wwPDB X-ray Structure Validation Summary Report (i)

Apr 20, 2024 – 11:44 pm BST

PDB ID	:	7OIS
Title	:	mPI3Kd in complex with compound 7
Authors	:	Petersen, J.
Deposited on	:	2021-05-12
Resolution	:	2.30 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 (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 (i)) were used in the production of this report:

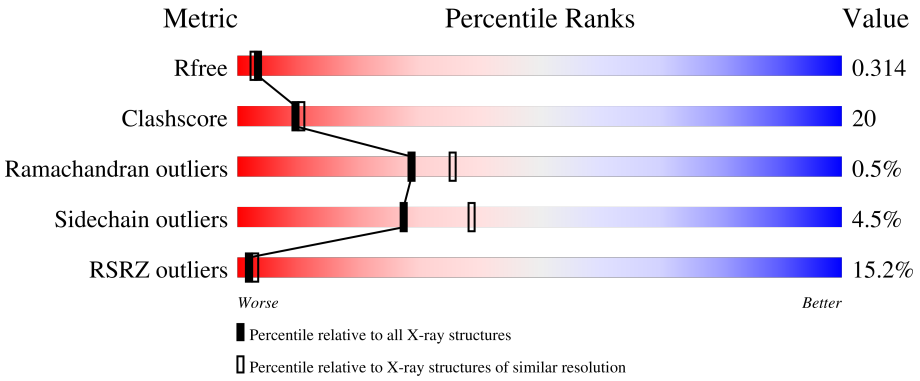
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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
1	AAA	1084	12% 55% 20% · 24%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8250 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

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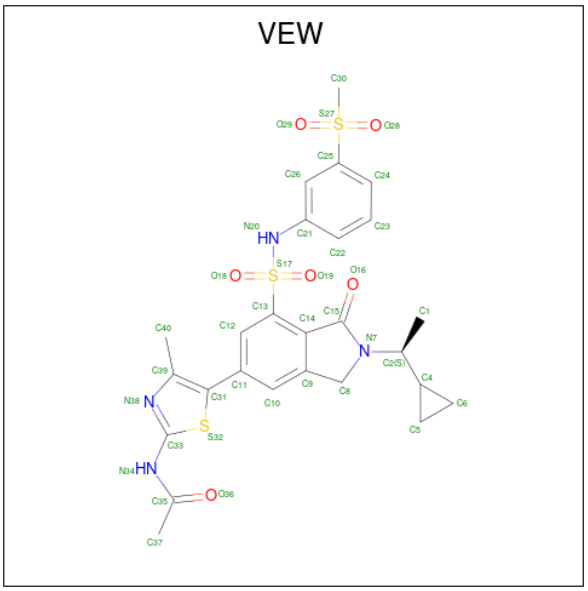
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-13	PHE	-	expression tag	UNP O35904
AAA	-12	GLN	-	expression tag	UNP O35904
AAA	-11	GLY	-	expression tag	UNP O35904
AAA	-10	ALA	-	expression tag	UNP O35904
AAA	-9	MET	-	expression tag	UNP O35904
AAA	-8	ASP	-	expression tag	UNP O35904
AAA	-7	LEU	-	expression 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 SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 3 is N-[5-[2-[(1S)-1-cyclopropylethyl]-7-[(3-methylsulfonylphenyl)sulfamoyl]-1-oxidanylidene-3H-isoindol-5-yl]-4-methyl-1,3-thiazol-2-yl]ethanamide (three-letter code: VEW) (formula: $C_{26}H_{28}N_4O_6S_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	AAA	1	Total	C	N	O	S	0	0
			39	26	4	6	3		

- Molecule 4 is water.

