WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

May 13, 2020 – 03:35 am BST

PDB ID	:	4KZI
Title	:	Crystal Structure of TR3 LBD in complex with DPDO
Authors	:	Li, F.; Zhang, Q.; Li, A.; Tian, X.; Cai, Q.; Wang, W.; Wang, Y.; Chen, H.; Xing, Y.; Wu, Q.; Lin, T.
Deposited on	:	2013-05-30
Resolution	:	2.41 Å(reported)

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

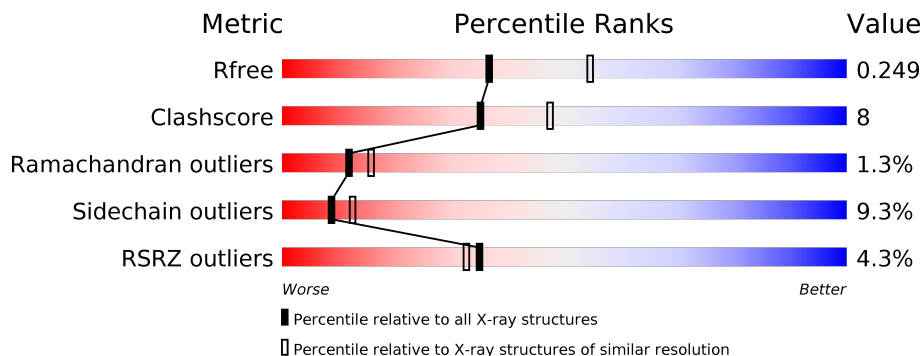|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.41 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	Percentile Ranks	Value
Rfree		0.249
Clashscore		8
Ramachandran outliers		1.3%
Sidechain outliers		9.3%
RSRZ outliers		4.3%

Worse　　　　　　　　　　　　　　　　*Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (2.44-2.40)

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 <=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	257	3%　　73%　　15%　•　10%
1	B	257	5%　　75%　　13%　•　9%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ZJ0	A	703	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3772 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 Nuclear receptor subfamily 4 group A member 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	234	Total	C	N	O	S	0	0	0
			1819	1175	309	328	7			
1	A	232	Total	C	N	O	S	0	0	0
			1822	1178	310	327	7			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	350	MET	-	expression tag	UNP P22736
B	599	LEU	-	expression tag	UNP P22736
B	600	GLU	-	expression tag	UNP P22736
B	601	HIS	-	expression tag	UNP P22736
B	602	HIS	-	expression tag	UNP P22736
B	603	HIS	-	expression tag	UNP P22736
B	604	HIS	-	expression tag	UNP P22736
B	605	HIS	-	expression tag	UNP P22736
B	606	HIS	-	expression tag	UNP P22736
A	350	MET	-	expression tag	UNP P22736
A	599	LEU	-	expression tag	UNP P22736
A	600	GLU	-	expression tag	UNP P22736
A	601	HIS	-	expression tag	UNP P22736
A	602	HIS	-	expression tag	UNP P22736
A	603	HIS	-	expression tag	UNP P22736
A	604	HIS	-	expression tag	UNP P22736
A	605	HIS	-	expression tag	UNP P22736
A	606	HIS	-	expression tag	UNP P22736

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

C3

OH O3

C1   C2

HO
O1

OH
O2

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total 6	C 3	O 3	0	0
2	A	1	Total 6	C 3	O 3	0	0
2	A	1	Total 6	C 3	O 3	0	0

- Molecule 3 is 1-(3,5-dimethoxyphenyl)decan-1-one (three-letter code: ZJ0) (formula: $C_{18}H_{28}O_3$).

ZJ0

C21

C5   O18

O19   C6   C4   C20

C7   C3

C2

C1

C9   O8

C11   C10

C13   C12

C15   C14

C16

C17
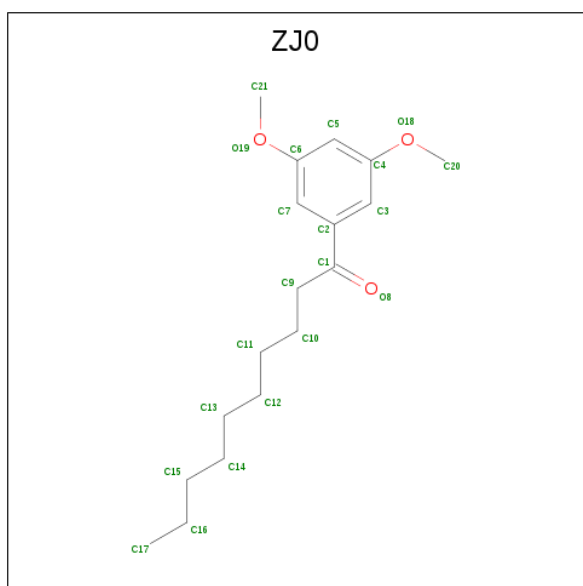
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 21	C 18	O 3	0	0

