	All	0.27	0/5354	0.46	2/7272 (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	A	342	ARG	NE-CZ-NH1	-8.07	116.27	120.30
1	A	342	ARG	NE-CZ-NH2	5.21	122.90	120.30

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	A	2624	0	2577	18	0
1	B	2624	0	2577	40	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	23	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	23	0	0	0	0
5	A	127	0	0	4	0
5	B	82	0	0	2	0
All	All	5507	0	5154	58	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.

All (58) 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:B:105:HIS:HB3	1:B:108:ARG:HD3	1.44	0.97
1:B:108:ARG:HD2	1:B:108:ARG:H	1.35	0.92
1:B:105:HIS:HB3	1:B:108:ARG:CD	2.08	0.81
1:B:338:GLU:OE2	1:B:342:ARG:NH2	2.13	0.81
1:B:108:ARG:HD2	1:B:108:ARG:N	1.95	0.81
1:B:147:MET:SD	5:B:773:HOH:O	2.44	0.74
1:A:252:LEU:O	5:A:701:HOH:O	2.05	0.74
1:B:293:THR:HG22	1:B:295:SER:H	1.57	0.69
1:B:292:VAL:HG12	1:B:298:LEU:HA	1.75	0.67
1:B:282:ASP:HB3	1:B:308:GLN:OE1	1.95	0.66
1:B:105:HIS:CB	1:B:108:ARG:HD3	2.24	0.63
1:B:104:LEU:HD22	1:B:170:GLN:HG3	1.83	0.59
1:A:254:LYS:HE2	1:A:254:LYS:HA	1.85	0.59
1:B:107:PHE:H	1:B:108:ARG:HH11	1.51	0.58
1:A:105:HIS:HE1	1:A:107:PHE:HB2	1.70	0.56
1:B:108:ARG:H	1:B:108:ARG:CD	2.16	0.56
1:A:338:GLU:HG3	5:A:818:HOH:O	2.06	0.56
1:A:105:HIS:CE1	1:A:107:PHE:HB2	2.42	0.55
1:B:182:GLU:N	5:B:703:HOH:O	2.40	0.55
1:B:107:PHE:N	1:B:108:ARG:HH11	2.06	0.53
1:B:293:THR:HG22	1:B:295:SER:N	2.24	0.52
1:B:87:GLU:HG3	1:B:90:ASP:H	1.76	0.51
1:B:105:HIS:HB3	1:B:108:ARG:NE	2.26	0.50
1:B:345:ASP:OD1	1:B:348:ARG:NH2	2.45	0.50
1:B:185:PHE:O	1:B:189:GLU:HB2	2.12	0.49
1:B:177:SER:HA	1:B:182:GLU:HB2	1.95	0.49
1:B:107:PHE:H	1:B:108:ARG:NH1	2.11	0.49
1:A:104:LEU:HD22	1:A:170:GLN:HG3	1.94	0.48
1:B:105:HIS:C	1:B:108:ARG:HD3	2.33	0.48
1:B:182:GLU:HA	1:B:183:ALA:HA	1.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:LEU:O	1:B:178:THR:HG22	2.15	0.47
1:A:321:ASN:HB2	1:A:322:PRO:HD3	1.96	0.47
1:B:254:LYS:O	1:B:258:GLN:HG3	2.15	0.46
1:A:158:ALA:HB2	5:A:818:HOH:O	2.16	0.46
1:A:130:ASP:HA	1:A:133:LYS:NZ	2.31	0.46
1:B:321:ASN:HB2	1:B:322:PRO:HD3	1.98	0.46
1:B:254:LYS:HD3	1:B:258:GLN:OE1	2.17	0.45
1:B:275:LYS:HA	1:B:275:LYS:HD2	1.80	0.45
1:B:104:LEU:HG	1:B:105:HIS:N	2.33	0.43
1:B:306:ARG:HH11	1:B:306:ARG:HG3	1.83	0.43
1:B:316:CYS:HB3	1:B:381:TRP:CZ2	2.54	0.43
1:B:189:GLU:HG2	1:B:263:MET:SD	2.59	0.42
1:A:105:HIS:CD2	5:A:710:HOH:O	2.72	0.42
1:A:176:LEU:HD13	1:A:190:ILE:HG23	2.01	0.42
1:A:364:SER:OG	1:A:367:LYS:HB2	2.20	0.42
1:A:301:ASP:HB3	1:A:302:ASN:HD22	1.85	0.42
1:B:121:ILE:HD12	1:B:166:ALA:HB1	2.02	0.42
1:A:348:ARG:NH2	1:A:360:LYS:HE2	2.35	0.41
1:B:396:LEU:O	1:B:400:GLU:HG3	2.20	0.41
1:B:290:LYS:HG3	1:B:298:LEU:HD11	2.02	0.41
1:A:300:LEU:HD13	1:A:306:ARG:HA	2.03	0.41
1:B:373:ILE:HA	1:B:377:VAL:HB	2.01	0.41
1:B:139:VAL:O	1:B:143:ILE:HG12	2.21	0.41
1:B:253:THR:O	1:B:257:ARG:HG3	2.20	0.41
1:A:286:MET:HB2	1:A:286:MET:HE3	1.95	0.41
1:B:136:LYS:HG3	1:B:251:ASN:ND2	2.35	0.41
1:A:201:ASP:O	1:A:204:HIS:HB2	2.22	0.40
1:A:373:ILE:HA	1:A:377:VAL:HB	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	322/506 (64%)	317 (98%)	5 (2%)	0	100	100
1	B	322/506 (64%)	314 (98%)	7 (2%)	1 (0%)	37	37
All	All	644/1012 (64%)	631 (98%)	12 (2%)	1 (0%)	44	45

