



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 21, 2024 – 06:41 am BST

PDB ID : 7OIJ  
Title : mPI3Kd in complex with an inhibitor  
Authors : Petersen, J.  
Deposited on : 2021-05-11  
Resolution : 1.80 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>.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36.2  
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) : 2.36.2

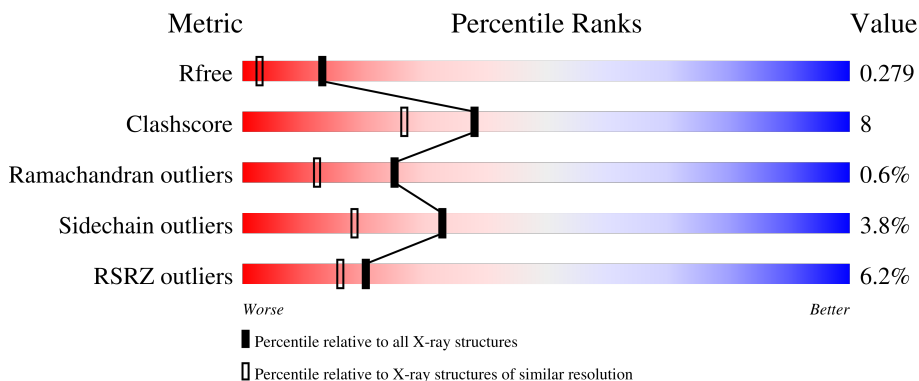
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	AAA	1084	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6982 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 Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit delta isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AAA	827	6678	4281	1131	1211	55	3	1	0

There are 41 discrepancies between the modelled and reference sequences:

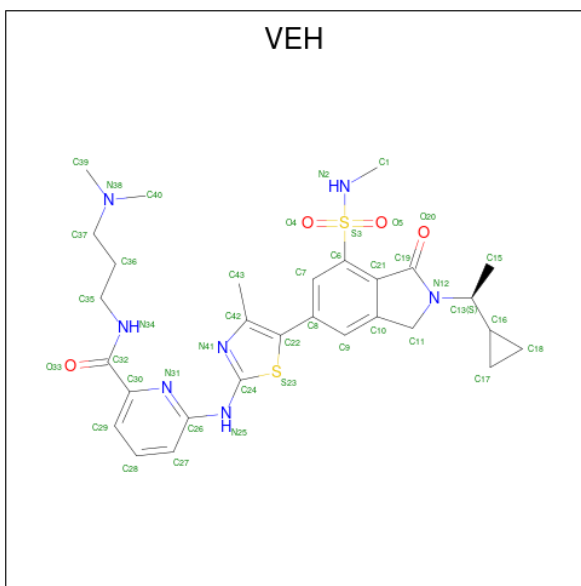
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-39	MET	-	initiating methionine	UNP O35904
AAA	-38	SER	-	expression tag	UNP O35904
AAA	-37	TYR	-	expression tag	UNP O35904
AAA	-36	HIS	-	expression tag	UNP O35904
AAA	-35	ASN	-	expression tag	UNP O35904
AAA	-34	HIS	-	expression tag	UNP O35904
AAA	-33	ASN	-	expression tag	UNP O35904
AAA	-32	HIS	-	expression tag	UNP O35904
AAA	-31	ASN	-	expression tag	UNP O35904
AAA	-30	HIS	-	expression tag	UNP O35904
AAA	-29	ASN	-	expression tag	UNP O35904
AAA	-28	HIS	-	expression tag	UNP O35904
AAA	-27	ASN	-	expression tag	UNP O35904
AAA	-26	HIS	-	expression tag	UNP O35904
AAA	-25	ASN	-	expression tag	UNP O35904
AAA	-24	ASP	-	expression tag	UNP O35904
AAA	-23	TYR	-	expression tag	UNP O35904
AAA	-22	ASP	-	expression tag	UNP O35904
AAA	-21	ILE	-	expression tag	UNP O35904
AAA	-20	PRO	-	expression tag	UNP O35904
AAA	-19	THR	-	expression tag	UNP O35904
AAA	-18	THR	-	expression tag	UNP O35904
AAA	-17	GLU	-	expression tag	UNP O35904
AAA	-16	ASN	-	expression tag	UNP O35904
AAA	-15	LEU	-	expression tag	UNP O35904
AAA	-14	TYR	-	expression tag	UNP O35904

