



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 01:56 PM UTC

PDB ID : 7WR5 / pdb_00007wr5
Title : Crystal structure of OspC3-calmodulin-caspase-4 complex binding with 2'-aF-NAD⁺
Authors : Hou, Y.J.; Zeng, H.; Shao, F.; Ding, J.
Deposited on : 2022-01-26
Resolution : 3.10 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

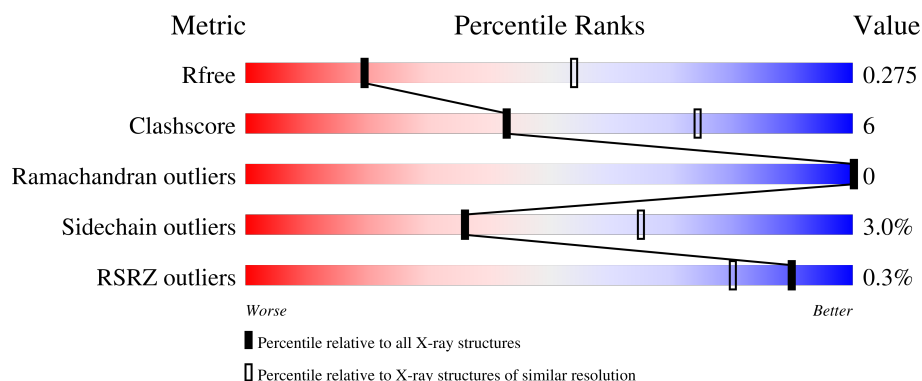
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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 ≥ 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	430	 84% 14% .
2	B	149	 73% 19% 7%
3	C	280	 66% 18% . 15%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6534 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 OspC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	424	Total	C	N	O	S	0	0	0
			3467	2198	601	655	13			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	45	GLY	-	expression tag	UNP R4X5L7
A	46	PRO	-	expression tag	UNP R4X5L7
A	47	LEU	-	expression tag	UNP R4X5L7
A	48	GLY	-	expression tag	UNP R4X5L7
A	49	SER	-	expression tag	UNP R4X5L7
A	50	GLY	-	expression tag	UNP R4X5L7
A	51	ARG	-	expression tag	UNP R4X5L7
A	52	PRO	-	expression tag	UNP R4X5L7

- Molecule 2 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	138	Total	C	N	O	S	0	0	0
			1093	672	176	236	9			

- Molecule 3 is a protein called Caspase-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	237	Total	C	N	O	S	0	0	0
			1930	1226	333	357	14			

There are 5 discrepancies between the modelled and reference sequences:

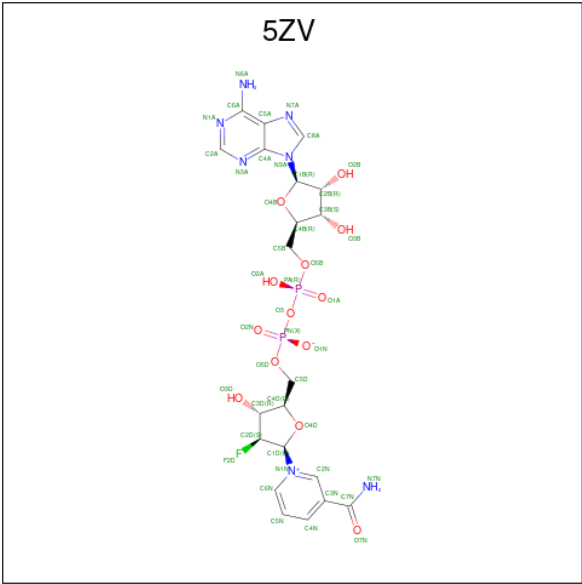
Chain	Residue	Modelled	Actual	Comment	Reference
C	98	SER	-	expression tag	UNP P49662
C	99	GLY	-	expression tag	UNP P49662

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Chain	Residue	Modelled	Actual	Comment	Reference
C	100	ARG	-	expression tag	UNP P49662
C	101	PRO	-	expression tag	UNP P49662
C	258	ALA	CYS	engineered mutation	UNP P49662

- Molecule 4 is [[(2 {R},3 {R},4 {S},5 {R})-5-(3-aminocarbonylpyridin-1-yl)-4-fluoranyl-3-oxidanyl-oxolan-2-yl]methoxy-oxidanyl-phosphoryl] [(2 {R},3 {S},4 {R},5 {R})-5-(6-aminopurin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methyl hydrogen phosphate (CCD ID: 5ZV) (formula: C₂₁H₂₇FN₇O₁₃P₂) (labeled as "Ligand of Interest" by depositor).