- Molecule 4 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	38	Total 38	O 38	0	0
4	A	54	Total 54	O 54	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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: Nuclear receptor subfamily 4 group A member 1
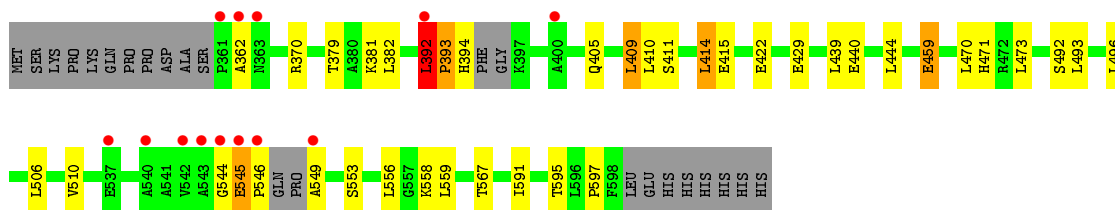
- Molecule 1: Nuclear receptor subfamily 4 group A member 1
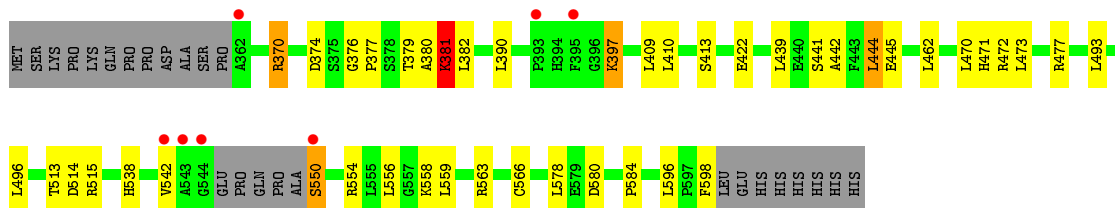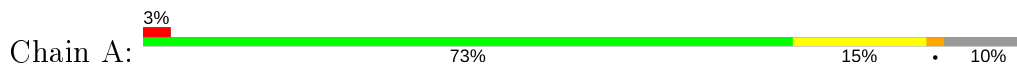
4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	74.72Å 76.51Å 128.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.28 – 2.41 37.25 – 2.41	Depositor EDS
% Data completeness (in resolution range)	99.1 (37.28-2.41) 99.2 (37.25-2.41)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.23 (at 2.39Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.206 , 0.249 0.206 , 0.249	Depositor DCC
R_{free} test set	1486 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	47.9	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 36.0	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.034 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3772	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, ZJ0

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	0.85	0/1860	0.83	0/2518
1	B	0.76	0/1857	0.86	1/2517 (0.0%)
All	All	0.81	0/3717	0.85	1/5035 (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	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	392	LEU	C-N-CD	-12.12	93.94	120.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	392	LEU	Peptide

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	1822	0	1869	44	1
1	B	1819	0	1848	17	1
2	A	12	0	16	1	0
2	B	6	0	8	0	0
3	A	21	0	28	23	0
4	A	54	0	0	4	0
4	B	38	0	0	2	0
All	All	3772	0	3769	61	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 8.

The worst 5 of 61 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:A:397:LYS:HD2	1:A:477:ARG:HH12	1.21	1.01
1:A:445:GLU:OE1	3:A:703:ZJ0:C9	2.15	0.94
3:A:703:ZJ0:H23	4:A:826:HOH:O	1.70	0.90
1:A:445:GLU:OE1	3:A:703:ZJ0:C10	2.23	0.87
1:A:514:ASP:O	3:A:703:ZJ0:H4	1.74	0.86

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)
1:B:459:GLU:OE1	1:A:580:ASP:OD2[3_544]	2.05	0.15

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	228/257 (89%)	221 (97%)	5 (2%)	2 (1%)	17	24
1	B	228/257 (89%)	219 (96%)	5 (2%)	4 (2%)	8	10
All	All	456/514 (89%)	440 (96%)	10 (2%)	6 (1%)	12	16

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	362	ALA
1	B	393	PRO
1	A	381	LYS
1	A	379	THR
1	B	545	GLU

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	A	200/223 (90%)	180 (90%)	20 (10%)	7	10
1	B	198/223 (89%)	181 (91%)	17 (9%)	10	15
All	All	398/446 (89%)	361 (91%)	37 (9%)	9	12

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	556	LEU
1	A	390	LEU
1	A	559	LEU
1	A	370	ARG
1	A	381	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	471	HIS

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Continued from previous page...

