Full wwPDB X-ray Structure Validation Report (i)

Aug 23, 2023 – 08:42 AM EDT

PDB ID	:	3CJF
Title	:	Crystal structure of VEGFR2 in complex with a 3,4,5-trimethoxy aniline containing pyrimidine
Authors	:	Nolte, R.T.
Deposited on	:	2008-03-12
Resolution	:	2.15 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 (i)) were used in the production of this report:

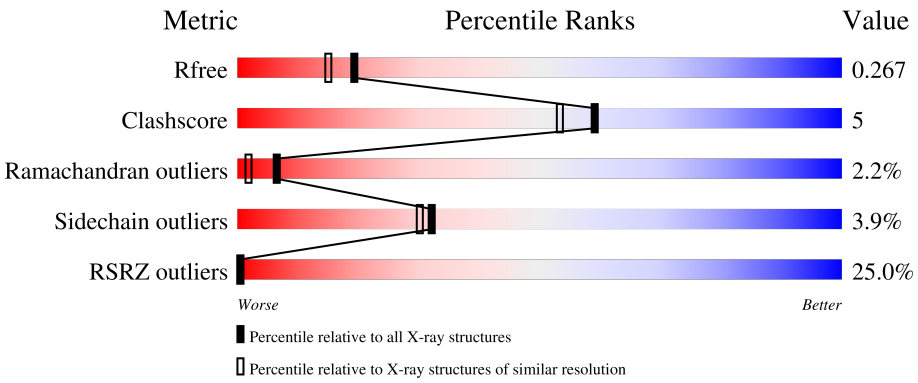
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	A	309	22%, 81%, 9%, •, 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	4	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2428 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.

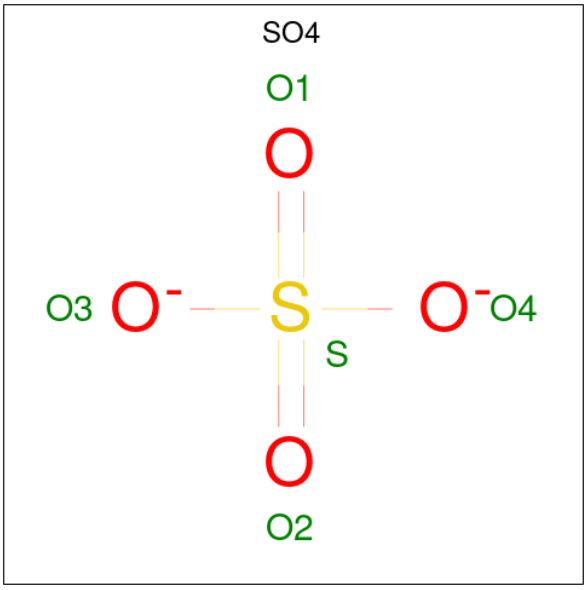
- Molecule 1 is a protein called Vascular endothelial growth factor receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	281	2296	1460	406	412	18	0	7	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	833	ASN	LYS	See remark 999	UNP P35968

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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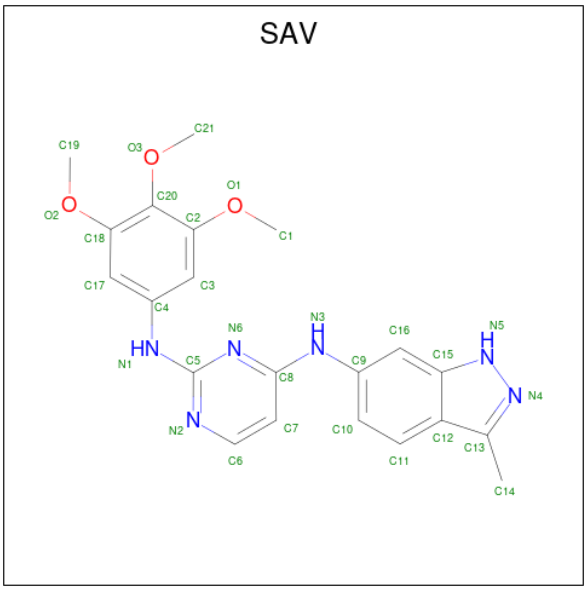
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0

- Molecule 3 is N 4 -(3-methyl-1H-indazol-6-yl)-N 2 -(3,4,5-trimethoxyphenyl)pyrimidine-2,4-diamine (three-letter code: SAV) (formula: $C_{21}H_{22}N_6O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	30	21	6	3	0	0

- Molecule 4 is water.