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	186	THR

### 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	296/466 (64%)	293 (99%)	3 (1%)	73	79
1	B	296/466 (64%)	294 (99%)	2 (1%)	81	87
All	All	592/932 (64%)	587 (99%)	5 (1%)	79	84

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	130	ASP
1	A	297	VAL
1	A	301	ASP
1	B	108	ARG
1	B	254	LYS

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

Mol	Chain	Res	Type
1	B	258	GLN

### 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 6 ligands modelled in this entry, 4 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	$\# Z  > 2$
4	A1D8O	B	603	-	25,25,25	0.20	0	32,35,35	0.52	0
4	A1D8O	A	603	-	25,25,25	0.22	0	32,35,35	0.80	1 (3%)

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
4	A1D8O	B	603	-	-	2/9/21/21	0/3/3/3
4	A1D8O	A	603	-	-	0/9/21/21	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	603	A1D8O	C4-C3-C12	-2.29	121.51	132.05

There are no chirality outliers.

All (2) torsion outliers are listed below:

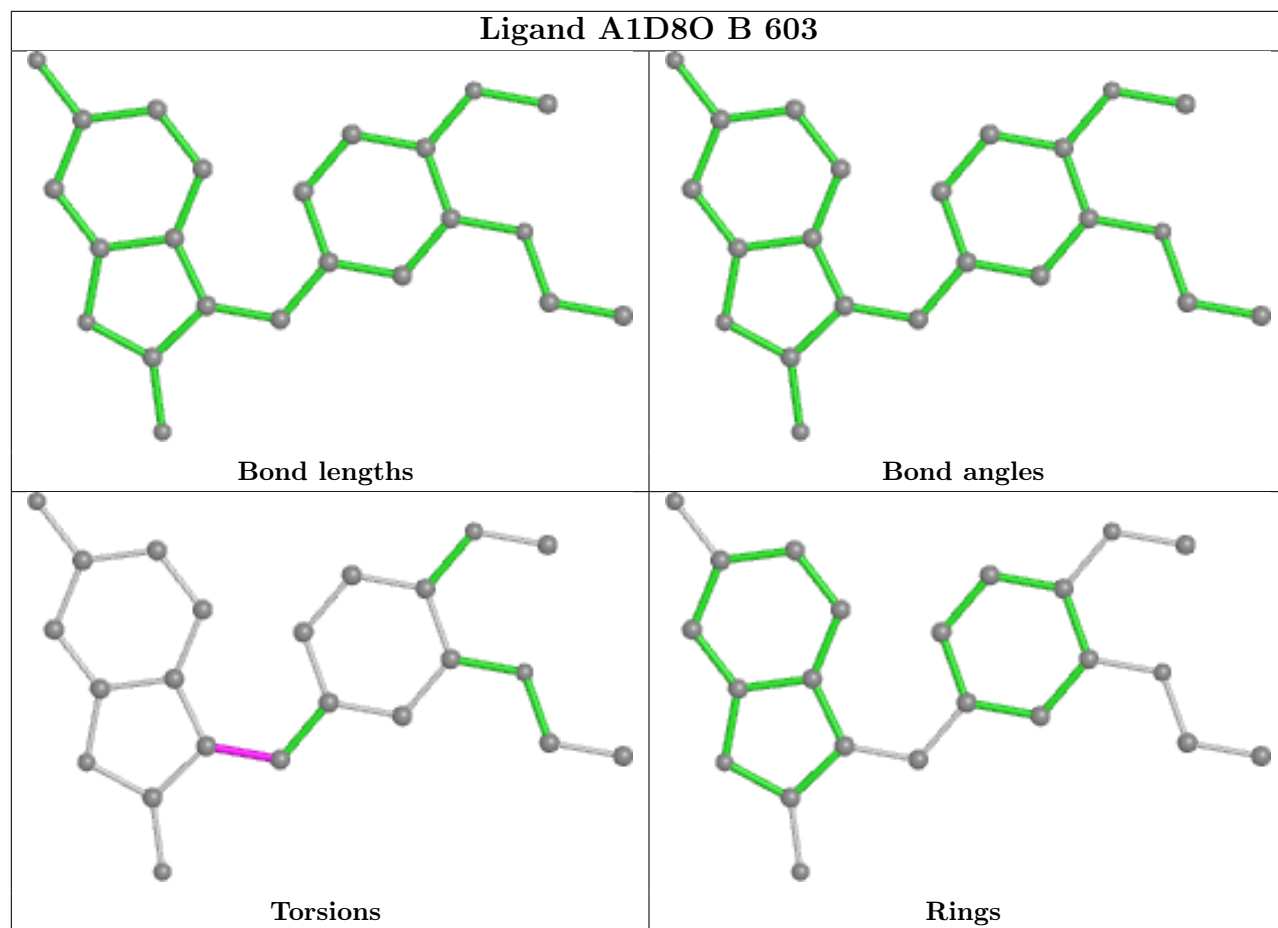
Mol	Chain	Res	Type	Atoms
4	B	603	A1D8O	C13-C12-C3-C4
4	B	603	A1D8O	C13-C12-C3-C2

