

Full wwPDB X-ray Structure Validation Report (i)

Oct 25, 2023 – 01:19 pm BST

PDB ID : 80EG

Title: PDE4B bound to MAPI compound 92a

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Deposited on : 2023-03-10

Resolution : 1.89 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
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

MolProbity: 4.02b-467

Mogul : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.36

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)

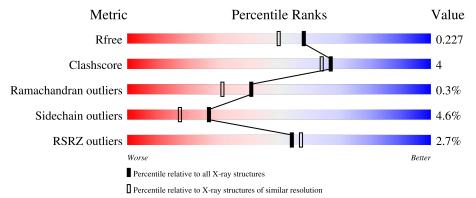
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 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 $(\# \mathrm{Entries})$	Similar resolution $(\# \text{Entries, resolution range}(\text{\AA}))$
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 <=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			
			2%			
1	A	421	65%	13%	•	20%



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 2881 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 4B.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Λ	336	Total	С	N	О	S	0	0	0
1	A	330	2714	1711	460	524	19	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	245	MET	-	initiating methionine	UNP Q07343
A	295	LYS	SER	conflict	UNP Q07343
A	296	VAL	PRO	conflict	UNP Q07343
A	298	ALA	GLN	conflict	UNP Q07343
A	299	GLU	LYS	$\operatorname{conflict}$	UNP Q07343
A	300	GLU	ASP	$\operatorname{conflict}$	UNP Q07343
A	?	-	ARG	deletion	UNP Q07343
A	?	-	GLU	deletion	UNP Q07343
A	?	-	LYS	deletion	UNP Q07343
A	?	-	LYS	deletion	UNP Q07343
A	?	-	LYS	deletion	UNP Q07343
A	301	ALA	LYS	$\operatorname{conflict}$	UNP Q07343
A	302	PRO	GLN	$\operatorname{conflict}$	UNP Q07343
A	304	PRO	LEU	$\operatorname{conflict}$	UNP Q07343
A	660	HIS	-	expression tag	UNP Q07343
A	661	HIS	-	expression tag	UNP Q07343
A	662	HIS	-	expression tag	UNP Q07343
A	663	HIS	-	expression tag	UNP Q07343
A	664	HIS	-	expression tag	UNP Q07343
A	665	HIS	-	expression tag	UNP Q07343

• Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

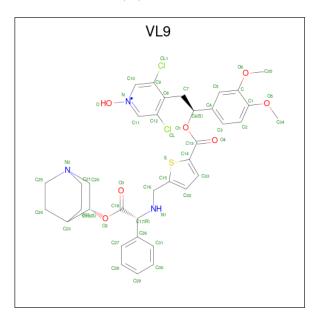


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0

• Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

• Molecule 4 is $[(1 \{S\})-2-[3,5-bis(chloranyl)-1-oxidanyl-pyridin-4-yl]-1-(3,4-dimethoxyph enyl)ethyl]$ 5- $[[(1 \{R\})-2-[[(3 \{R\})-1-azabicyclo[2.2.2]octan-3-yl]oxy]-2-oxidanylidene-1-phenyl-ethyl]amino]methyl]thiophene-2-carboxylate (three-letter code: VL9) (formula: <math>C_{36}H_{38}Cl_2N_3O_7S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
4	A	1	Total 49	C 36	Cl 2	N 3	O 7	S 1	0	0

• Molecule 5 is water.