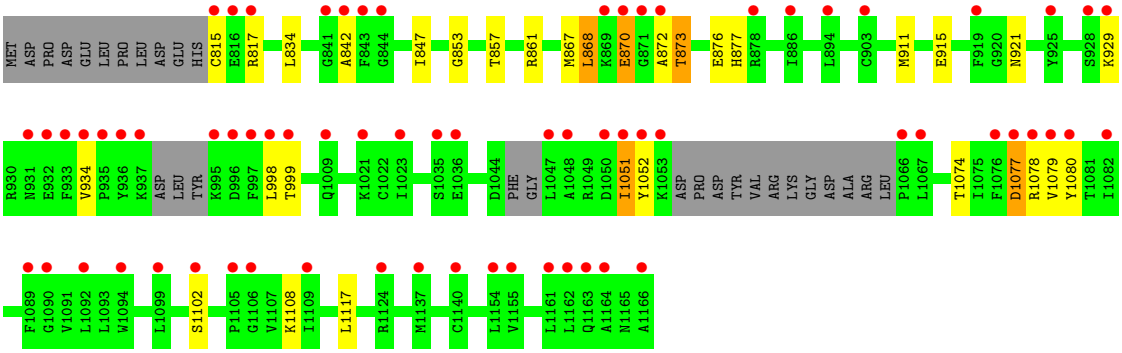
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	82	82	82	0	0

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: Vascular endothelial growth factor receptor 2

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	37.44Å 94.74Å 96.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.92 – 2.15 34.91 – 2.15	Depositor EDS
% Data completeness (in resolution range)	96.2 (34.92-2.15) 96.2 (34.91-2.15)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.72 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.204 , 0.258 0.212 , 0.267	Depositor DCC
R_{free} test set	601 reflections (3.23%)	wwPDB-VP
Wilson B-factor (Å^2)	44.7	Xtriage
Anisotropy	0.544	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 88.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.011 for -h,l,k	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	2428	wwPDB-VP
Average B, all atoms (Å^2)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.43% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, SAV, CSO

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	0.54	0/2299	0.63	0/3093

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
1	A	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1051	ILE	Peptide
1	A	872	ALA	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	2296	0	2280	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	20	0	0	0	0
3	A	30	0	22	5	0
4	A	82	0	0	1	0
All	All	2428	0	2302	22	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 5.

All (22) 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:834:LEU:HD22	1:A:847:ILE:HD11	1.17	1.13
1:A:834:LEU:HD22	1:A:847:ILE:CD1	1.94	0.98
1:A:834:LEU:CD2	1:A:847:ILE:HD11	1.99	0.92
1:A:873:THR:HG22	1:A:876:GLU:H	1.49	0.77
1:A:1052:TYR:CB	4:A:1240:HOH:O	2.40	0.69
1:A:868:LEU:HD11	1:A:877:HIS:HA	1.83	0.60
1:A:834:LEU:HB3	1:A:847:ILE:HD12	1.86	0.56
1:A:834:LEU:HD13	1:A:847:ILE:CD1	2.36	0.56
1:A:929:LYS:HE2	1:A:998:LEU:HD13	1.90	0.54
1:A:867:MET:HB3	1:A:911:MET:HG2	1.93	0.51
1:A:934:VAL:O	1:A:999:THR:HA	2.13	0.48
1:A:834:LEU:HD13	1:A:847:ILE:HD11	1.96	0.48
1:A:1074:THR:O	1:A:1078:ARG:N	2.45	0.47
3:A:1167:SAV:N6	3:A:1167:SAV:H3	2.30	0.46
1:A:915:GLU:O	3:A:1167:SAV:H6	2.18	0.44
1:A:1052:TYR:CB	1:A:1080:TYR:HB2	2.47	0.44
1:A:934:VAL:HG23	1:A:999:THR:HG22	1.99	0.43
3:A:1167:SAV:H21B	3:A:1167:SAV:O2	2.17	0.43
3:A:1167:SAV:H17	3:A:1167:SAV:H19B	1.78	0.43
1:A:853:GLY:HA2	1:A:857:THR:O	2.19	0.43
1:A:1077:ASP:N	1:A:1077:ASP:OD1	2.53	0.42
3:A:1167:SAV:N6	3:A:1167:SAV:C3	2.82	0.42

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	274/309 (89%)	258 (94%)	9 (3%)	7 (3%)	5 1