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-13	PHE	-	expression tag	UNP O35904
AAA	-12	GLN	-	expression tag	UNP O35904
AAA	-11	GLY	-	expression tag	UNP O35904
AAA	-10	ALA	-	expression tag	UNP O35904
AAA	-9	MET	-	expression tag	UNP O35904
AAA	-8	ASP	-	expression tag	UNP O35904
AAA	-7	LEU	-	expression tag	UNP O35904
AAA	99	GLU	-	insertion	UNP O35904
AAA	100	ASN	-	insertion	UNP O35904
AAA	101	LEU	-	insertion	UNP O35904
AAA	102	TYR	-	insertion	UNP O35904
AAA	103	PHE	-	insertion	UNP O35904
AAA	104	GLN	-	insertion	UNP O35904
AAA	105	GLY	-	insertion	UNP O35904
AAA	510A	GLN	-	insertion	UNP O35904

- Molecule 2 is 6-[[5-[2-[(1S)-1-cyclopropylethyl]-7-(methylsulfamoyl)-1-oxidanylidene-3H-isoindol-5-yl]-4-methyl-1,3-thiazol-2-yl]amino]-N-[3-(dimethylamino)propyl]pyridine-2-carboxamide (three-letter code: VEH) (formula: C<sub>29</sub>H<sub>37</sub>N<sub>7</sub>O<sub>4</sub>S<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).

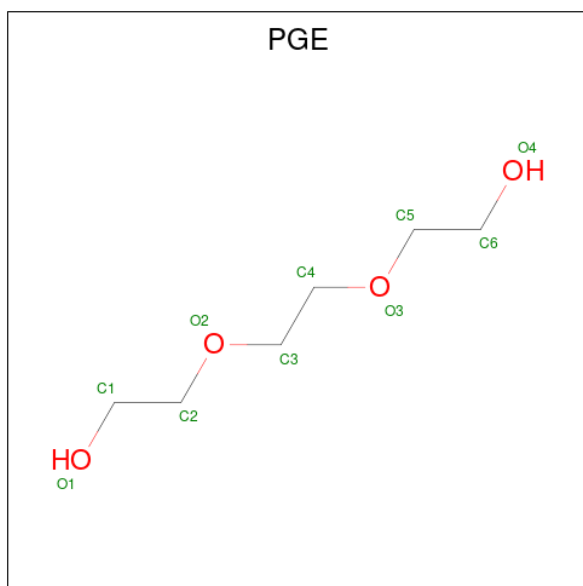


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	AAA	1	42	29	7	4	2	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total Na 1 1	0	0

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	1	Total C O 4 2 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	257	Total O 257 257	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	141.81Å 64.84Å 116.58Å 90.00° 103.66° 90.00°	Depositor
Resolution (Å)	42.97 – 1.80 42.97 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.2 (42.97-1.80) 99.2 (42.97-1.80)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.17 (at 1.79Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.236 , 0.276 0.241 , 0.279	Depositor DCC
$R_{free}$ test set	4709 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.9	Xtrriage
Anisotropy	0.074	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 40.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6982	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.29% 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: NA, PGE, VEH

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	AAA	0.71	0/6824	0.81	0/9207

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	AAA	6678	0	6656	101	1
2	AAA	42	0	0	1	0
3	AAA	1	0	0	0	0
4	AAA	4	0	5	1	0
5	AAA	257	0	0	3	0
All	All	6982	0	6661	102	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.

