



wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 04:17 am BST

PDB ID : 4Q5V
Title : Crystal structure of the catalytic core of human DNA polymerase alpha in ternary complex with an RNA-primed DNA template and aphidicolin
Authors : Baranovskiy, A.G.; Babayeva, N.D.; Suwa, Y.; Gu, J.; Tahirov, T.H.
Deposited on : 2014-04-17
Resolution : 2.52 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 : 2.11
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

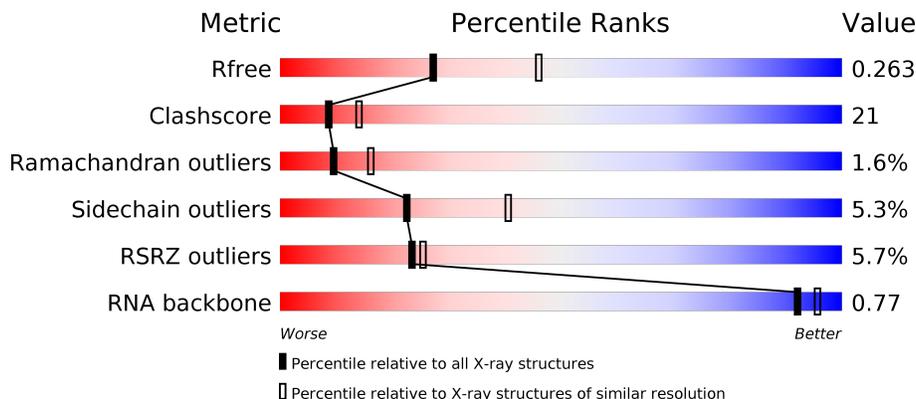
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.52 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	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)
RNA backbone	3102	1020 (2.86-2.18)

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	A	922	 7% 60% 30% 6%
1	E	922	 4% 56% 34% 6%
2	B	11	 9% 82% 9%
2	F	11	 36% 55% 9%

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Mol	Chain	Length	Quality of chain				
3	C	21		10%	52%	38%	
3	G	21		14%	43%	5%	38%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 15085 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 DNA polymerase alpha catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	865	6947	4470	1162	1274	41	0	0	0
1	E	865	6947	4470	1162	1274	41	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	516	ALA	VAL	ENGINEERED MUTATION	UNP P09884
E	516	ALA	VAL	ENGINEERED MUTATION	UNP P09884

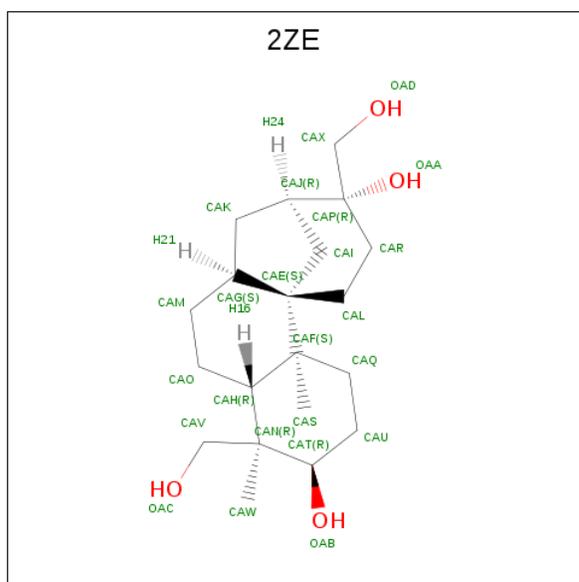
- Molecule 2 is a RNA chain called RNA primer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	11	232	105	44	73	10	0	0	0
2	F	11	232	105	44	73	10	0	0	0

- Molecule 3 is a DNA chain called DNA template.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	C	13	264	125	52	75	12	0	0	0
3	G	13	264	125	52	75	12	0	0	0

- Molecule 4 is (3R,4R,4aR,6aS,8R,9R,11aS,11bS)-4,9-bis(hydroxymethyl)-4,11b-dimethyl tetradecahydro-8,11a-methanocyclohepta[a]naphthalene-3,9-diol (three-letter code: 2ZE) (formula: C₂₀H₃₄O₄).

