Full wwPDB X-ray Structure Validation Report

Apr 2, 2025 – 02:48 am BST

PDB ID	:	8B2A / pdb_00008b2a
Title	:	Crystal structure of type I dehydroquinase from Staphylococcus aureus inhibited by a hydroxylamine derivative
Authors	:	Otero, J.M.; Rodriguez, A.; Maneiro, M.; Lence, E.; Thompson, P.; Hawkins, A.R.; Gonzalez-Bello, C.; van Raaij, M.J.
Deposited on	:	2022-09-13
Resolution	:	1.65 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 ⓘ 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:

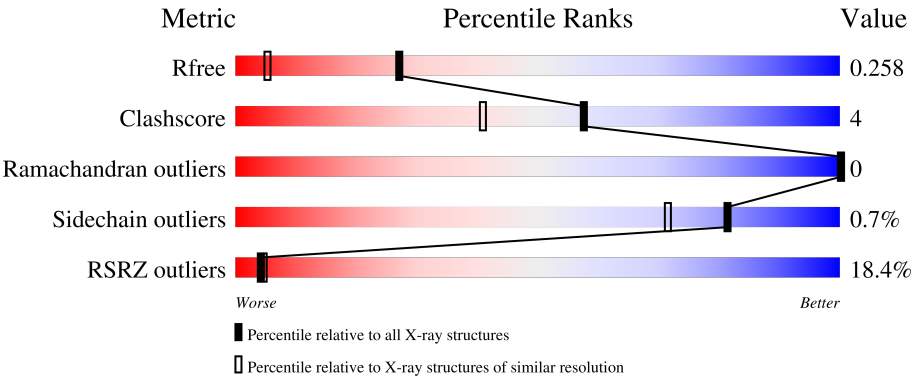
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 1.65 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}	164625	2328 (1.66-1.66)
Clashscore	180529	2515 (1.66-1.66)
Ramachandran outliers	177936	2475 (1.66-1.66)
Sidechain outliers	177891	2475 (1.66-1.66)
RSRZ outliers	164620	2328 (1.66-1.66)

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	238	7% 90% 9%
1	BBB	238	30% 87% 13%

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
4	CL	AAA	303	-	-	X	-

2 Entry composition

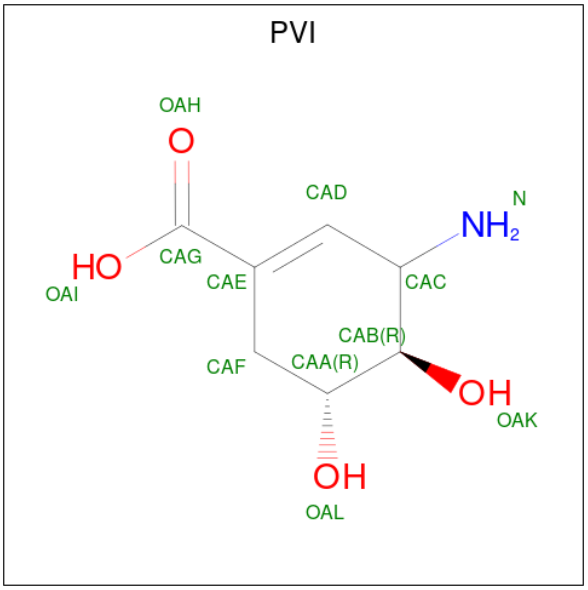
There are 5 unique types of molecules in this entry. The entry contains 3916 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 3-dehydroquinate dehydratase.

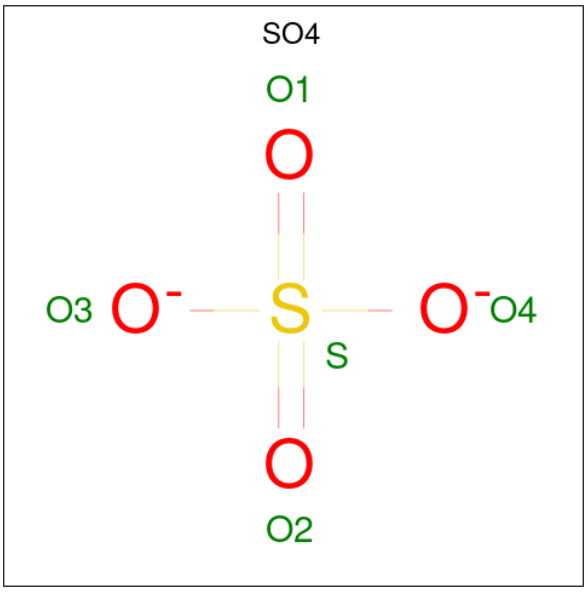
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	236	Total	C	N	O	S	0	3	0
			1872	1201	309	352	10			
1	BBB	238	Total	C	N	O	S	0	3	0
			1861	1189	310	352	10			

- Molecule 2 is (4R,5R)-3-amino-4,5-dihydroxy-cyclohexene-1-carboxylic acid (CCD ID: PVI) (formula: $C_7H_{11}NO_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	AAA	1	Total	C	O	0	0
			11	7	4		
2	BBB	1	Total	C	O	0	0
			11	7	4		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total O S 5 4 1	0	0
3	BBB	1	Total O S 5 4 1	0	0

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	1	Total Cl 1 1	0	0

- Molecule 5 is water.