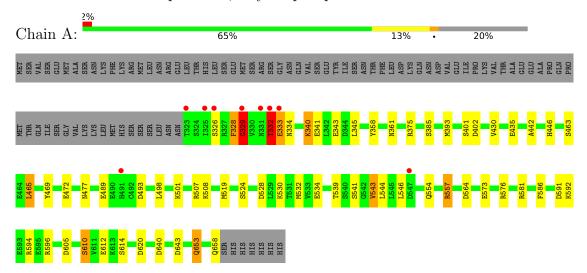
\mathbf{Mol}	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	116	Total O 116 116	0	0



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 4B





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants	95.76Å 95.76Å 85.46Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	83.07 - 1.89	Depositor
Resolution (A)	82.93 - 1.89	EDS
% Data completeness	99.5 (83.07-1.89)	Depositor
(in resolution range)	99.5 (82.93-1.89)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.70 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
D.D.	0.158 , 0.195	Depositor
R, R_{free}	0.191 , 0.227	DCC
R_{free} test set	1771 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	29.0	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.37, 36.9	EDS
L-test for twinning ²	$< L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2881	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.36% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: VL9, MG, ZN

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	Bo	nd lengths	Bo	ond angles
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z >5
1	A	1.38	$14/2770 \ (0.5\%)$	1.31	$33/3757 \ (0.9\%)$

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 maintenain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	Ideal(Å)
1	A	524	SER	CB-OG	-9.04	1.30	1.42
1	A	329	GLY	N-CA	6.90	1.56	1.46
1	A	329	GLY	CA-C	6.47	1.62	1.51
1	A	576	ARG	CD-NE	-6.39	1.35	1.46
1	A	401	SER	CB-OG	-6.12	1.34	1.42
1	A	653	GLN	CG-CD	-5.71	1.38	1.51
1	A	557	ARG	CD-NE	-5.60	1.36	1.46
1	A	612	GLU	CD-OE2	-5.50	1.19	1.25
1	A	592	LYS	CE-NZ	5.34	1.62	1.49
1	A	472	GLU	CD-OE2	5.22	1.31	1.25
1	A	472	GLU	CG-CD	5.19	1.59	1.51
1	A	343	GLU	CG-CD	5.15	1.59	1.51
1	A	341	GLU	CD-OE2	-5.11	1.20	1.25
1	A	463	SER	CB-OG	5.05	1.48	1.42

All (33) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	576	ARG	NE-CZ-NH1	14.25	127.42	120.30
1	A	576	ARG	NE-CZ-NH2	-11.75	114.42	120.30
1	A	605	ASP	CB-CG-OD2	-9.81	109.47	118.30
1	A	328	PHE	C-N-CA	-9.69	101.95	122.30
1	A	507	ARG	NE-CZ-NH1	9.63	125.12	120.30
1	A	605	ASP	CB-CG-OD1	8.34	125.80	118.30
1	A	402	ASP	CB-CG-OD1	7.46	125.01	118.30
1	A	591	ASP	CB-CG-OD1	7.42	124.98	118.30
1	A	435	GLU	OE1-CD-OE2	-6.98	114.92	123.30
1	A	596	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	A	581	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	A	393	MET	CG-SD-CE	-6.67	89.52	100.20
1	A	643	ASP	CB-CG-OD1	6.64	124.27	118.30
1	A	493	ASP	CB-CG-OD1	6.57	124.22	118.30
1	A	489	GLU	OE1-CD-OE2	6.18	130.72	123.30
1	A	528	ASP	CB-CG-OD1	5.91	123.62	118.30
1	A	544	LEU	CB-CG-CD1	-5.77	101.19	111.00
1	A	596	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	345	LEU	CB-CG-CD2	-5.59	101.50	111.00
1	A	375	ARG	NE-CZ-NH2	5.55	123.07	120.30
1	A	640	ASP	CB-CG-OD1	5.52	123.27	118.30
1	A	557	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	465	LEU	CB-CG-CD1	5.49	120.34	111.00
1	A	524	SER	CB-CA-C	-5.49	99.67	110.10
1	A	498	LEU	CB-CG-CD1	5.27	119.95	111.00
1	A	564	ASP	CB-CG-OD1	5.27	123.04	118.30
1	A	614	SER	N-CA-CB	5.25	118.38	110.50
1	A	586	PHE	CB-CG-CD2	-5.25	117.12	120.80
1	A	581	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	A	620	ASP	CB-CG-OD2	5.11	122.89	118.30
1	A	329	GLY	N-CA-C	5.04	125.71	113.10
1	A	594	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	A	564	ASP	CB-CG-OD2	-5.02	113.78	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group	
1	A	329 GLY		Peptide	
1	A	332	THR	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	2714	0	2639	21	0
2	A	1 0 0		0	0	0
3	A	1	0	0	0	0
4	A	49	0	0	1	0
5	A	116	0	0	4	0
All	All	2881	0	2639	21	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 4.