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	817[A]	ARG
1	A	817[B]	ARG
1	A	873	THR
1	A	868	LEU
1	A	1051	ILE
1	A	842	ALA
1	A	870	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	239/264 (90%)	229 (96%)	10 (4%)	30 28

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	815	CYS
1	A	861[A]	ARG
1	A	861[B]	ARG
1	A	870	GLU

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Mol	Chain	Res	Type
1	A	921	ASN
1	A	1077	ASP
1	A	1079	VAL
1	A	1102	SER
1	A	1108	LYS
1	A	1117	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1038	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)

6 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	CSO	A	860[B]	1	3,6,7	0.70	0	0,6,8	-	-
1	CSO	A	860[A]	1	3,6,7	0.37	0	0,6,8	-	-
1	CSO	A	1022	1	3,6,7	0.40	0	0,6,8	-	-
1	CSO	A	1005	1	3,6,7	0.64	0	0,6,8	-	-
1	CSO	A	1043	1	3,6,7	0.85	0	0,6,8	-	-
1	CSO	A	1114	1	3,6,7	0.83	0	0,6,8	-	-

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
1	CSO	A	860[B]	1	-	0/1/5/7	-
1	CSO	A	860[A]	1	-	0/1/5/7	-
1	CSO	A	1022	1	-	1/1/5/7	-
1	CSO	A	1005	1	-	0/1/5/7	-
1	CSO	A	1043	1	-	0/1/5/7	-
1	CSO	A	1114	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1022	CSO	N-CA-CB-SG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

5 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	$\#\|Z\| > 2$
2	SO4	A	1	-	4,4,4	0.13	0	6,6,6	0.28	0
3	SAV	A	1167	-	31,33,33	1.14	4 (12%)	39,46,46	2.33	14 (35%)
2	SO4	A	4	-	4,4,4	0.12	0	6,6,6	0.13	0
2	SO4	A	3	-	4,4,4	0.16	0	6,6,6	0.11	0
2	SO4	A	2	-	4,4,4	0.15	0	6,6,6	0.07	0

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	SAV	A	1167	-	-	4/14/14/14	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1167	SAV	C14-C13	-2.98	1.48	1.50
3	A	1167	SAV	C16-C15	-2.57	1.37	1.41
3	A	1167	SAV	C5-N1	2.27	1.41	1.36
3	A	1167	SAV	C11-C12	-2.02	1.38	1.42

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1167	SAV	C1-O1-C2	-8.02	105.43	117.53
3	A	1167	SAV	C19-O2-C18	-6.07	108.36	117.53
3	A	1167	SAV	C9-C16-C15	-3.97	116.17	120.50
3	A	1167	SAV	C21-O3-C20	-3.22	105.94	114.78
3	A	1167	SAV	C10-C11-C12	-2.96	117.01	121.13
3	A	1167	SAV	O1-C2-C3	-2.82	119.26	124.12
3	A	1167	SAV	O2-C18-C20	2.82	120.12	115.16
3	A	1167	SAV	O2-C18-C17	-2.68	119.51	124.12
3	A	1167	SAV	O1-C2-C20	2.53	119.61	115.16
3	A	1167	SAV	C16-C15-C12	2.40	124.25	121.16
3	A	1167	SAV	N2-C5-N6	-2.22	124.44	126.55
3	A	1167	SAV	N3-C8-N6	2.18	123.10	116.95
3	A	1167	SAV	C7-C8-N6	-2.09	119.64	123.16
3	A	1167	SAV	C9-N3-C8	-2.07	123.31	128.74

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1167	SAV	C20-C2-O1-C1
3	A	1167	SAV	C3-C2-O1-C1
3	A	1167	SAV	C20-C18-O2-C19
3	A	1167	SAV	C17-C18-O2-C19