All (102) 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:AAA:495:ILE:HG23	1:AAA:563:GLN:HA	1.38	1.05
1:AAA:495:ILE:CG2	1:AAA:563:GLN:HA	2.02	0.90
1:AAA:495:ILE:HD13	1:AAA:562:ALA:O	1.78	0.84
1:AAA:495:ILE:CD1	1:AAA:562:ALA:O	2.28	0.81
1:AAA:367:SER:HB3	1:AAA:368:GLU:C	2.05	0.77
1:AAA:912:PHE:CB	1:AAA:913:GLY:HA3	2.15	0.77
1:AAA:642:LYS:HE3	4:AAA:1103:PGE:O4	1.86	0.76
1:AAA:495:ILE:HG12	1:AAA:562:ALA:C	2.08	0.74
1:AAA:495:ILE:HG21	1:AAA:566:TYR:CB	2.17	0.73
1:AAA:549:LEU:HG	1:AAA:564:MET:HE3	1.70	0.72
1:AAA:387:MET:HE3	1:AAA:590:CYS:HB3	1.71	0.71
1:AAA:756:MET:CE	1:AAA:781:GLY:HA3	2.21	0.69
1:AAA:495:ILE:HG21	1:AAA:566:TYR:HB3	1.76	0.68
1:AAA:387:MET:HE2	1:AAA:590:CYS:SG	2.35	0.66
1:AAA:549:LEU:HG	1:AAA:564:MET:CE	2.26	0.66
1:AAA:495:ILE:HG12	1:AAA:562:ALA:O	1.98	0.64
1:AAA:495:ILE:HG21	1:AAA:566:TYR:HB2	1.79	0.64
1:AAA:495:ILE:CG1	1:AAA:562:ALA:O	2.45	0.64
1:AAA:756:MET:HE3	1:AAA:781:GLY:HA3	1.81	0.62
1:AAA:912:PHE:HB2	1:AAA:913:GLY:HA3	1.82	0.61
1:AAA:912:PHE:HB3	1:AAA:913:GLY:HA3	1.82	0.61
1:AAA:332:LYS:HE3	1:AAA:333:VAL:N	2.17	0.60
1:AAA:495:ILE:CG2	1:AAA:566:TYR:HB2	2.32	0.60
1:AAA:154:ARG:HD2	1:AAA:165:TYR:CE2	2.37	0.59
2:AAA:1101:VEH:N31	2:AAA:1101:VEH:S23	2.76	0.58
1:AAA:833:THR:OG1	1:AAA:836:ASN:HB2	2.02	0.58
1:AAA:194:VAL:HG21	1:AAA:216:LEU:HD21	1.86	0.58
1:AAA:495:ILE:O	1:AAA:497:GLU:N	2.37	0.56
1:AAA:534:MET:CE	1:AAA:534:MET:HA	2.35	0.56
1:AAA:841:LYS:HG2	1:AAA:844:MET:HG3	1.88	0.56
1:AAA:367:SER:CB	1:AAA:368:GLU:C	2.75	0.55
1:AAA:601:ARG:HD2	5:AAA:1407:HOH:O	2.05	0.55
1:AAA:495:ILE:HB	1:AAA:566:TYR:HB2	1.88	0.55
1:AAA:495:ILE:CG2	1:AAA:566:TYR:CB	2.84	0.55
1:AAA:1006:LYS:HB3	1:AAA:1010:GLU:HB2	1.89	0.55
1:AAA:495:ILE:HG12	1:AAA:562:ALA:HB1	1.88	0.54
1:AAA:495:ILE:CB	1:AAA:566:TYR:HB2	2.37	0.54
1:AAA:491:ILE:HG22	1:AAA:495:ILE:HD11	1.89	0.54
1:AAA:491:ILE:O	1:AAA:495:ILE:HG13	2.07	0.54
1:AAA:496:THR:HG22	1:AAA:566:TYR:CE1	2.43	0.54
1:AAA:330:GLY:C	1:AAA:331:ARG:HG3	2.27	0.54
1:AAA:332:LYS:HE3	1:AAA:332:LYS:C	2.29	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:892:GLY:O	1:AAA:894:ARG:HG2	2.09	0.53
1:AAA:495:ILE:HG23	1:AAA:563:GLN:CA	2.27	0.52
1:AAA:434:THR:HG21	1:AAA:477:GLU:HA	1.93	0.51
1:AAA:154:ARG:HD2	1:AAA:165:TYR:CZ	2.45	0.51
1:AAA:331:ARG:O	1:AAA:469:ALA:HA	2.10	0.51
1:AAA:756:MET:HE2	1:AAA:781:GLY:HA3	1.89	0.51
1:AAA:495:ILE:CG1	1:AAA:562:ALA:HB1	2.41	0.51
1:AAA:358:VAL:HG22	1:AAA:377:PHE:CE2	2.46	0.51
1:AAA:366:CYS:O	1:AAA:367:SER:CB	2.59	0.51
1:AAA:492:LEU:HA	1:AAA:495:ILE:HD12	1.93	0.50
1:AAA:188:ARG:HD2	1:AAA:189:ALA:N	2.26	0.50
1:AAA:743:GLU:HG2	1:AAA:764:SER:O	2.12	0.49
1:AAA:271:THR:O	1:AAA:273:HIS:HD2	1.95	0.48
1:AAA:581:GLU:HB2	1:AAA:976:HIS:CE1	2.48	0.48
1:AAA:489:GLU:HG3	1:AAA:490:LYS:N	2.28	0.48
1:AAA:859:LEU:HD21	1:AAA:905:GLY:HA2	1.94	0.48
1:AAA:1012:LEU:O	1:AAA:1016:ARG:HG3	2.13	0.48
1:AAA:356:LYS:HE3	1:AAA:378:ASP:HB2	1.96	0.47
1:AAA:491:ILE:O	1:AAA:495:ILE:CD1	2.62	0.47
1:AAA:172:GLU:HG3	1:AAA:263:CYS:SG	2.55	0.47
1:AAA:841:LYS:HD3	1:AAA:841:LYS:H	1.79	0.46
1:AAA:495:ILE:C	1:AAA:497:GLU:N	2.68	0.46
1:AAA:435:GLY:O	1:AAA:475:LEU:N	2.25	0.46
1:AAA:617:GLN:HE21	1:AAA:984:ALA:HA	1.80	0.46
1:AAA:349:HIS:HE1	5:AAA:1241:HOH:O	1.99	0.46
1:AAA:617:GLN:HE22	1:AAA:620:LYS:NZ	2.14	0.45
1:AAA:247:HIS:HB2	1:AAA:738:SER:HA	1.98	0.45
1:AAA:157:LEU:HD22	1:AAA:161:GLU:HB3	1.97	0.45
1:AAA:419:ALA:HB3	1:AAA:441:MET:HE3	1.97	0.45
1:AAA:188:ARG:NH2	1:AAA:266:LEU:HD22	2.31	0.45
1:AAA:367:SER:HA	1:AAA:368:GLU:HB3	1.99	0.45
1:AAA:192:VAL:HG13	1:AAA:272:PRO:HB2	1.99	0.45
1:AAA:912:PHE:CB	1:AAA:913:GLY:CA	2.91	0.44
1:AAA:368:GLU:N	1:AAA:369:PRO:CD	2.81	0.44
1:AAA:784:LEU:O	1:AAA:788:MET:HG2	2.17	0.44
1:AAA:387:MET:CE	1:AAA:590:CYS:SG	3.04	0.44
1:AAA:423:LEU:H	1:AAA:423:LEU:HD12	1.82	0.44
1:AAA:553:THR:HB	1:AAA:564:MET:HE2	2.00	0.44
1:AAA:423:LEU:HD12	1:AAA:423:LEU:N	2.33	0.44
1:AAA:495:ILE:HG12	1:AAA:562:ALA:CB	2.47	0.44
1:AAA:587:PHE:HB3	1:AAA:592:VAL:HG11	1.99	0.43