- Molecule 1: OspC3

GLY	PHO	LEU	GLY	SER	GLY	RS1	K60	L63	S66	L67	Q70	G79	F82	L85	N86	L87	E90	R96	R100	V108	S109	R110	T116	V120	E127	R128	L131	T135	S147	N151	N152	T153	L154	K161	T178	H184	G187	
V449	M455	M474	L200	P201	T208	M235	V240	F241	Y242	F249	E255	V256	V257	H265	G269	N277	M281	T290	D298	S314	I318	F321	S334	I341	D384	L390	E402	K405	M406	R407	N408	V415	V433	F434	I435	V440	D441	H442

Amino Acid	Count
MET	1
ALA	1
ASP	1
GLN	1
LEU	1
THR	1
GLU	88
G9	9
I110	110
F20	20
D25	25
E32	32
L33	33
V36	36
M37	37
M52	52
I53	53
M54	54
E55	55
V56	56
D57	57
ALA	1
ASP	1
GLY	1
M61	61
E68	68
M72	72
S82	82
E83	83
I86	86
R87	87
K96	96
D96	96
L106	106
M10	10
E115	115
I121	121
V122	122
E123	123
E124	124
M125	125
E128	128
L129	129
Q144	1
M145	1
M146	1
T147	1
A148	1
LYS	1

L339	V252	SER
E340	T253	GLY
E341	T254	ARG
V342	V255	PRO
	V256	SER
V346	V257	THR
	A258	ASP
T352	R259	ALA
P353	GLY	LEU
R354	ALA	LYS
A355	ASN	LEU
K356	ARG	CYS
	GLY	P110
R364	GLY	R121
L365	LEU	
F371	TRP	E130
	VAL	
G376	ARG	R134
ASN	ASP	
	SER	L137
	PRO	
	ALA	F146
	SER	
	LEU	D158
	GLU	
	VAL	L179
	ALA	
	SER	D183
	SER	
	GLN	A190
	SER	
	SER	R194
	GLU	P195
	ASN	E196
	LEU	H197
	GLU	K198
	D199	S199
	G289	
	K293	M208
		S209
	V296	T216
	I301	
	A302	T219
		V220
	H309	H221
	N310	ASP
	V311	E223
	S312	K224
	W313	
	R314	D227
	S320	D232
		T233
	L326	I234
	C337	L246
	H338	

4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	52.32Å 120.07Å 141.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.07 – 3.10 49.07 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.07-3.10) 94.6 (49.07-3.10)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.226 , 0.272 0.232 , 0.275	Depositor DCC
R_{free} test set	1679 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	77.0	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6534	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% 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: 5ZV

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	0.11	0/3541	0.29	0/4766
2	B	0.09	0/1104	0.24	0/1480
3	C	0.11	0/1972	0.32	0/2660
All	All	0.11	0/6617	0.29	0/8906

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3467	0	3404	37	0
2	B	1093	0	1026	18	0
3	C	1930	0	1906	32	0
4	A	44	0	0	0	0
All	All	6534	0	6336	80	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 80 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:C:221:HIS:HB2	3:C:227:ASP:HB3	1.76	0.67
2:B:83:GLU:OE2	2:B:87:ARG:NH2	2.28	0.67
1:A:60:LYS:NZ	2:B:115:GLU:O	2.27	0.66
2:B:87:ARG:HH12	2:B:144:GLN:HG3	1.60	0.66
3:C:337:CYS:HB3	3:C:341:GLU:HB2	1.78	0.65

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	422/430 (98%)	409 (97%)	13 (3%)	0	100	100
2	B	134/149 (90%)	131 (98%)	3 (2%)	0	100	100
3	C	231/280 (82%)	222 (96%)	9 (4%)	0	100	100
All	All	787/859 (92%)	762 (97%)	25 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	392/395 (99%)	383 (98%)	9 (2%)	44	70
2	B	119/127 (94%)	113 (95%)	6 (5%)	22	53
3	C	216/252 (86%)	209 (97%)	7 (3%)	34	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	727/774 (94%)	705 (97%)	22 (3%)	36 65

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	132	ASP
3	C	216	ILE
3	C	199	SER
3	C	223	GLU
1	A	408	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	338	HIS
3	C	221	HIS
2	B	112	ASN
1	A	245	HIS
2	B	138	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	5ZV	A	501	-	47,48,48	4.70	18 (38%)	67,73,73	1.78	15 (22%)

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	5ZV	A	501	-	-	14/30/62/62	0/5/5/5