All (21) 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:332:THR:HG23	2:THR:HG23 1:A:358:TYR:O		1.14
1:A:539:THR:HG22	1:A:543:VAL:H	1.42	0.82
1:A:610:SER:HB3	5:A:860:HOH:O	1.81	0.80
1:A:610:SER:CB	5:A:860:HOH:O	2.31	0.79
1:A:539:THR:HG23	1:A:541:SER:H	1.56	0.70
1:A:332:THR:CG2	1:A:358:TYR:O	2.34	0.69
1:A:539:THR:HG23	1:A:541:SER:N	2.15	0.61
1:A:328:PHE:O	1:A:329:GLY:C	2.41	0.59
1:A:508:LYS:HD2	5:A:843:HOH:O	2.11	0.50
1:A:610:SER:HB2	5:A:860:HOH:O	2.03	0.50
1:A:539:THR:CG2	1:A:541:SER:OG	2.62	0.47
1:A:539:THR:HG21	1:A:541:SER:OG	2.14	0.47
1:A:554:GLN:NE2	1:A:557:ARG:NH1	2.64	0.46
1:A:530:LYS:O	1:A:534:GLU:HG3	2.15	0.46
1:A:332:THR:HG22	1:A:334:ASN:HB2	1.99	0.45
1:A:519:MET:HG2	4:A:703:VL9:C11	2.48	0.44
1:A:442:ALA:O	1:A:446:HIS:HB3	2.19	0.41
1:A:469:TYR:CE1	1:A:477:ASN:HB3	2.56	0.41
1:A:340:LYS:HD3	1:A:340:LYS:O	2.21	0.41
1:A:430:VAL:HG11	1:A:546:LEU:HD12	2.03	0.41
1:A:332:THR:HG22	1:A:334:ASN:H	1.85	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	334/421 (79%)	328 (98%)	5 (2%)	1 (0%)	41 31	

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	\mathbf{Type}	
1	A	333	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	305/385~(79%)	291 (95%)	14 (5%)	27 17	

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	326	SER
1	A	332	THR
1	A	333	GLU
1	A	340	LYS
1	A	361	ASN
1	A	385	SER
1	A	465	LEU

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Mol	Chain	Res	Type
1	A	501	LYS
1	A	532	MET
1	A	543	VAL
1	A	573	GLU
1	A	610	SER
1	A	653	GLN
1	A	658	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	334	ASN
1	A	548	ASN
1	A	588	GLN
1	A	653	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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).



Mal	Type	Chain	n Res	Link	Bond lengths			Bond angles		
MIOI	туре	Chain		Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	VL9	A	703	-	51,54,54	2.10	14 (27%)	58,76,76	1.88	9 (15%)

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.

\mathbf{Mol}	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	VL9	A	703	-	-	4/33/71/71	0/7/6/6