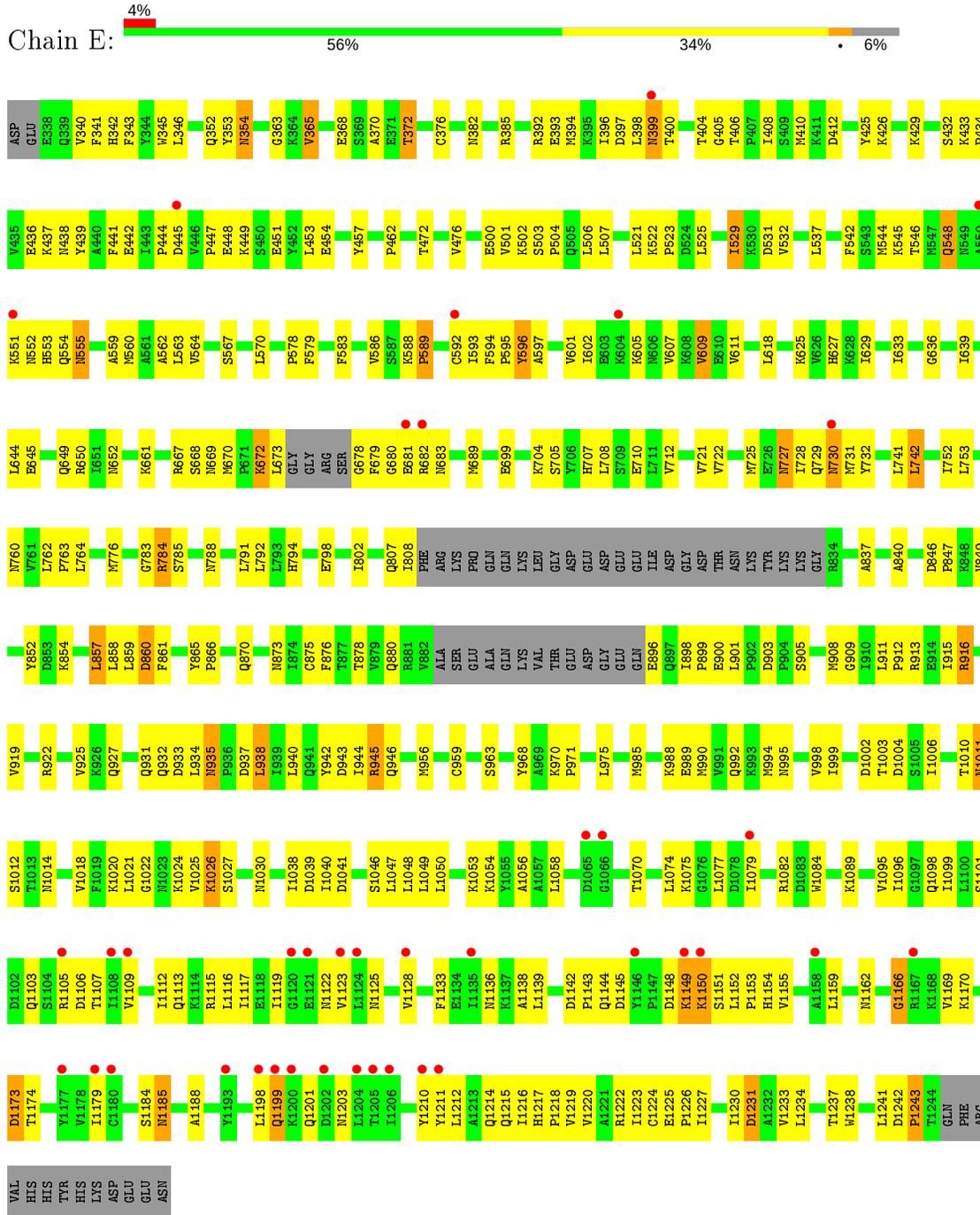


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
4	A	1	Total	C	O	0	0
			24	20	4		
4	E	1	Total	C	O	0	0
			24	20	4		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	80	Total	O	0	0
			80	80		
5	B	1	Total	O	0	0
			1	1		
5	C	3	Total	O	0	0
			3	3		
5	E	62	Total	O	0	0
			62	62		
5	F	3	Total	O	0	0
			3	3		
5	G	2	Total	O	0	0
			2	2		

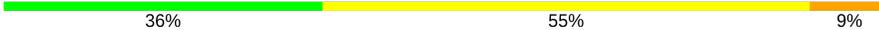
• Molecule 1: DNA polymerase alpha catalytic subunit