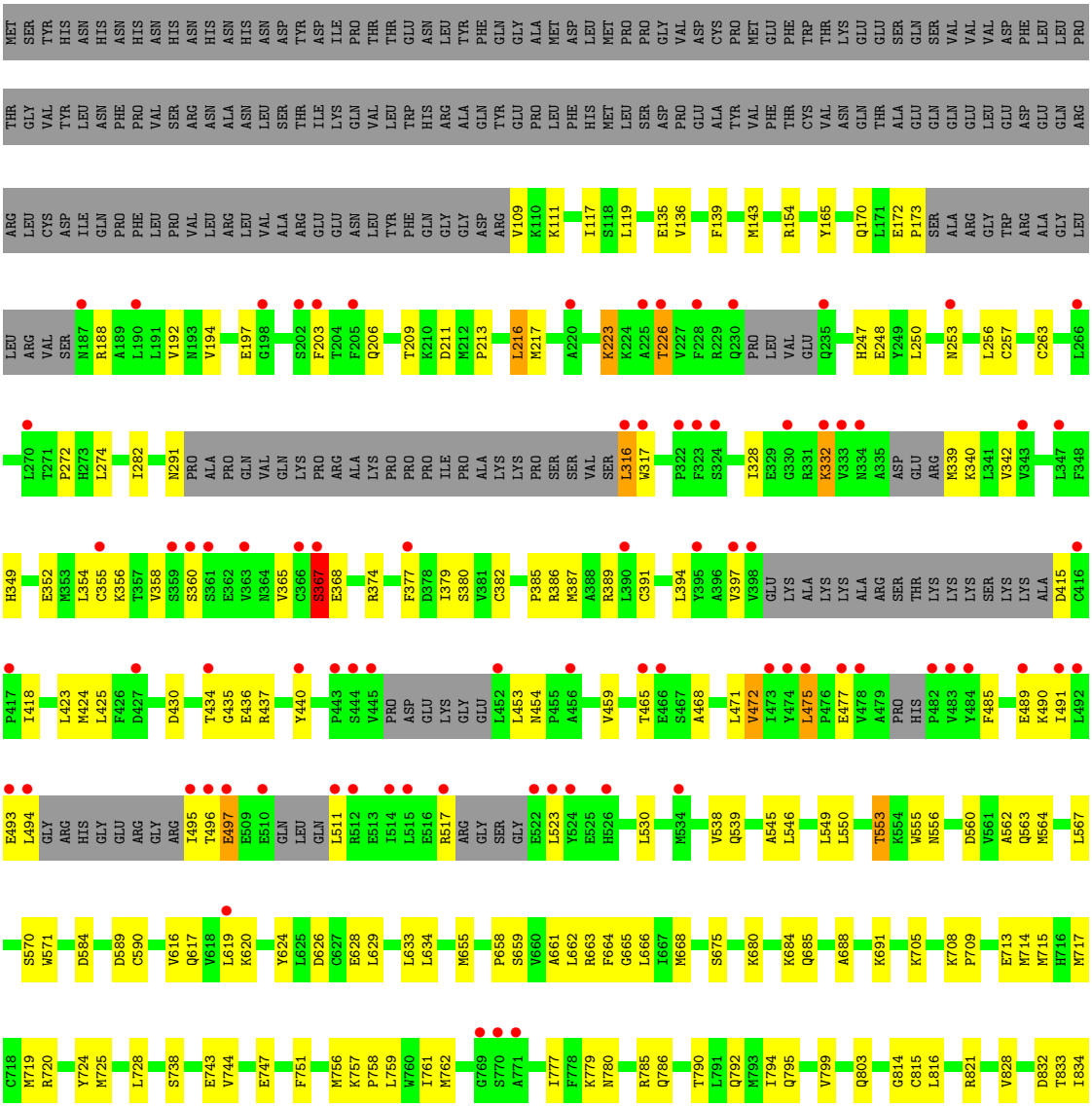
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	1532	Total	O	0	0
			1532	1532		

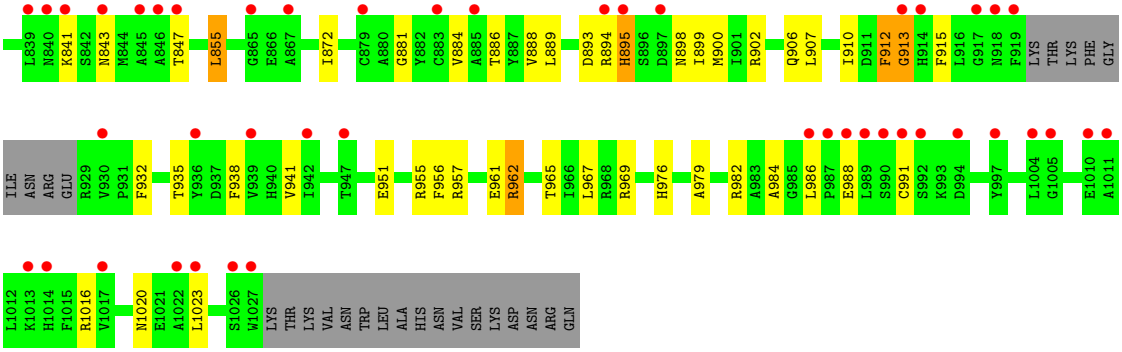
3 Residue-property plots (i)