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:579:ALA:HB1	1:AAA:600:LEU:HG	2.00	0.43
1:AAA:238:GLU:HB3	1:AAA:278:HIS:CE1	2.53	0.43
1:AAA:281:SER:O	1:AAA:285:MET:HG3	2.18	0.43
1:AAA:329:GLU:O	1:AAA:472:VAL:HG22	2.18	0.43
1:AAA:930:VAL:HG22	1:AAA:997:TYR:OH	2.18	0.43
1:AAA:534:MET:HA	1:AAA:534:MET:HE2	2.00	0.43
1:AAA:496:THR:HG22	1:AAA:566:TYR:CZ	2.54	0.43
1:AAA:913:GLY:CA	1:AAA:914:HIS:HB2	2.49	0.43
1:AAA:316:LEU:HA	5:AAA:1424:HOH:O	2.18	0.43
1:AAA:515:LEU:HD12	1:AAA:515:LEU:C	2.39	0.42
1:AAA:367:SER:HB2	1:AAA:369:PRO:N	2.35	0.42
1:AAA:495:ILE:O	1:AAA:496:THR:C	2.58	0.42
1:AAA:637:ALA:HB1	1:AAA:644:GLY:HA2	2.02	0.42
1:AAA:617:GLN:NE2	1:AAA:984:ALA:HA	2.35	0.42
1:AAA:913:GLY:N	1:AAA:914:HIS:HB2	2.35	0.42
1:AAA:523:LEU:O	1:AAA:528:LYS:HE3	2.21	0.41
1:AAA:550:LEU:O	1:AAA:553:THR:CG2	2.68	0.41
1:AAA:511:LEU:O	1:AAA:514:ILE:HG22	2.21	0.41
1:AAA:915:PHE:CD1	1:AAA:915:PHE:C	2.94	0.41