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	501	5ZV	C2D-C3D	-18.93	1.27	1.52
4	A	501	5ZV	C2D-C1D	13.21	1.68	1.53
4	A	501	5ZV	O4D-C1D	-8.94	1.29	1.40
4	A	501	5ZV	C3B-C4B	-8.84	1.30	1.53
4	A	501	5ZV	O4B-C4B	8.08	1.62	1.45

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	5ZV	C5A-C4A-N3A	-5.64	118.95	126.72
4	A	501	5ZV	N1A-C2A-N3A	-4.42	121.89	128.58
4	A	501	5ZV	C3D-C2D-C1D	4.22	108.00	103.10
4	A	501	5ZV	C2A-N3A-C4A	3.85	121.24	111.83
4	A	501	5ZV	C4D-O4D-C1D	-3.67	106.56	109.92

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	5ZV	C2D-C1D-N1N-C6N
4	A	501	5ZV	C2D-C1D-N1N-C2N
4	A	501	5ZV	PA-O3-PN-O5D
4	A	501	5ZV	C5B-O5B-PA-O3

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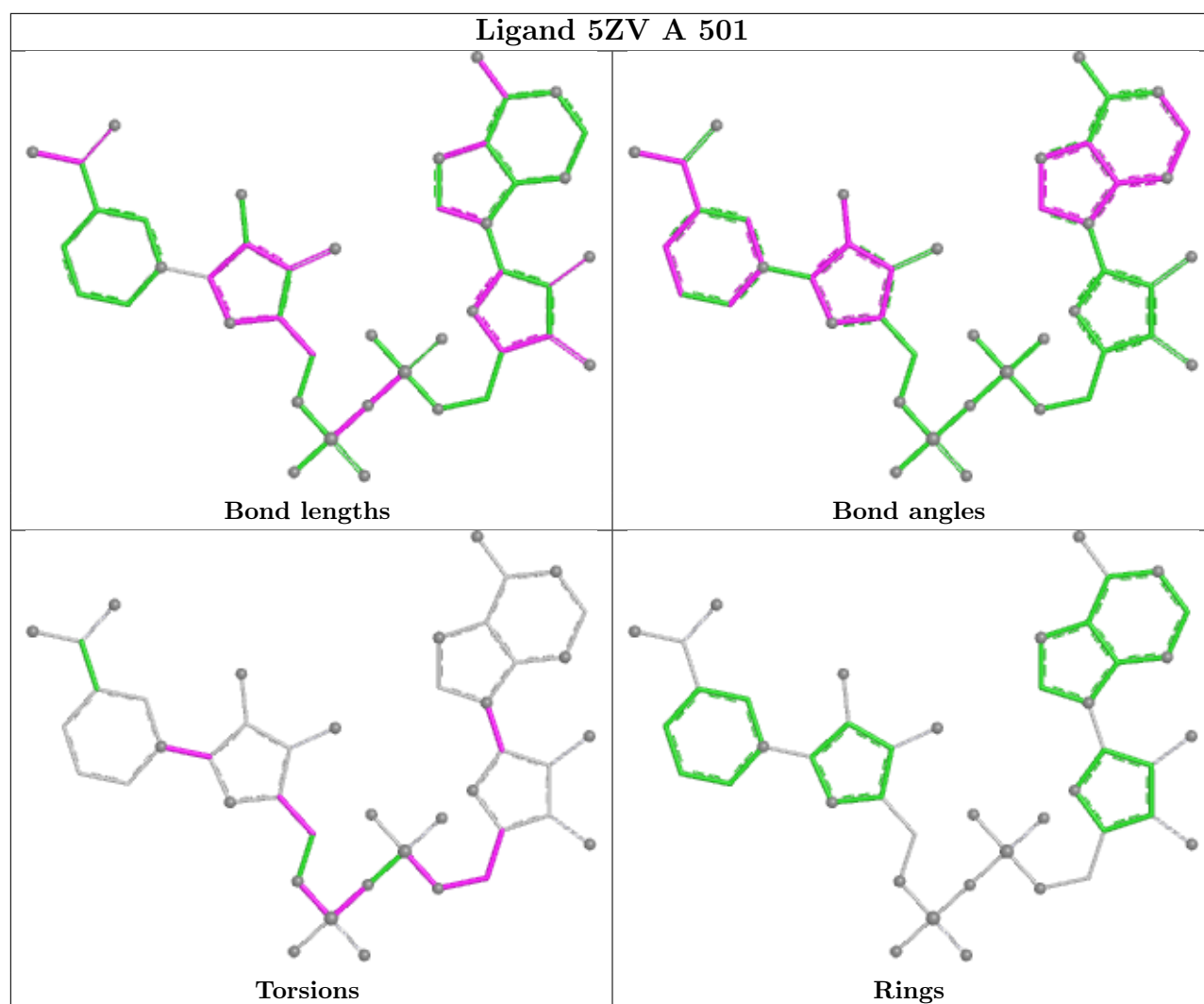
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Mol	Chain	Res	Type	Atoms
4	A	501	5ZV	C5B-O5B-PA-O2A

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.