• Molecule 2: RNA primer



• Molecule 2: RNA primer

Chain F:  36% 55% 9%

G201
C202
C203
G208
C209
G210
C211

- Molecule 3: DNA template

Chain C:  10% 52% 38%

DA	A109
DT	G110
DA	G111
DC	G112
DT	G113
DA	C114
DT	T115
	C116
	A117
	G118
	G119
	G120
	C121

- Molecule 3: DNA template

Chain G:  14% 43% 5% 38%

DA	A309	T315
DT	G310	C316
DA	G311	C317
DC	C312	A318
DT		G319
DA		G320
DT		C321

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.05Å 116.43Å 233.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	78.02 – 2.52 78.02 – 2.52	Depositor EDS
% Data completeness (in resolution range)	96.0 (78.02-2.52) 96.1 (78.02-2.52)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	189.48 (at 2.51Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.233 , 0.268 0.228 , 0.263	Depositor DCC
R_{free} test set	4714 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	42.8	Xtrriage
Anisotropy	0.254	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 46.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15085	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section:
2ZE

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	0.45	0/7089	0.68	4/9582 (0.0%)
1	E	0.47	0/7089	0.67	4/9582 (0.0%)
2	B	0.45	0/259	0.89	2/402 (0.5%)
2	F	0.51	0/259	0.86	2/402 (0.5%)
3	C	0.46	0/296	0.81	0/455
3	G	0.45	0/296	0.77	0/455
All	All	0.46	0/15288	0.69	12/20878 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	G	0	1

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	553	HIS	N-CA-C	7.66	131.67	111.00
2	B	8	G	O4'-C1'-N9	6.90	113.72	108.20
2	F	208	G	N9-C1'-C2'	6.16	122.01	114.00
1	A	552	ASN	N-CA-C	5.98	127.15	111.00
1	A	442	GLU	N-CA-C	5.67	126.31	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	G	320	DG	Sidechain

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	6947	0	7092	268	0
1	E	6947	0	7092	297	0
2	B	232	0	120	9	0
2	F	232	0	120	6	0
3	C	264	0	146	15	0
3	G	264	0	146	15	0
4	A	24	0	34	8	0
4	E	24	0	34	6	0
5	A	80	0	0	12	0
5	B	1	0	0	0	0
5	C	3	0	0	2	0
5	E	62	0	0	7	0
5	F	3	0	0	0	0
5	G	2	0	0	2	0
All	All	15085	0	14784	611	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 21.

The worst 5 of 611 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)
3:G:315:DT:H2''	3:G:316:DC:H5''	1.30	1.14
1:E:908:MET:HE2	1:E:916:ARG:HH11	1.13	1.08
1:A:652:ASN:HD22	1:A:670:MET:HE3	1.19	1.04
1:A:1233:VAL:HG13	1:A:1243:PRO:HB3	1.36	1.03
1:E:555:ASN:H	1:E:555:ASN:HD22	1.08	1.01

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	857/922 (93%)	785 (92%)	56 (6%)	16 (2%)	8	12
1	E	857/922 (93%)	783 (91%)	62 (7%)	12 (1%)	11	19
All	All	1714/1844 (93%)	1568 (92%)	118 (7%)	28 (2%)	9	16

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	551	LYS
1	A	553	HIS
1	A	589	PRO
1	A	1101	SER
1	A	1149	LYS

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	778/827 (94%)	740 (95%)	38 (5%)	25	45
1	E	778/827 (94%)	734 (94%)	44 (6%)	20	37
All	All	1556/1654 (94%)	1474 (95%)	82 (5%)	22	40

5 of 82 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1243	PRO

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Mol	Chain	Res	Type
1	E	529	ILE
1	E	1098	GLN
1	E	343	PHE
1	E	365	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 71 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1181	GLN
1	E	554	GLN
1	E	1132	GLN
1	A	1185	ASN
1	A	1209	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	9/11 (81%)	0	0
2	F	9/11 (81%)	0	0
All	All	18/22 (81%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 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
4	2ZE	A	1301	-	27,27,27	1.02	4 (14%)	43,46,46	1.63	7 (16%)
4	2ZE	E	1301	-	27,27,27	1.02	3 (11%)	43,46,46	1.65	5 (11%)

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	2ZE	A	1301	-	-	3/6/72/72	0/5/4/4
4	2ZE	E	1301	-	-	3/6/72/72	0/5/4/4