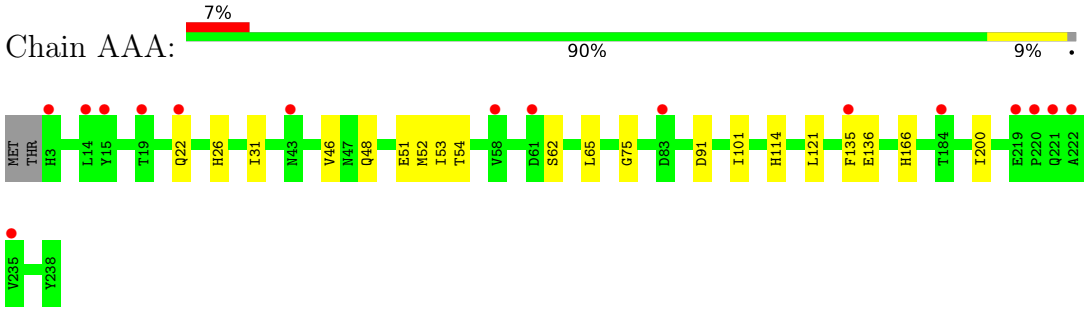
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	105	Total O 105 105	0	0
5	BBB	45	Total O 45 45	0	0

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.

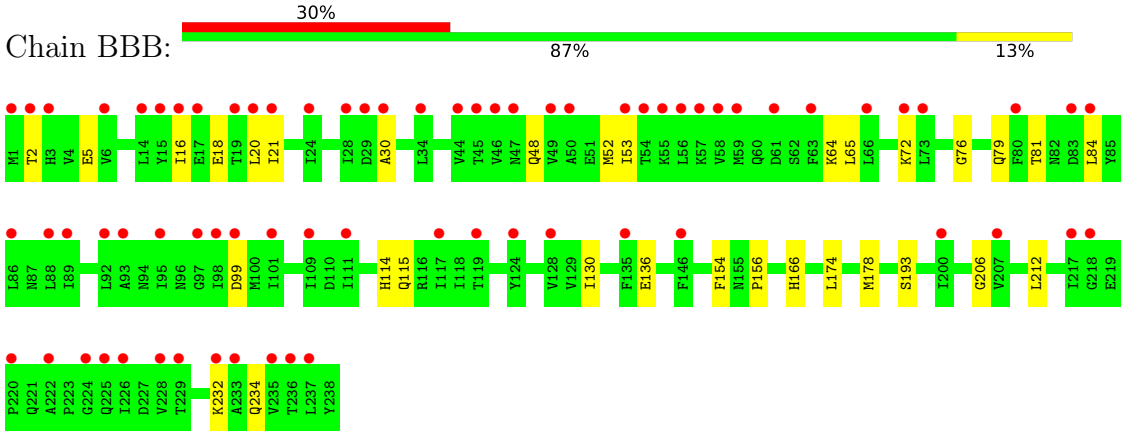
• Molecule 1: 3-dehydroquinate dehydratase

Chain AAA:



• Molecule 1: 3-dehydroquinate dehydratase

Chain BBB:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	36.38Å 79.57Å 83.53Å 90.00° 101.17° 90.00°	Depositor
Resolution (Å)	79.70 – 1.65 79.70 – 1.65	Depositor EDS
% Data completeness (in resolution range)	97.8 (79.70-1.65) 97.8 (79.70-1.65)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.02 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.219 , 0.255 0.225 , 0.258	Depositor DCC
R_{free} test set	2833 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	25.8	Xtriage
Anisotropy	0.691	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 27.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	3916	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.24% 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: SO4, CL, PVI

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	0.70	0/1914	0.84	0/2595
1	BBB	0.70	0/1904	0.77	0/2586
All	All	0.70	0/3818	0.81	0/5181

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

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	1872	0	1887	13	0
1	BBB	1861	0	1830	20	0
2	AAA	11	0	0	0	0
2	BBB	11	0	0	0	0
3	AAA	5	0	0	0	0
3	BBB	5	0	0	0	0
4	AAA	1	0	0	2	0
5	AAA	105	0	0	1	1
5	BBB	45	0	0	1	0
All	All	3916	0	3717	33	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 4.