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:AAA:714:MET:SD	1:AAA:714:MET:SD[2_555]	1.48	0.72

## 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	AAA	806/1084 (74%)	778 (96%)	23 (3%)	5 (1%)	25 12

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	367	SER
1	AAA	893	ASP
1	AAA	1026	SER
1	AAA	368	GLU
1	AAA	496	THR

### 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	AAA	734/962 (76%)	706 (96%)	28 (4%)	33 18

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	111	LYS
1	AAA	190	LEU
1	AAA	203	PHE
1	AAA	212	MET
1	AAA	291	ASN
1	AAA	316	LEU
1	AAA	332	LYS
1	AAA	340	LYS
1	AAA	352	GLU
1	AAA	356	LYS
1	AAA	360	SER
1	AAA	423	LEU
1	AAA	453	LEU
1	AAA	517	ARG
1	AAA	530	LEU
1	AAA	534	MET
1	AAA	553	THR
1	AAA	634	LEU
1	AAA	743	GLU
1	AAA	752	MET

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type
1	AAA	756	MET
1	AAA	779	LYS
1	AAA	795	GLN
1	AAA	836	ASN
1	AAA	841	LYS
1	AAA	898	ASN
1	AAA	915	PHE
1	AAA	1026	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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, 1 is 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	PGE	AAA	1103	-	3,3,9	0.55	0	2,2,8	0.25	0
2	VEH	AAA	1101	-	39,46,46	1.21	2 (5%)	46,68,68	2.61	13 (28%)

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	PGE	AAA	1103	-	-	0/1/1/7	-
2	VEH	AAA	1101	-	-	4/34/50/50	0/5/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	1101	VEH	C9-C10	-3.42	1.33	1.39
2	AAA	1101	VEH	C29-C30	2.69	1.44	1.39