There are no ring outliers.

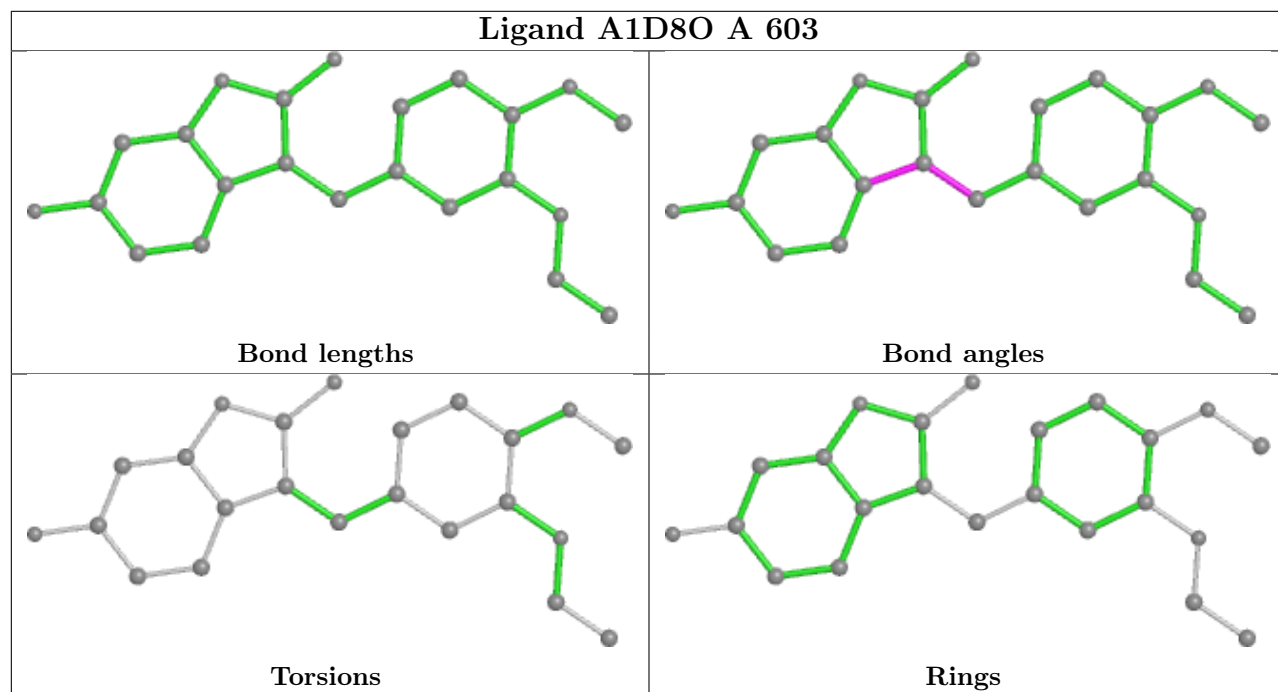
No monomer is involved in short contacts.