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: Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit delta isoform

Chain AAA:




L839 N840 K841 S842 N843 M844 A845 A846 T847 L865 G865 E866 A867 I872 C879 A880 G881 Y882 C883 V884 A885 T886 Y887 V888 L889 D893 R894 H895 S896 D897 N898 I899 M900 I901 R902 Q906 L907 I910 D911 F912 G913 H914 F915 L916 G917 N918 F919 LYS THR LYS PHE GLY
ILE ASN ARG GLU R929 V930 P931 F932 T935 Y936 D937 F938 V939 H940 V941 I942 T947 E951 R955 F956 R957 E961 R962 T965 I966 L967 R968 R969 H976 A979 R982 A983 A984 G985 L986 P987 E988 L989 S990 C991 S992 K993 D994 Y997 L1004 G1005 E1010 A1011
L1012 K1013 H1014 F1015 R1016 V1017 N1020 E1021 A1022 L1023 S1026 W1027 LYS THR LYS VAL ASN TRP LEU ALA HIS ASN VAL SER LYS ASP ASN ARG GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	141.90Å 64.96Å 116.14Å 90.00° 103.59° 90.00°	Depositor
Resolution (Å)	31.02 – 2.30 31.01 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (31.02-2.30) 99.9 (31.01-2.30)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.12 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.208 , 0.306 0.216 , 0.314	Depositor DCC
R_{free} test set	2316 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	18.0	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 51.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	8250	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.44% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: VEW, NA

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	0.68	0/6824	0.77	1/9207 (0.0%)

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	AAA	912	PHE	CB-CA-C	6.55	123.50	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	258	1
2	AAA	1	0	0	0	0
3	AAA	39	0	0	4	0
4	AAA	1532	0	0	187	4
All	All	8250	0	6656	261	5

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 20.

The worst 5 of 261 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:900:MET:SD	4:AAA:2359:HOH:O	1.96	1.20
1:AAA:900:MET:SD	4:AAA:1624:HOH:O	1.98	1.19
1:AAA:900:MET:CG	4:AAA:2359:HOH:O	1.90	1.16
1:AAA:900:MET:HG2	4:AAA:2359:HOH:O	1.44	1.15
1:AAA:910:ILE:HG13	4:AAA:2101:HOH:O	1.48	1.13

All (5) 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]	1.63	0.57
4:AAA:1450:HOH:O	4:AAA:1808:HOH:O[2_555]	2.00	0.20
4:AAA:1609:HOH:O	4:AAA:2241:HOH:O[4_445]	2.12	0.08
4:AAA:1825:HOH:O	4:AAA:2151:HOH:O[3_545]	2.17	0.03
4:AAA:2475:HOH:O	4:AAA:2628:HOH:O[3_455]	2.18	0.02

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%)	768 (95%)	34 (4%)	4 (0%)	29 35

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	496	THR
1	AAA	893	ASP
1	AAA	367	SER
1	AAA	913	GLY

5.3.2 Protein sidechains

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%)	701 (96%)	33 (4%)	27 39

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	843	ASN
1	AAA	855	LEU
1	AAA	962	ARG
1	AAA	367	SER
1	AAA	356	LYS

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

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 1 is 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	VEW	AAA	1102	-	37,43,43	1.16	4 (10%)	45,67,67	3.76	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
3	VEW	AAA	1102	-	-	10/31/47/47	0/5/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AAA	1102	VEW	C10-C9	-2.68	1.34	1.39
3	AAA	1102	VEW	C33-N34	2.65	1.41	1.36
3	AAA	1102	VEW	C12-C13	-2.64	1.35	1.39
3	AAA	1102	VEW	C21-N20	-2.43	1.39	1.43

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	AAA	1102	VEW	C9-C8-N7	16.36	107.63	102.18
3	AAA	1102	VEW	C8-N7-C15	-11.73	108.30	113.12
3	AAA	1102	VEW	O28-S27-C25	-8.89	101.00	108.25
3	AAA	1102	VEW	C37-C35-N34	4.73	121.92	114.98
3	AAA	1102	VEW	O29-S27-C25	4.26	111.72	108.25