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(A)	$\operatorname{Ideal}(\text{\AA})$
4	A	703	VL9	O2-C18	5.62	1.47	1.34
4	A	703	VL9	C20-N2	5.19	1.55	1.46
4	A	703	VL9	O-N	4.99	1.55	1.36
4	A	703	VL9	C7-C6	4.09	1.59	1.53
4	A	703	VL9	C12-C8	3.82	1.46	1.39
4	A	703	VL9	C10-C9	3.49	1.42	1.38
4	A	703	VL9	C21-N2	3.35	1.56	1.46
4	A	703	VL9	C26-C17	-3.03	1.47	1.52
4	A	703	VL9	C24-C23	2.94	1.60	1.53
4	A	703	VL9	C23-C19	2.65	1.58	1.52
4	A	703	VL9	C11-C12	-2.55	1.36	1.38
4	A	703	VL9	C7-C8	-2.35	1.48	1.51
4	A	703	VL9	C25-N2	2.10	1.52	1.46
4	A	703	VL9	C16-C15	2.01	1.54	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
4	A	703	VL9	C19-O2-C18	6.96	128.34	117.89
4	A	703	VL9	C35-O6-C	4.96	125.02	117.53
4	A	703	VL9	C25-N2-C20	4.15	115.86	109.52
4	A	703	VL9	O2-C18-C17	3.53	121.12	110.83
4	A	703	VL9	C10-C9-CL1	3.42	121.73	118.01
4	A	703	VL9	C18-C17-N1	-3.07	102.84	109.74
4	A	703	VL9	O2-C18-O3	-2.99	118.35	123.94
4	A	703	VL9	C21-N2-C20	-2.50	105.70	109.52
4	A	703	VL9	C26-C17-C18	-2.12	102.50	109.86

There are no chirality outliers.



All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	703	VL9	C23-C19-O2-C18
4	A	703	VL9	C20-C19-O2-C18
4	A	703	VL9	C18-C17-N1-C16
4	A	703	VL9	C7-C6-O1-C13

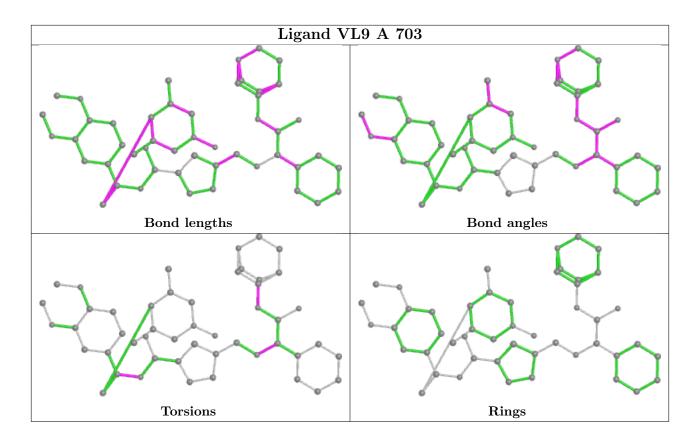
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	703	VL9	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 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.





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, 95^{th} 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	$OWAB(A^2)$	Q < 0.9
1	A	336/421 (79%)	-0.05	9 (2%) 54 57	13, 20, 35, 54	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	491	HIS	3.4
1	A	323	THR	3.2
1	A	333	GLU	3.1
1	A	332	THR	2.4
1	A	331	ASN	2.3
1	A	329	GLY	2.3
1	A	326	SER	2.2
1	A	547	ASP	2.2
1	A	325	ILE	2.2

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.

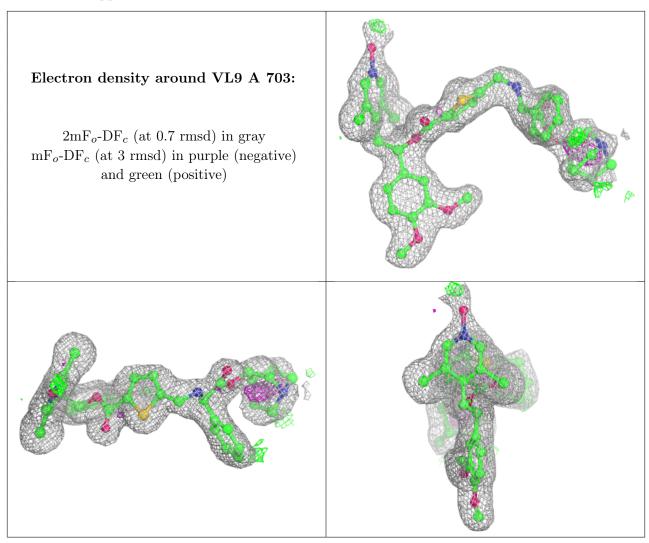
6.4 Ligands (i)

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^{th} 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.