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 A1D8O B 603



## Ligand A1D8O A 603



## 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 ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	324/506 (64%)	-0.14	9 (2%) 55 57	8, 18, 38, 52	0
1	B	324/506 (64%)	0.49	33 (10%) 13 14	11, 26, 47, 73	0
All	All	648/1012 (64%)	0.18	42 (6%) 26 28	8, 22, 44, 73	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	294	SER	4.7
1	B	183	ALA	4.4
1	B	297	VAL	3.9
1	B	296	GLY	3.5
1	B	105	HIS	3.4
1	B	182	GLU	3.4
1	B	293	THR	3.4
1	B	180	ALA	3.3
1	B	91	VAL	3.2
1	B	108	ARG	3.1
1	B	184	VAL	3.1
1	A	133	LYS	3.0
1	B	179	PRO	3.0
1	A	130	ASP	3.0
1	B	295	SER	3.0
1	A	342	ARG	2.9
1	B	390	PRO	2.9
1	B	133	LYS	2.9
1	A	348	ARG	2.8
1	A	349	GLU	2.8
1	A	301	ASP	2.8
1	B	88	GLN	2.8
1	B	181	LEU	2.8
1	B	178	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	292	VAL	2.7
1	B	289	THR	2.5
1	B	132	LEU	2.5
1	A	105	HIS	2.4
1	B	90	ASP	2.3
1	B	87	GLU	2.3
1	B	104	LEU	2.3
1	B	362	ASN	2.3
1	B	185	PHE	2.2
1	B	351	GLY	2.1
1	B	287	VAL	2.1
1	B	298	LEU	2.1
1	B	389	HIS	2.1
1	A	87	GLU	2.1
1	B	131	LEU	2.1
1	A	363	ALA	2.0
1	B	186	THR	2.0
1	B	286	MET	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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
4	A1D8O	B	603	23/23	0.85	0.13	19,31,50,54	0
4	A1D8O	A	603	23/23	0.86	0.12	16,24,38,42	0
3	MG	A	602	1/1	0.96	0.06	10,10,10,10	0
2	ZN	B	601	1/1	0.99	0.04	19,19,19,19	0
2	ZN	A	601	1/1	1.00	0.01	16,16,16,16	0

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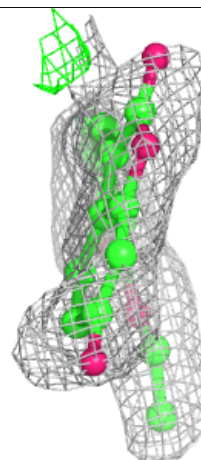
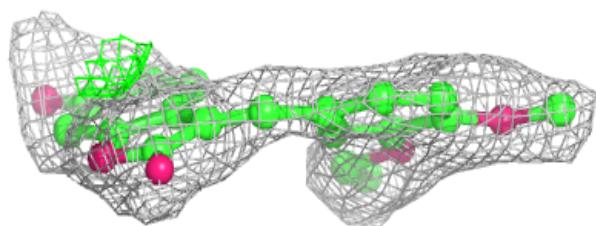
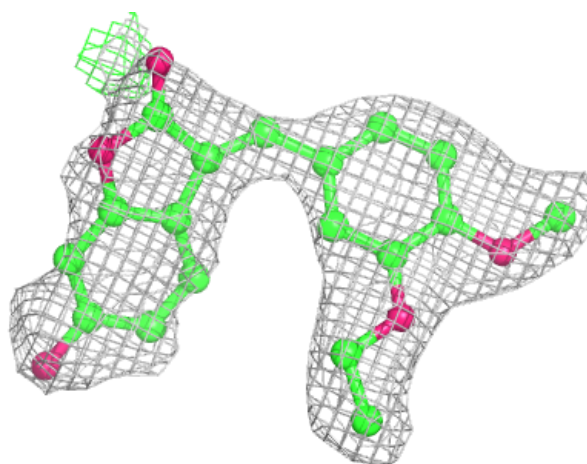
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	B	602	1/1	1.00	0.02	11,11,11,11	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.

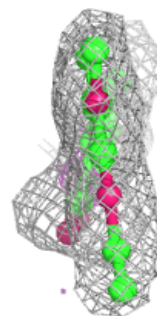
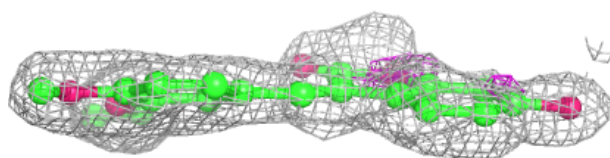
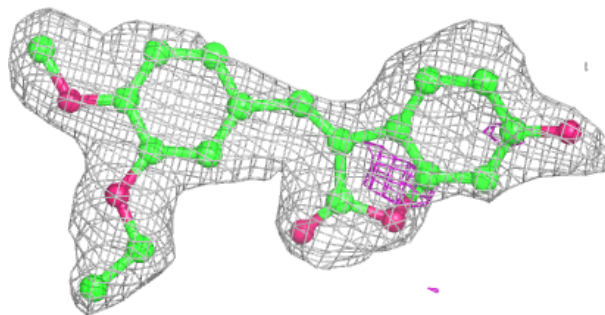
**Electron density around A1D8O B 603:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around A1D8O A 603:**

$2mF_o-DF_c$  (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.