Mol	Chain	Res	Type
1	A	538	HIS
1	A	494	HIS
1	B	519	GLN
1	A	519	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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	GOL	A	701	-	5,5,5	0.85	0	5,5,5	1.35	1 (20%)
2	GOL	A	702	-	5,5,5	0.48	0	5,5,5	0.63	0
3	ZJ0	A	703	-	21,21,21	1.39	4 (19%)	25,25,25	2.08	7 (28%)
2	GOL	B	701	-	5,5,5	0.30	0	5,5,5	0.55	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	701	-	-	0/4/4/4	-
2	GOL	A	702	-	-	0/4/4/4	-
3	ZJ0	A	703	-	-	11/17/17/17	0/1/1/1
2	GOL	B	701	-	-	0/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	703	ZJ0	C2-C1	4.07	1.55	1.49
3	A	703	ZJ0	C3-C2	2.62	1.43	1.39
3	A	703	ZJ0	O8-C1	2.60	1.26	1.22
3	A	703	ZJ0	C3-C4	2.09	1.42	1.38

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	703	ZJ0	O8-C1-C2	5.86	129.02	120.74
3	A	703	ZJ0	O8-C1-C9	-4.81	112.17	120.38
3	A	703	ZJ0	C21-O19-C6	3.05	124.12	117.51
3	A	703	ZJ0	C20-O18-C4	2.81	123.61	117.51
3	A	703	ZJ0	C2-C3-C4	2.61	122.35	119.57

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	703	ZJ0	C5-C4-O18-C20
3	A	703	ZJ0	C3-C4-O18-C20
3	A	703	ZJ0	C7-C6-O19-C21
3	A	703	ZJ0	C5-C6-O19-C21
3	A	703	ZJ0	C12-C13-C14-C15

There are no ring outliers.

2 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	702	GOL	1	0
3	A	703	ZJ0	23	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 then 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 ZJ0 A 703

Bond lengths

Bond angles

Torsions

Rings
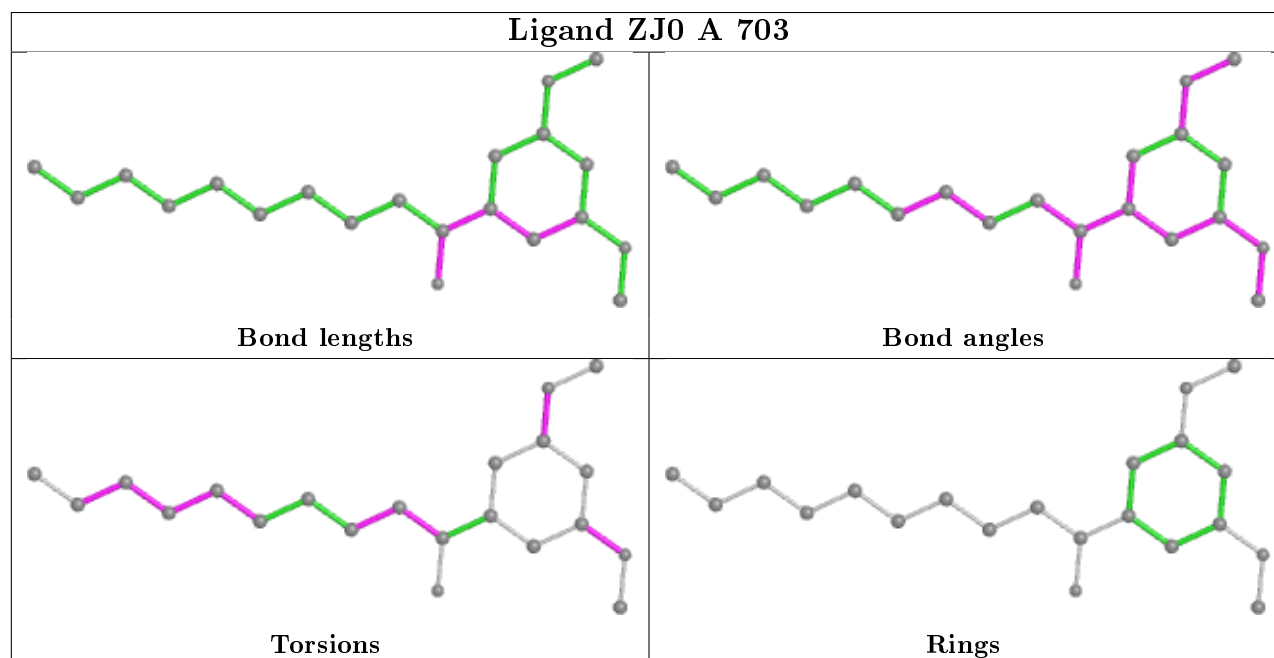
5.7 Other polymers (i)