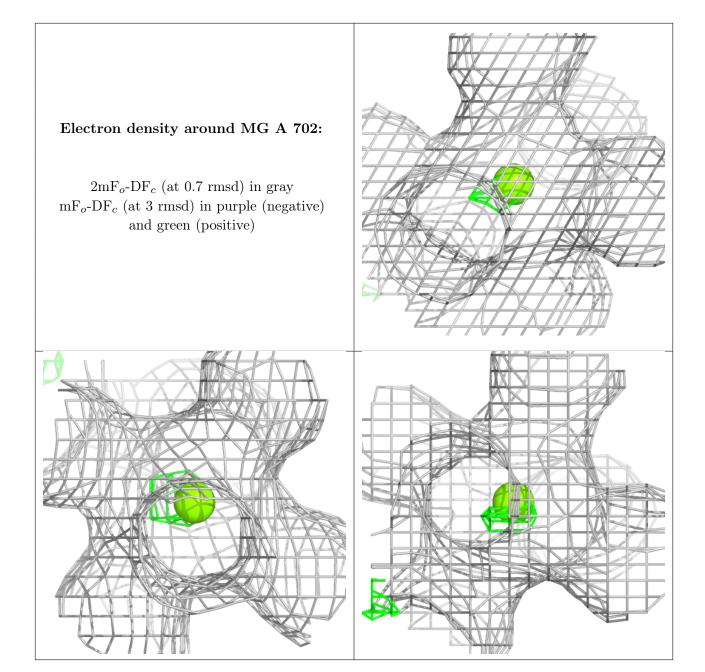


Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
4	VL9	A	703	49/49	0.95	0.11	17,25,48,52	0
3	MG	A	702	1/1	1.00	0.20	11,11,11,11	0
2	ZN	A	701	1/1	1.00	0.16	19,19,19,19	0

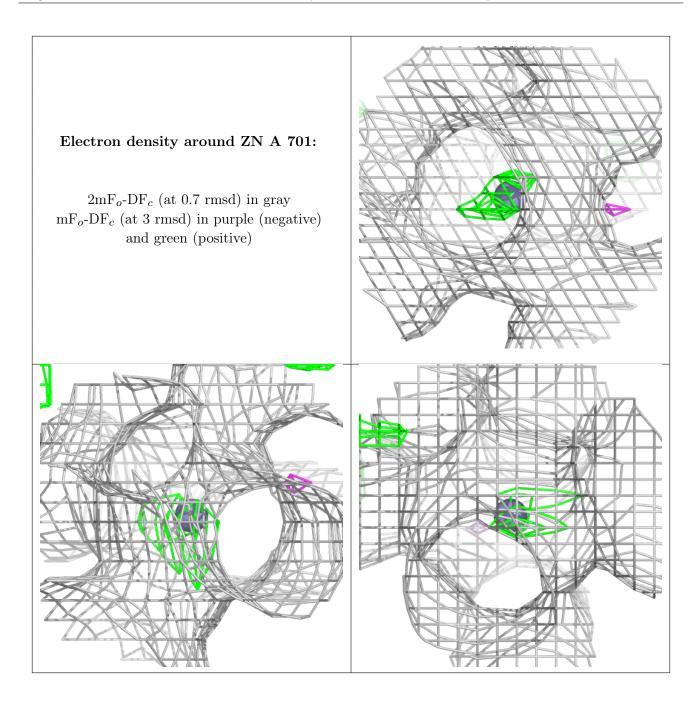
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.











6.5 Other polymers (i)

There are no such residues in this entry.