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1301	2ZE	CAF-CAE	-2.50	1.52	1.57
4	A	1301	2ZE	CAF-CAE	-2.45	1.52	1.57
4	A	1301	2ZE	CAF-CAH	-2.32	1.52	1.56
4	E	1301	2ZE	CAE-CAG	-2.27	1.51	1.55
4	E	1301	2ZE	CAN-CAH	-2.20	1.53	1.56

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1301	2ZE	CAL-CAE-CAI	6.16	111.50	105.08
4	E	1301	2ZE	CAL-CAE-CAI	6.11	111.46	105.08
4	A	1301	2ZE	CAK-CAJ-CAP	-3.41	107.84	111.07
4	E	1301	2ZE	CAK-CAJ-CAP	-3.36	107.89	111.07
4	A	1301	2ZE	CAU-CAT-CAN	-2.93	110.00	113.15

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	1301	2ZE	CAJ-CAP-CAX-OAD

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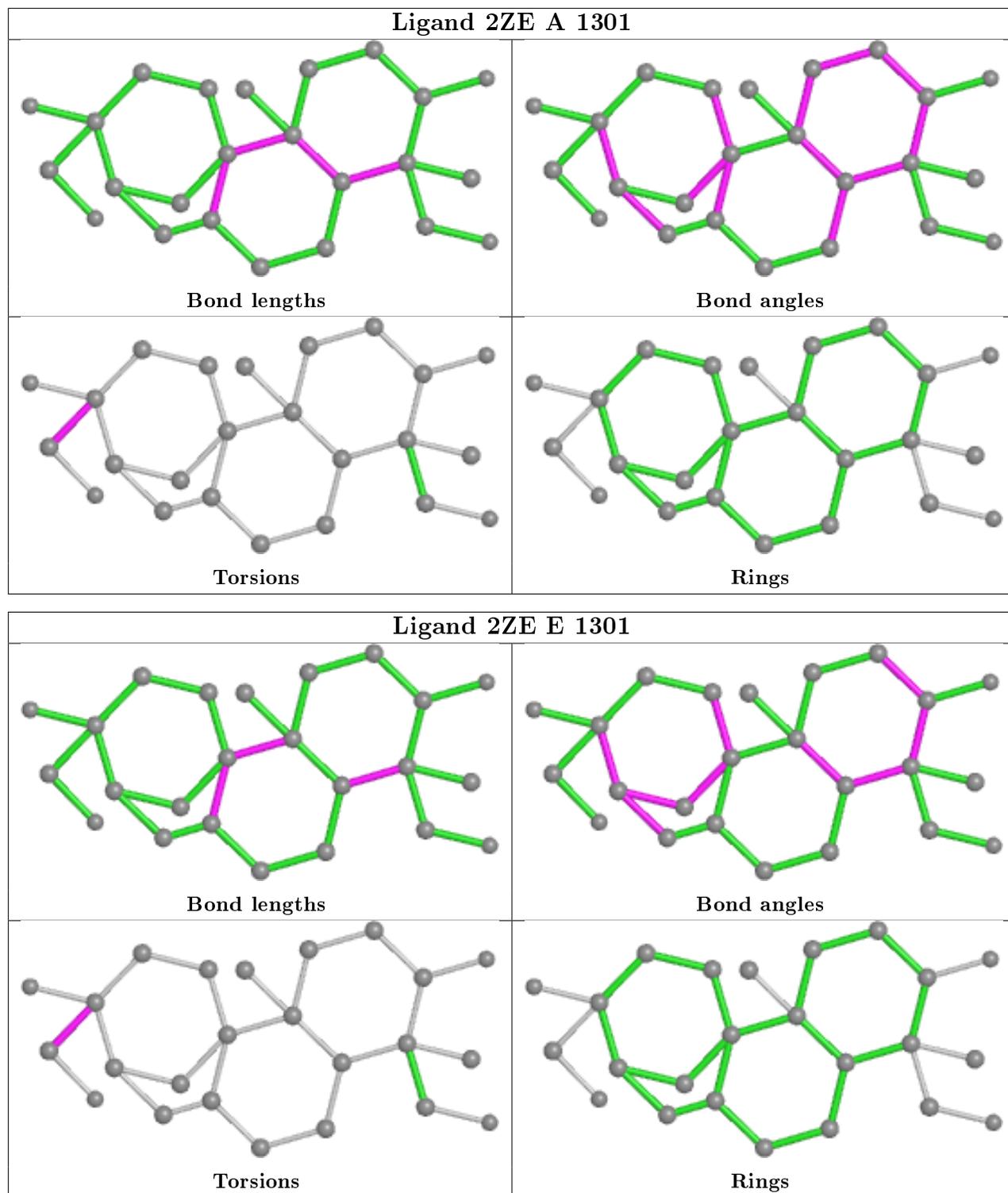
Mol	Chain	Res	Type	Atoms
4	E	1301	2ZE	CAR-CAP-CAX-OAD
4	E	1301	2ZE	OAA-CAP-CAX-OAD
4	A	1301	2ZE	OAA-CAP-CAX-OAD
4	A	1301	2ZE	CAR-CAP-CAX-OAD