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AAA	1101	VEH	C10-C11-N12	10.77	105.77	102.18
2	AAA	1101	VEH	C11-N12-C19	-8.29	109.71	113.12
2	AAA	1101	VEH	C30-C32-N34	4.00	121.18	115.59
2	AAA	1101	VEH	C13-N12-C19	3.83	127.02	122.91
2	AAA	1101	VEH	C29-C28-C27	-3.01	115.98	120.25
2	AAA	1101	VEH	C29-C30-N31	-2.96	119.45	122.92
2	AAA	1101	VEH	C35-N34-C32	2.87	128.63	122.08
2	AAA	1101	VEH	C30-N31-C26	2.65	119.78	117.83
2	AAA	1101	VEH	O20-C19-C21	-2.50	125.53	129.09
2	AAA	1101	VEH	C28-C29-C30	2.42	121.55	118.63
2	AAA	1101	VEH	O5-S3-O4	2.31	122.38	119.55
2	AAA	1101	VEH	C29-C30-C32	2.20	123.15	119.57
2	AAA	1101	VEH	C17-C16-C13	-2.06	114.90	119.32

There are no chirality outliers.

All (4) torsion outliers are listed below:

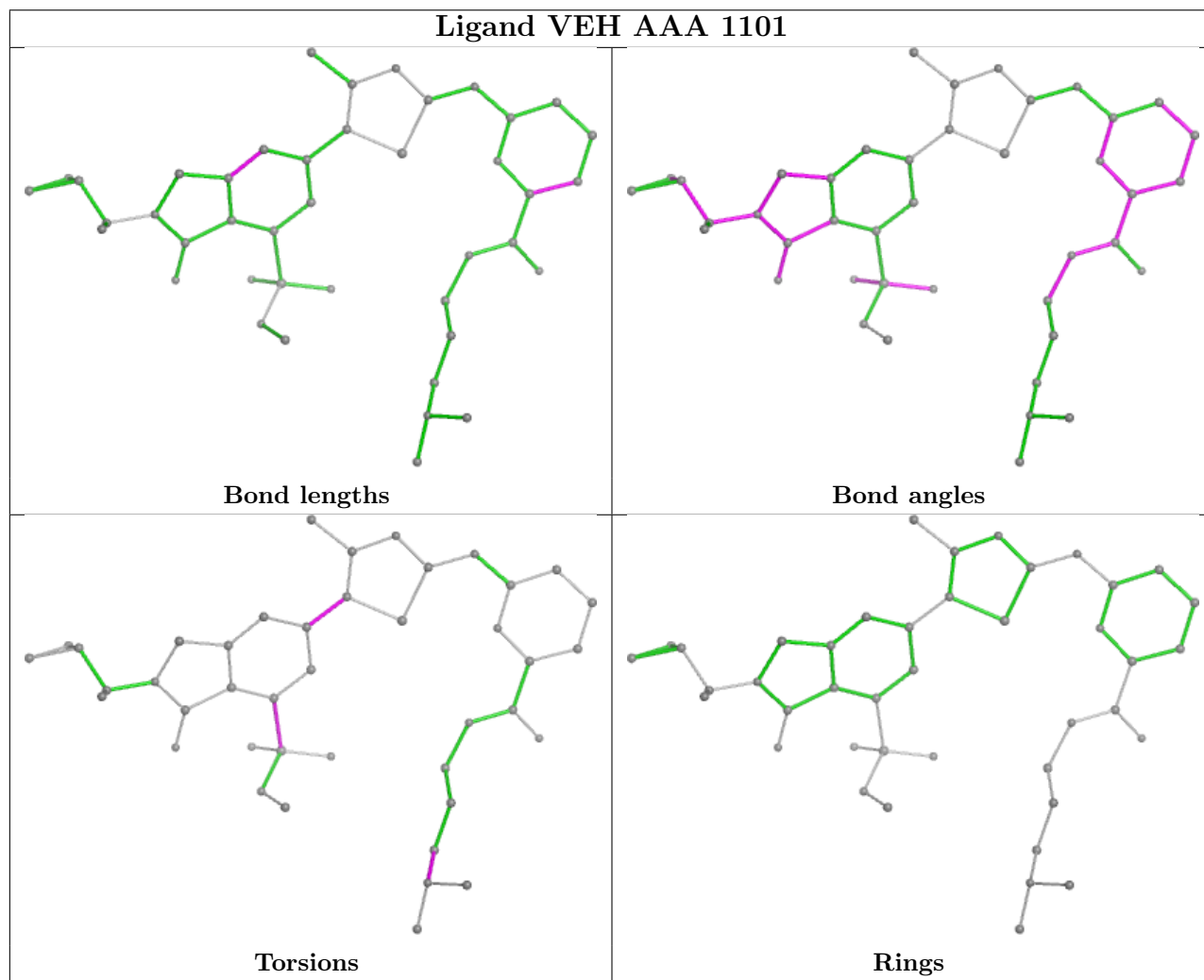
Mol	Chain	Res	Type	Atoms
2	AAA	1101	VEH	C42-C22-C8-C7
2	AAA	1101	VEH	C36-C37-N38-C40
2	AAA	1101	VEH	C21-C6-S3-O4
2	AAA	1101	VEH	C42-C22-C8-C9