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	424/430 (98%)	-0.28	1 (0%) 91 83	41, 64, 102, 142	0
2	B	138/149 (92%)	-0.09	0 100 100	60, 89, 118, 134	0
3	C	237/280 (84%)	0.14	1 (0%) 88 76	59, 102, 164, 189	0
All	All	799/859 (93%)	-0.12	2 (0%) 90 80	41, 80, 135, 189	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	200	LEU	2.6
3	C	311	VAL	2.4

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

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

6.3 Carbohydrates [i](#)

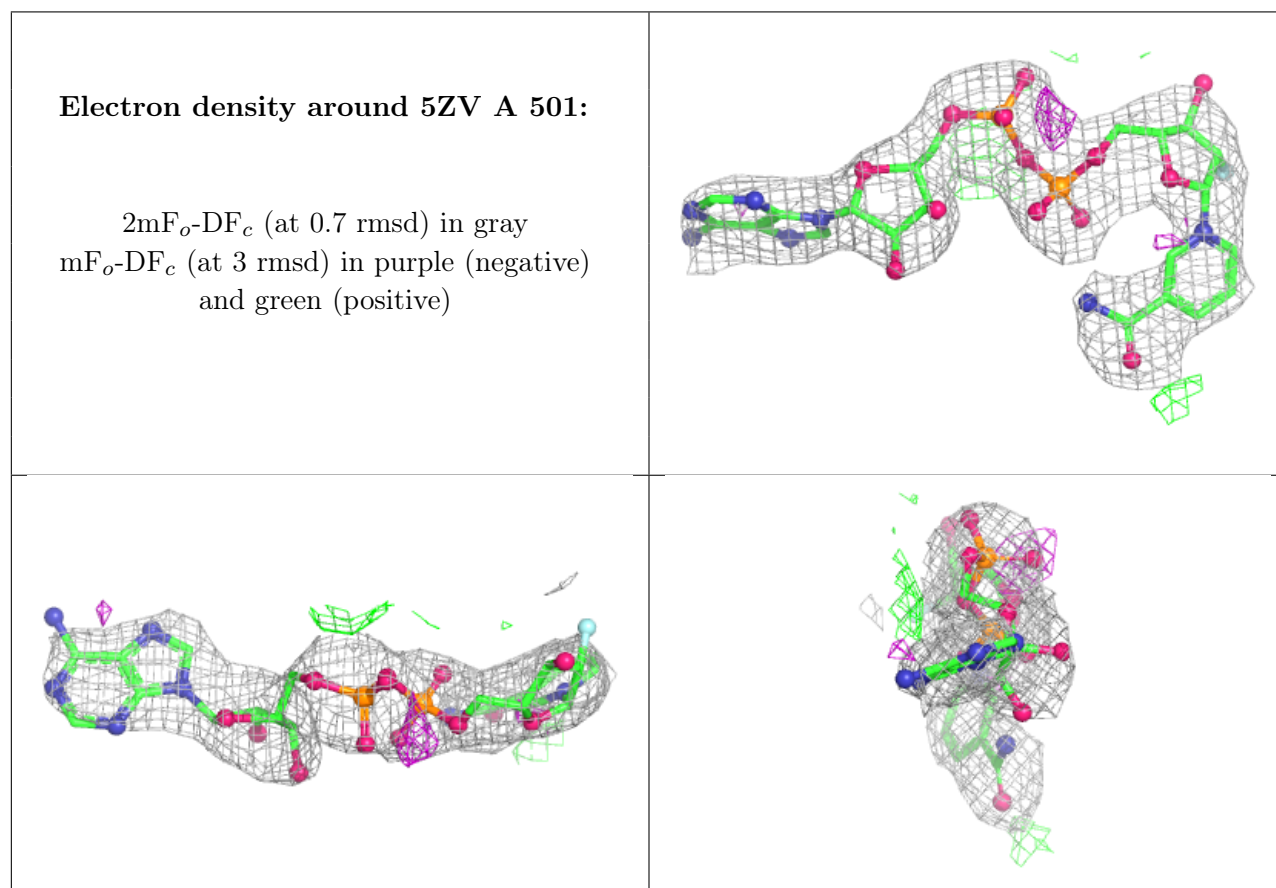
There are no oligosaccharides in this entry.

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	5ZV	A	501	44/44	0.85	0.10	54,90,109,113	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.