There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1301	2ZE	8	0
4	E	1301	2ZE	6	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

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	865/922 (93%)	0.38	63 (7%) 15 16	15, 54, 113, 128	0
1	E	865/922 (93%)	0.27	39 (4%) 33 36	18, 52, 105, 129	0
2	B	11/11 (100%)	-0.83	0 100 100	48, 62, 78, 87	0
2	F	11/11 (100%)	-0.63	0 100 100	43, 52, 79, 81	0
3	C	13/21 (61%)	-0.29	0 100 100	37, 59, 92, 101	0
3	G	13/21 (61%)	-0.34	0 100 100	42, 57, 76, 85	0
All	All	1778/1908 (93%)	0.30	102 (5%) 23 25	15, 53, 111, 129	0

The worst 5 of 102 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1241	LEU	9.0
1	A	1239	LEU	8.1
1	E	550	ALA	7.2
1	A	1180	CYS	6.8
1	A	1193	TYR	5.8

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](#)

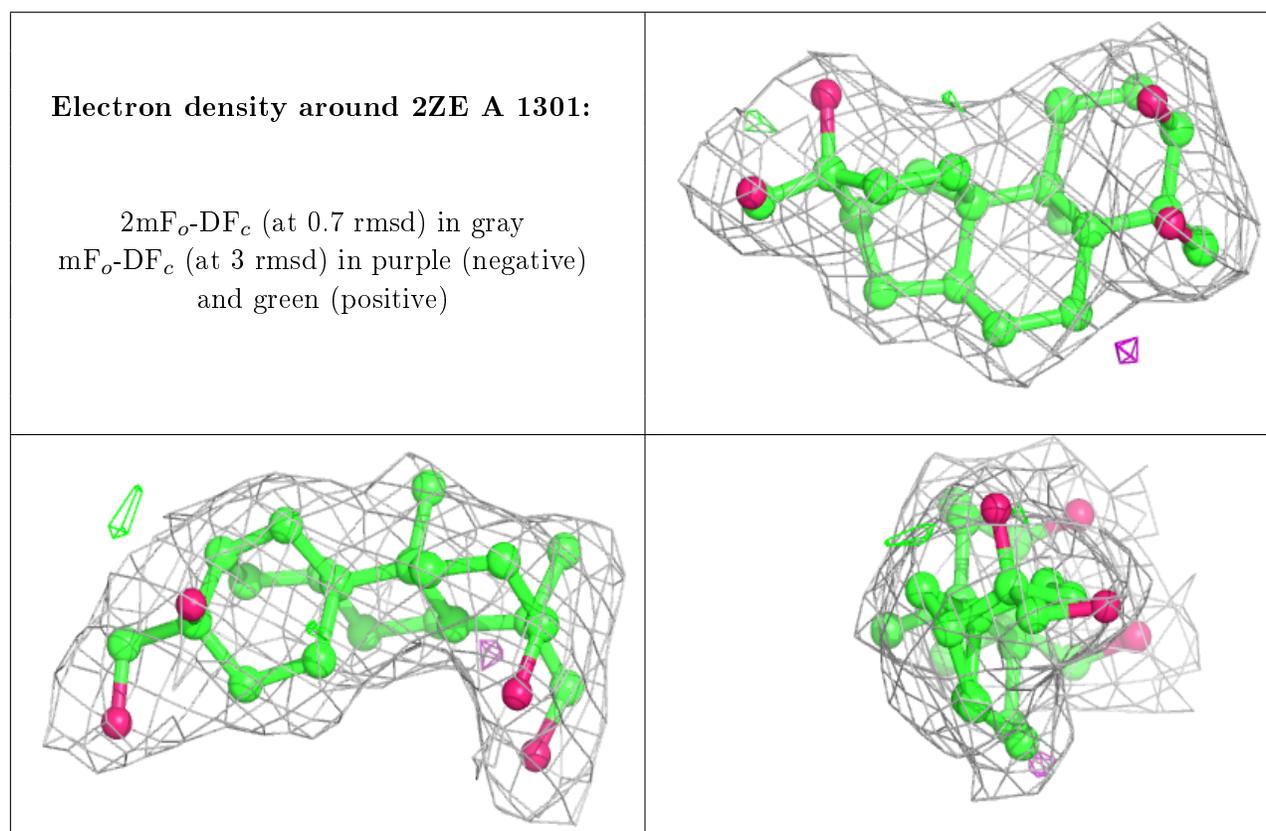
There are no carbohydrates in this entry.