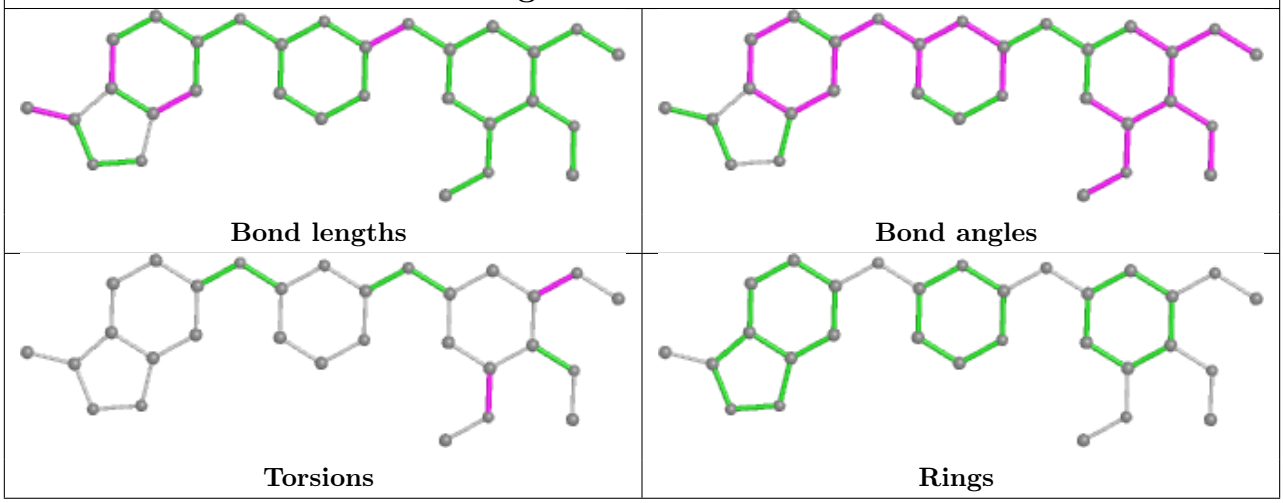
There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1167	SAV	5	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.

Ligand SAV A 1167



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	276/309 (89%)	1.68	69 (25%) 0 0	68, 74, 86, 94	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1052	TYR	10.9
1	A	997	PHE	10.7
1	A	815	CYS	10.4
1	A	843	PHE	9.9
1	A	841	GLY	8.8
1	A	1051	ILE	7.8
1	A	995	LYS	7.7
1	A	936	TYR	7.6
1	A	937	LYS	7.4
1	A	1050	ASP	7.3
1	A	816	GLU	6.3
1	A	1079	VAL	6.0
1	A	872	ALA	5.8
1	A	842	ALA	5.3
1	A	844	GLY	5.3
1	A	928	SER	5.2
1	A	1023	ILE	4.9
1	A	996	ASP	4.7
1	A	932	GLU	4.7
1	A	1047	LEU	4.6
1	A	1080	TYR	4.4
1	A	999	THR	4.3
1	A	1106	GLY	4.1
1	A	1163[A]	GLN	4.0
1	A	870	GLU	4.0
1	A	931	ASN	3.9
1	A	1048	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	1078	ARG	3.6
1	A	1164	ALA	3.5
1	A	925	TYR	3.5
1	A	1162	LEU	3.4
1	A	933	PHE	3.4
1	A	934	VAL	3.4
1	A	998	LEU	3.3
1	A	817[A]	ARG	3.2
1	A	1077	ASP	3.1
1	A	1053	LYS	3.1
1	A	1021	LYS	3.0
1	A	1076	PHE	2.9
1	A	1166	ALA	2.9
1	A	1067	LEU	2.7
1	A	871	GLY	2.7
1	A	919	PHE	2.7
1	A	935	PRO	2.6
1	A	1092	LEU	2.5
1	A	1066	PRO	2.5
1	A	903	CYS	2.5
1	A	1036	GLU	2.5
1	A	1082	ILE	2.4
1	A	1137	MET	2.4
1	A	1154	LEU	2.4
1	A	1099	LEU	2.3
1	A	1161	LEU	2.3
1	A	1109	ILE	2.3
1	A	1094	TRP	2.3
1	A	869	LYS	2.2
1	A	1035	SER	2.2
1	A	929	LYS	2.2
1	A	878	ARG	2.2
1	A	1089	PHE	2.2
1	A	894	LEU	2.1
1	A	1155	VAL	2.1
1	A	1140	CYS	2.1
1	A	1102	SER	2.1
1	A	1090	GLY	2.1
1	A	1105	PRO	2.1
1	A	1009	GLN	2.1
1	A	886	ILE	2.0
1	A	1124[A]	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	CSO	A	1022	7/8	0.80	0.11	73,77,78,78	0
1	CSO	A	1114	7/8	0.80	0.14	73,74,75,75	0
1	CSO	A	1043	7/8	0.84	0.22	79,80,83,83	0
1	CSO	A	860[B]	7/8	0.85	0.19	66,70,70,70	7
1	CSO	A	860[A]	7/8	0.85	0.19	70,71,71,72	7
1	CSO	A	1005	7/8	0.88	0.15	70,71,71,72	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