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	AAA	1103	PGE	1	0
2	AAA	1101	VEH	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 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	AAA	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AAA	497:GLU	C	509:GLU	N	21.77



## 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	AAA	827/1084 (76%)	0.31	51 (6%) <span style="border: 1px solid red; padding: 2px;">20</span> <span style="border: 1px solid red; padding: 2px;">16</span>	17, 34, 64, 99	2 (0%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	495	ILE	8.5
1	AAA	228	PHE	7.4
1	AAA	366	CYS	6.1
1	AAA	317	TRP	5.8
1	AAA	514	ILE	5.1
1	AAA	515	LEU	4.8
1	AAA	227	VAL	4.3
1	AAA	1027	TRP	4.2
1	AAA	919	PHE	4.1
1	AAA	847	THR	3.9
1	AAA	225	ALA	3.9
1	AAA	398	VAL	3.7
1	AAA	367	SER	3.7
1	AAA	109	VAL	3.6
1	AAA	200	GLU	3.3
1	AAA	843	ASN	3.3
1	AAA	496	THR	3.2
1	AAA	395	TYR	3.1
1	AAA	205	PHE	3.1
1	AAA	396	ALA	3.0
1	AAA	893	ASP	3.0
1	AAA	230	GLN	2.9
1	AAA	846	ALA	2.9
1	AAA	203	PHE	2.8
1	AAA	478	VAL	2.8
1	AAA	913	GLY	2.8
1	AAA	397	VAL	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	AAA	132	ARG	2.7
1	AAA	417	PRO	2.7
1	AAA	198	GLY	2.5
1	AAA	792	GLN	2.5
1	AAA	934	LEU	2.5
1	AAA	745[A]	CYS	2.5
1	AAA	333	VAL	2.5
1	AAA	342	VAL	2.5
1	AAA	416	CYS	2.5
1	AAA	445	VAL	2.4
1	AAA	334	ASN	2.4
1	AAA	894	ARG	2.4
1	AAA	201	GLU	2.4
1	AAA	363	VAL	2.4
1	AAA	914	HIS	2.4
1	AAA	341	LEU	2.3
1	AAA	1017	VAL	2.2
1	AAA	510	GLU	2.2
1	AAA	1018	LYS	2.1
1	AAA	1014	HIS	2.1
1	AAA	917	GLY	2.1
1	AAA	493	GLU	2.0
1	AAA	895	HIS	2.0
1	AAA	1024	ARG	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](#)