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

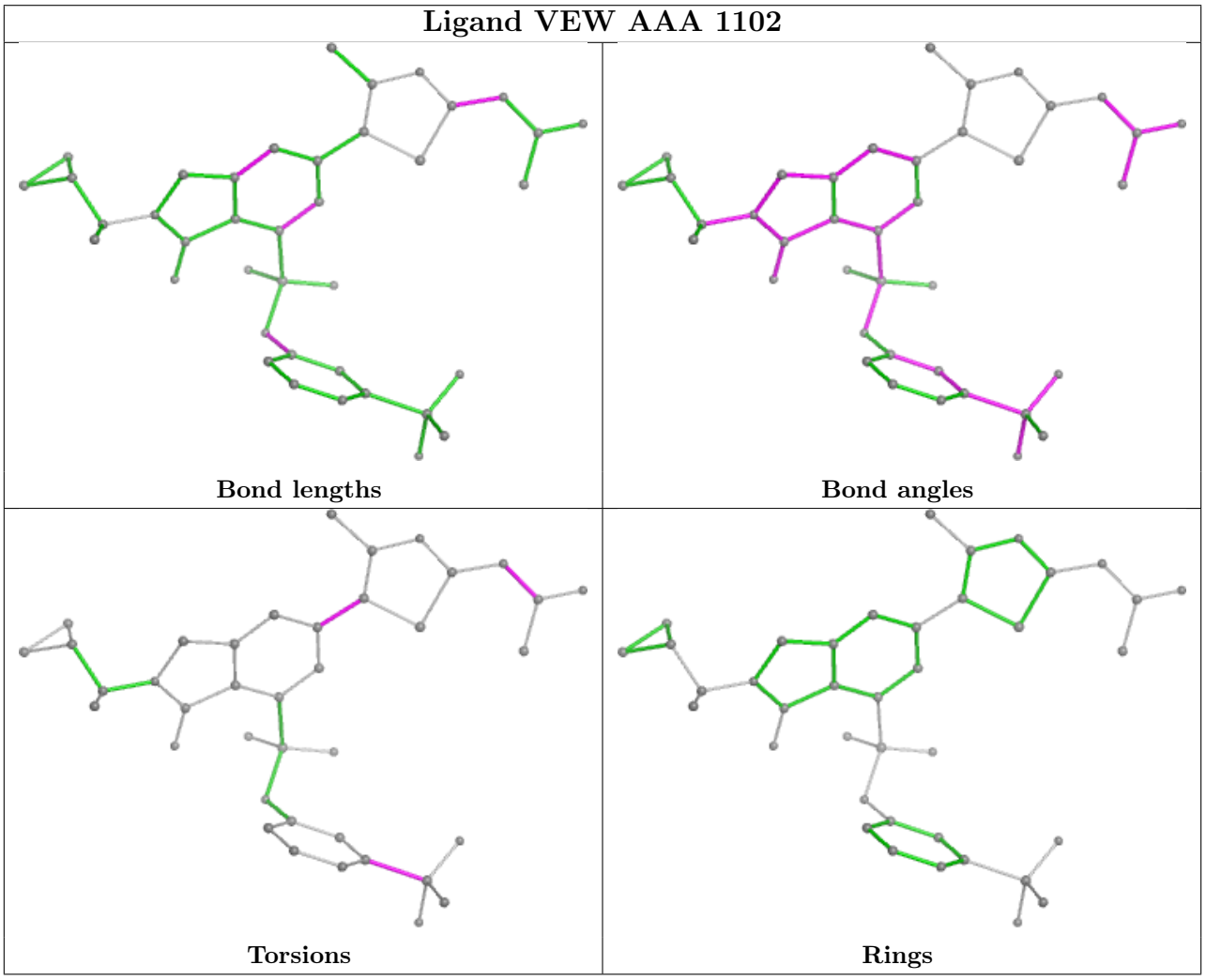
Mol	Chain	Res	Type	Atoms
3	AAA	1102	VEW	C24-C25-S27-C30
3	AAA	1102	VEW	C26-C25-S27-C30
3	AAA	1102	VEW	C24-C25-S27-O28
3	AAA	1102	VEW	C26-C25-S27-O28
3	AAA	1102	VEW	C37-C35-N34-C33

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AAA	1102	VEW	4	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)

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	22.95

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^{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(Å^2)	Q<0.9
1	AAA	827/1084 (76%)	0.98	126 (15%)	2	3	21, 43, 74, 99	2 (0%)