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	A	232/257 (90%)	-0.26	7 (3%)	50	48	37, 51, 92, 130	1 (0%)
1	B	234/257 (91%)	-0.19	13 (5%)	24	22	42, 59, 109, 175	0
All	All	466/514 (90%)	-0.23	20 (4%)	35	32	37, 56, 100, 175	1 (0%)

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	546	PRO	9.1
1	A	544	GLY	6.5
1	B	361	PRO	6.4
1	B	543	ALA	6.1
1	B	544	GLY	6.0

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

There are no non-standard protein/DNA/RNA residues in this entry.
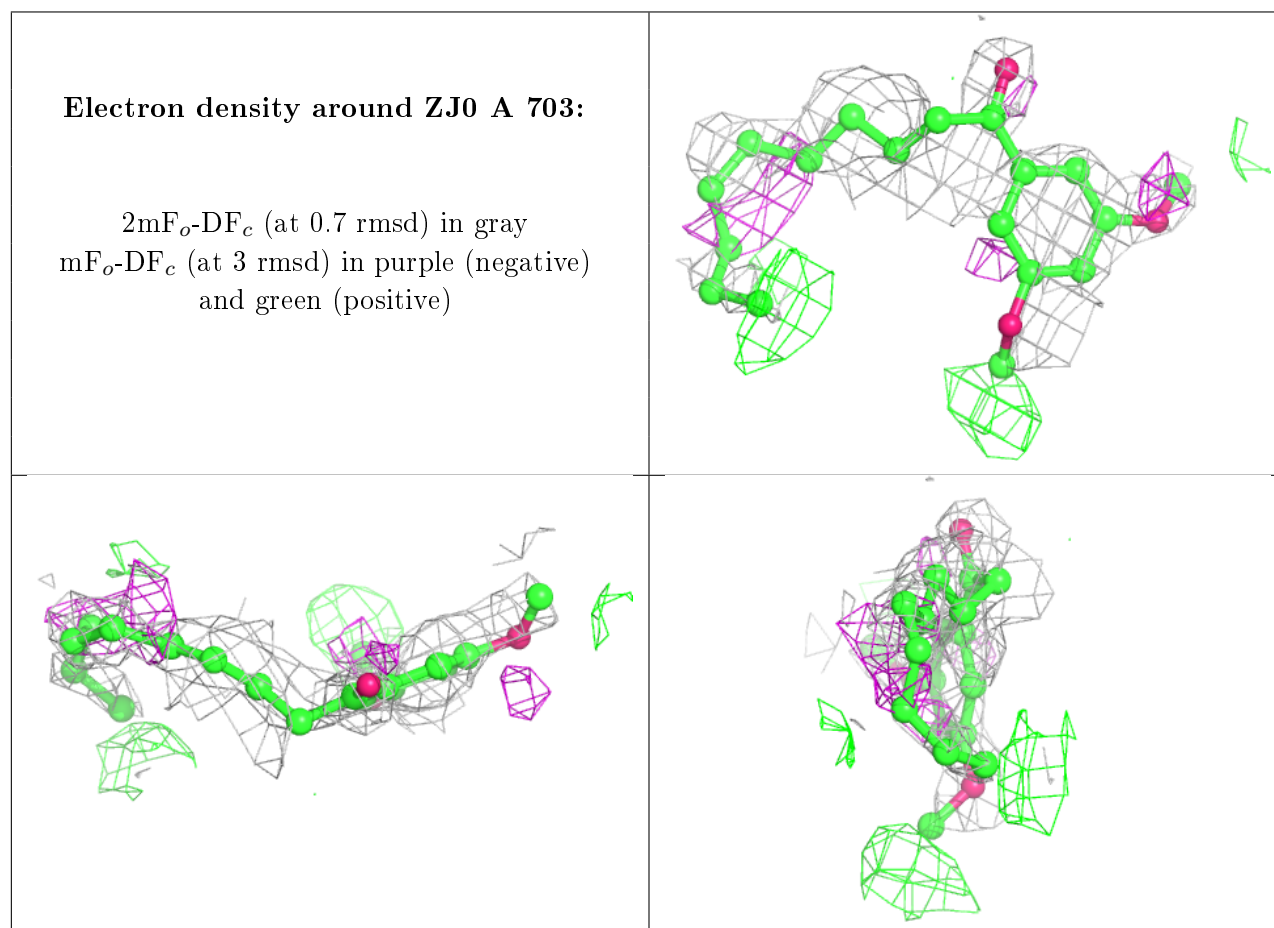
6.3 Carbohydrates (i)

There are no carbohydrates 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
3	ZJ0	A	703	21/21	0.68	0.32	51,87,115,121	0
2	GOL	A	701	6/6	0.77	0.28	64,70,75,77	0
2	GOL	A	702	6/6	0.94	0.16	61,63,66,69	0
2	GOL	B	701	6/6	0.96	0.11	45,58,61,63	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 ZJ0 A 703:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.