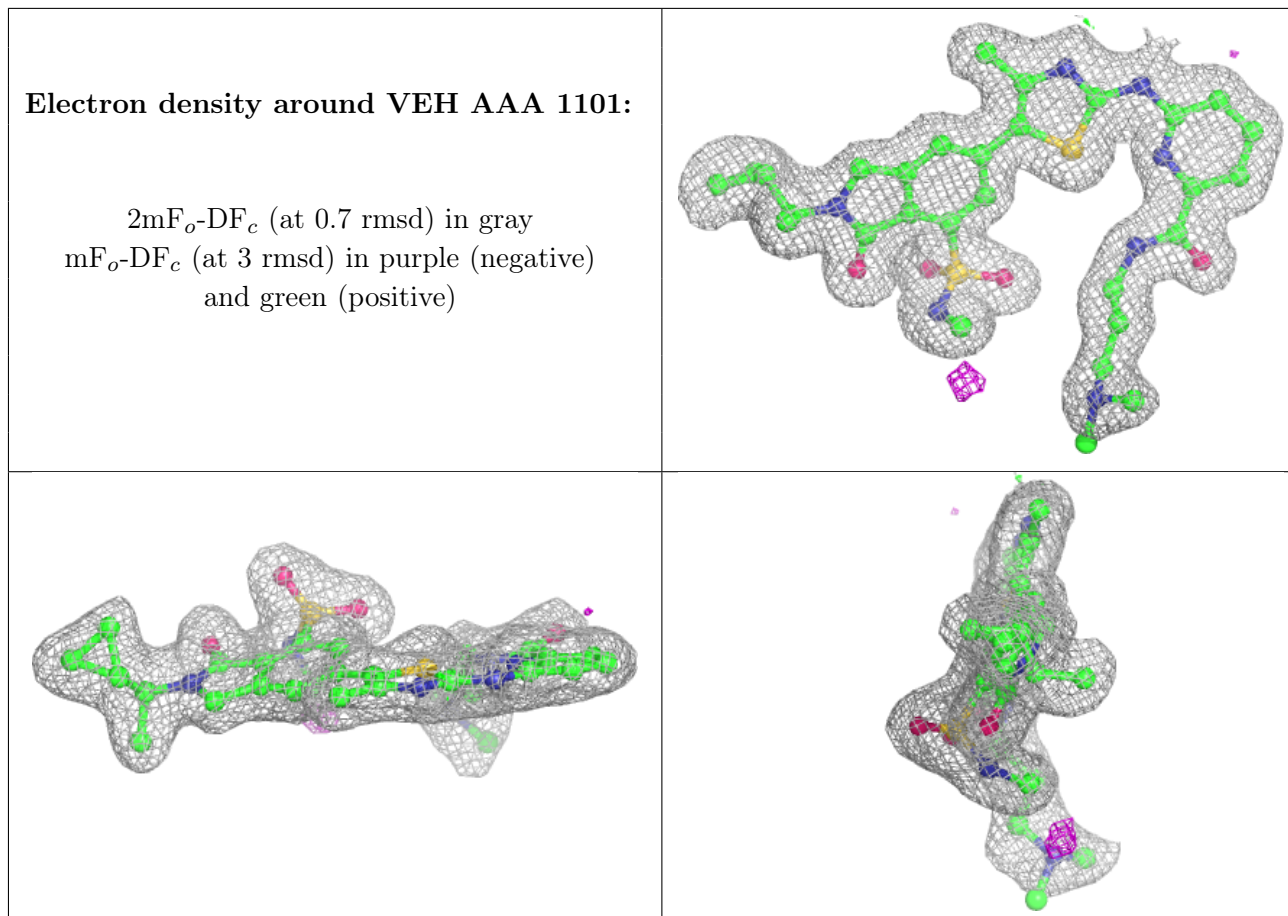
There are no monosaccharides in this entry.

## 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
3	NA	AAA	1102	1/1	0.91	0.22	54,54,54,54	0
4	PGE	AAA	1103	4/10	0.96	0.08	26,29,31,33	0
2	VEH	AAA	1101	42/42	0.98	0.12	16,21,44,53	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.