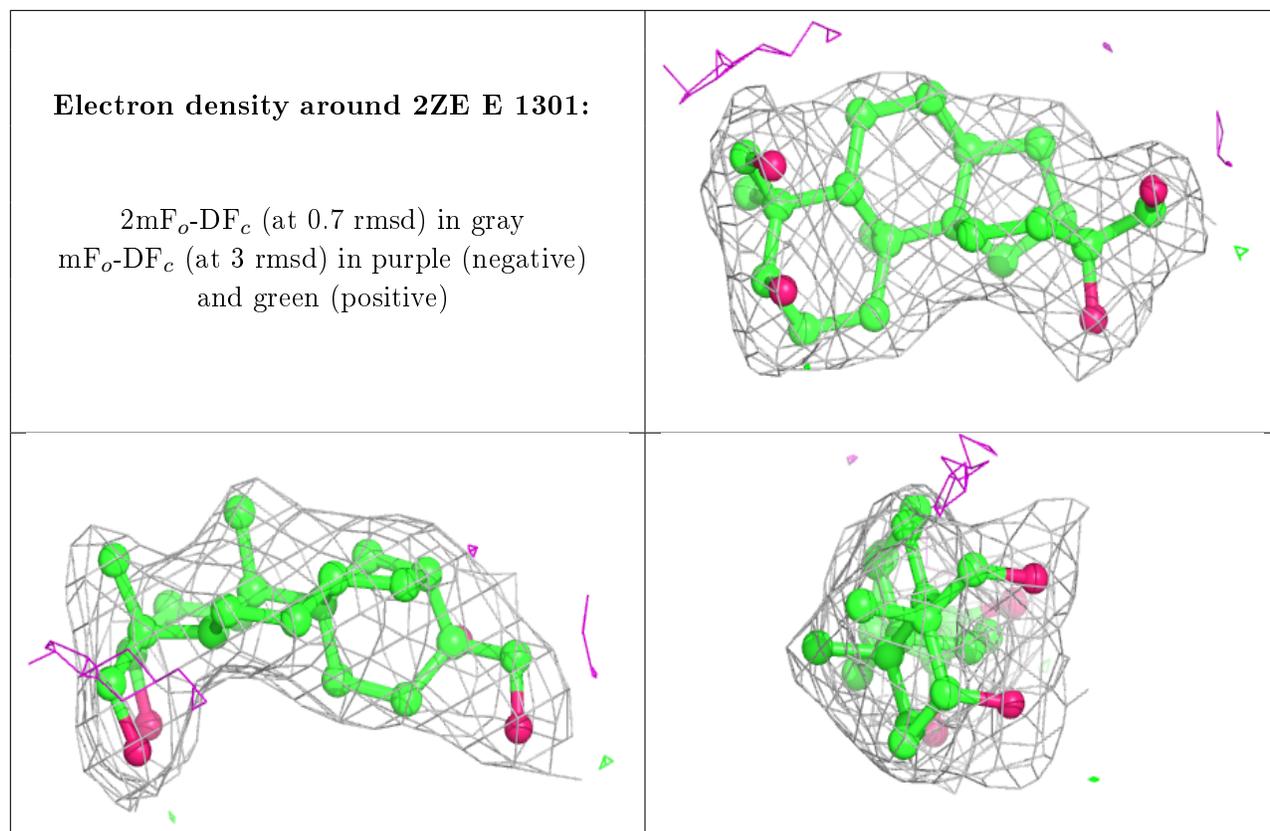
6.4 Ligands [i](#)

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
4	2ZE	A	1301	24/24	0.95	0.14	20,29,34,42	0
4	2ZE	E	1301	24/24	0.96	0.14	30,37,43,43	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.