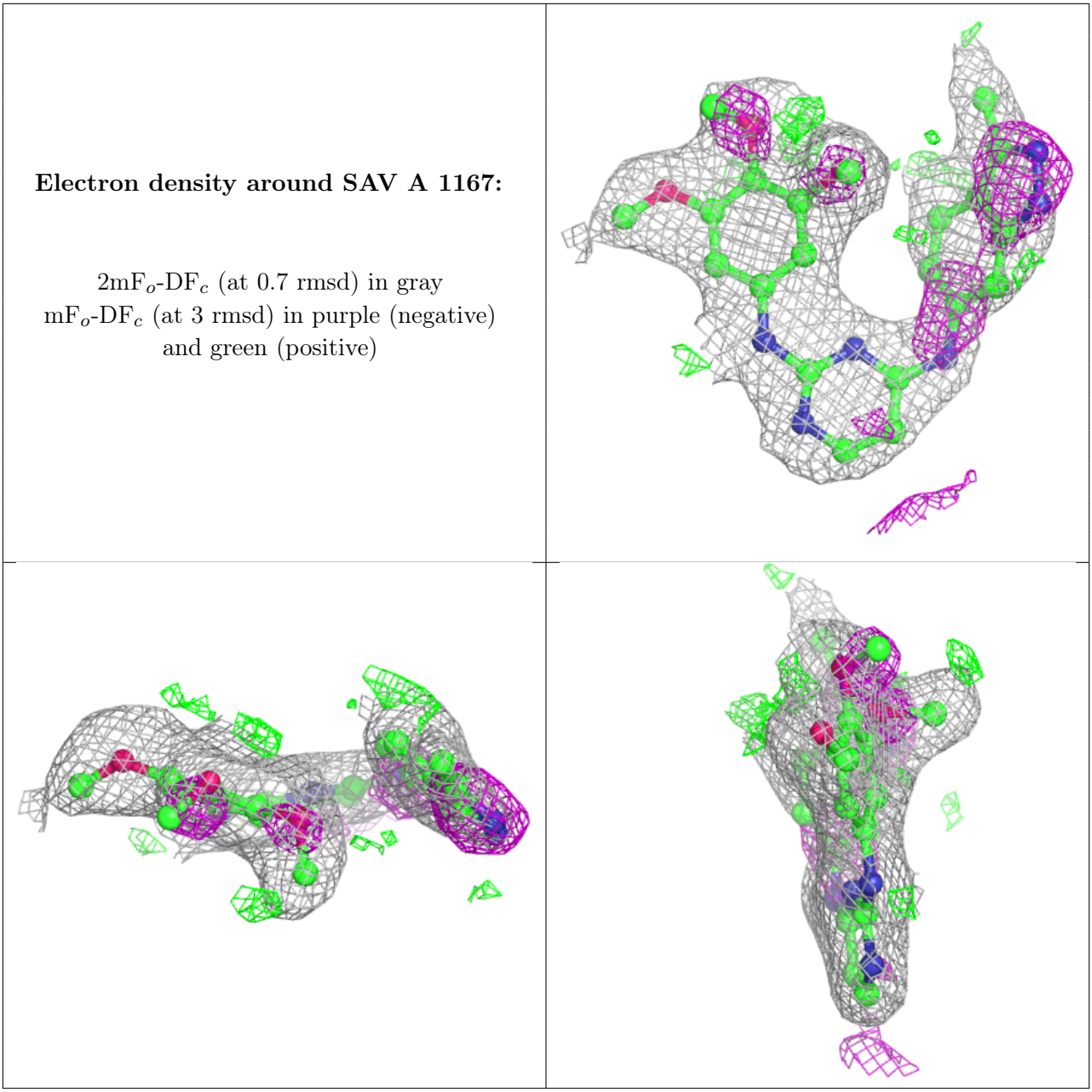
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	A	4	5/5	0.59	0.48	129,129,129,129	0
2	SO4	A	2	5/5	0.66	0.34	132,132,133,133	0
3	SAV	A	1167	30/30	0.80	0.26	67,74,80,80	0
2	SO4	A	1	5/5	0.87	0.20	115,115,116,116	0
2	SO4	A	3	5/5	0.94	0.16	114,114,115,115	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 SAV A 1167:

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.