The worst 5 of 126 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	913	GLY	8.7
1	AAA	514	ILE	7.8
1	AAA	919	PHE	7.3
1	AAA	228	PHE	6.8
1	AAA	333	VAL	6.4

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

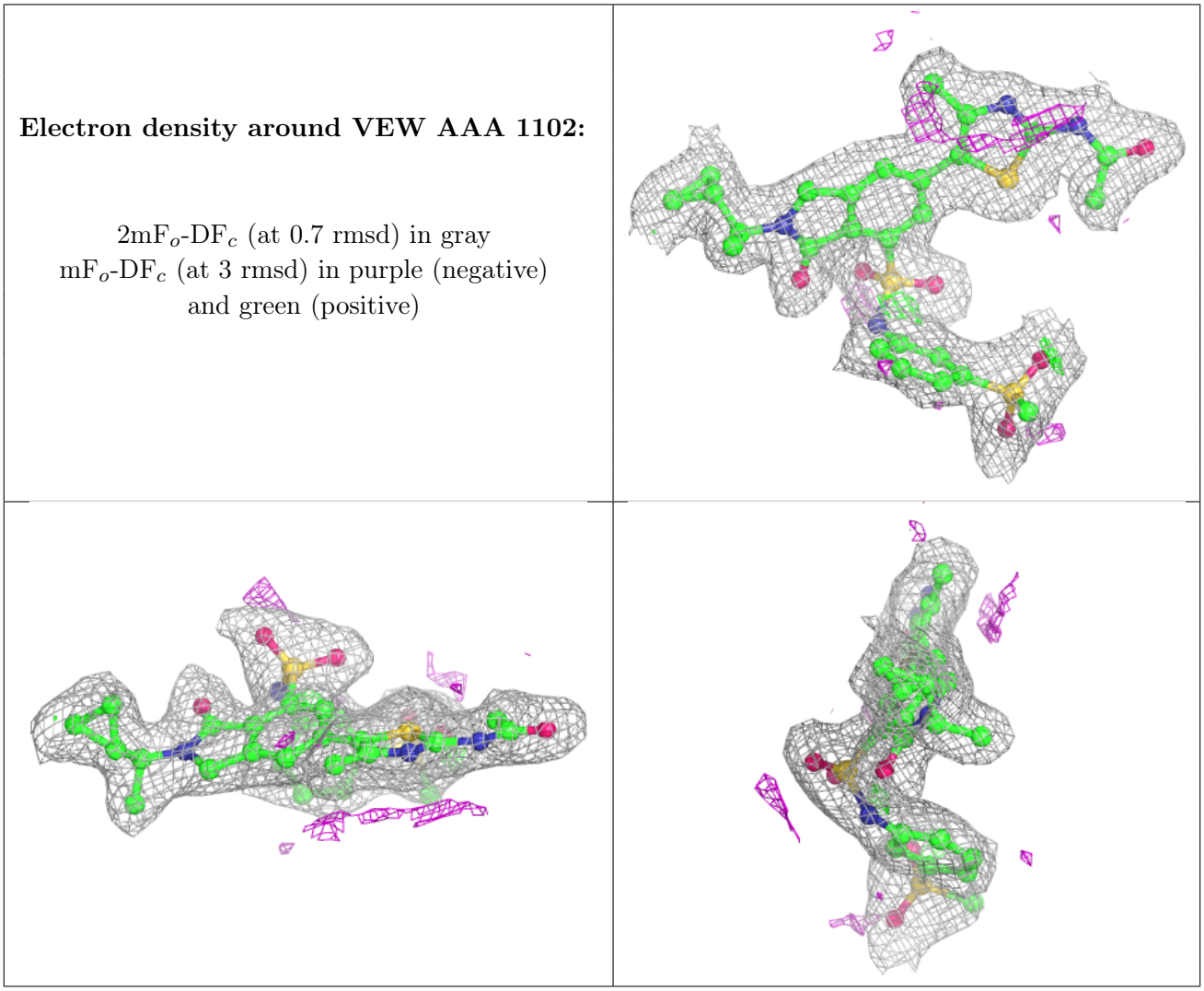
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NA	AAA	1101	1/1	0.83	0.23	72,72,72,72	0
3	VEW	AAA	1102	39/39	0.95	0.14	21,26,43,48	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 VEW AAA 1102:

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



6.5 Other polymers (i)

There are no such residues in this entry.