All (33) 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:62:SER:O	4:AAA:303:CL:CL	2.39	0.77
1:AAA:234:GLN:OE1	5:AAA:401:HOH:O	2.07	0.72
1:BBB:234:GLN:OE1	5:BBB:401:HOH:O	2.09	0.69
1:AAA:53:ILE:HG12	1:AAA:65:LEU:HD21	1.76	0.68
1:AAA:48:GLN:O	1:AAA:52:MET:HG3	1.95	0.66
1:AAA:31:ILE:O	4:AAA:303:CL:CL	2.50	0.66
1:BBB:5:GLU:HB2	1:BBB:212:LEU:HD23	1.79	0.65
1:BBB:30:ALA:HA	1:BBB:232:LYS:HG3	1.79	0.64
1:BBB:16:ILE:HG23	1:BBB:20:LEU:HD23	1.82	0.62
1:BBB:48:GLN:O	1:BBB:52:MET:HG3	2.04	0.57
1:AAA:22:GLN:HG3	1:AAA:26:HIS:CE1	2.40	0.56
1:BBB:18[B]:GLU:HA	1:BBB:18[B]:GLU:OE1	2.06	0.55
1:AAA:46[B]:VAL:HG11	1:AAA:91:ASP:CB	2.39	0.53
1:AAA:46[B]:VAL:HG11	1:AAA:91:ASP:HB3	1.92	0.52
1:BBB:174:LEU:CD2	1:BBB:193:SER:N	2.75	0.50
1:AAA:136:GLU:O	1:AAA:166:HIS:CE1	2.64	0.49
1:BBB:64:LYS:HA	1:BBB:99:ASP:OD2	2.14	0.48
1:BBB:53:ILE:HG12	1:BBB:65:LEU:HD21	1.96	0.47
1:BBB:130:ILE:CG2	1:BBB:156:PRO:HG3	2.46	0.46
1:BBB:5:GLU:HB2	1:BBB:212:LEU:CD2	2.43	0.46
1:BBB:16:ILE:HG22	1:BBB:21:ILE:HG13	1.99	0.45
1:BBB:115:GLN:HE22	1:BBB:154:PHE:HA	1.82	0.45
1:BBB:136:GLU:O	1:BBB:166[B]:HIS:NE2	2.50	0.44
1:BBB:2:THR:CG2	1:BBB:206:GLY:O	2.67	0.43
1:AAA:75:GLY:HA3	1:AAA:135:PHE:CE1	2.54	0.43
1:BBB:72:LYS:HA	1:BBB:76:GLY:O	2.18	0.43
1:BBB:130:ILE:HG21	1:BBB:156:PRO:HG3	2.00	0.42
1:AAA:101:ILE:HD12	1:AAA:121:LEU:HD22	2.03	0.41
1:AAA:200:ILE:HA	1:AAA:200:ILE:HD12	1.78	0.40
1:AAA:51:GLU:O	1:AAA:54:THR:OG1	2.31	0.40
1:BBB:81:THR:OG1	1:BBB:84:LEU:HG	2.21	0.40
1:BBB:178:MET:HB3	1:BBB:178:MET:HE2	1.94	0.40
1:BBB:174:LEU:HD22	1:BBB:193:SER:N	2.37	0.40

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)
5:AAA:494:HOH:O	5:AAA:495:HOH:O[2_656]	1.49	0.71

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	237/238 (100%)	235 (99%)	2 (1%)	0	100	100
1	BBB	239/238 (100%)	235 (98%)	4 (2%)	0	100	100
All	All	476/476 (100%)	470 (99%)	6 (1%)	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	AAA	209/214 (98%)	208 (100%)	1 (0%)	86	80
1	BBB	202/214 (94%)	200 (99%)	2 (1%)	73	59
All	All	411/428 (96%)	408 (99%)	3 (1%)	81	71

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	114	HIS
1	BBB	79	GLN
1	BBB	114	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	$\#\|Z\| > 2$
2	PVI	AAA	301	1	11,11,12	2.85	3 (27%)	12,15,17	1.79	4 (33%)
3	SO4	BBB	302	-	4,4,4	0.35	0	6,6,6	0.06	0
3	SO4	AAA	302	-	4,4,4	0.39	0	6,6,6	0.09	0
2	PVI	BBB	301	1	11,11,12	2.68	3 (27%)	12,15,17	1.52	3 (25%)

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
2	PVI	AAA	301	1	-	4/4/17/20	0/1/1/1
2	PVI	BBB	301	1	-	4/4/17/20	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	301	PVI	CAF-CAE	-6.84	1.39	1.51
2	BBB	301	PVI	CAF-CAE	-6.08	1.41	1.51
2	AAA	301	PVI	CAC-CAD	-4.40	1.40	1.50
2	BBB	301	PVI	CAC-CAD	-4.16	1.41	1.50
2	BBB	301	PVI	CAG-CAE	-3.92	1.39	1.49
2	AAA	301	PVI	CAG-CAE	-3.85	1.40	1.49

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	BBB	301	PVI	OAI-CAG-CAE	3.64	123.20	115.49
2	AAA	301	PVI	OAH-CAG-CAE	-3.59	115.41	121.59
2	AAA	301	PVI	OAI-CAG-CAE	3.35	122.59	115.49
2	AAA	301	PVI	CAF-CAE-CAD	2.39	124.49	119.68
2	BBB	301	PVI	OAI-CAG-OAH	-2.15	118.70	123.61
2	AAA	301	PVI	CAC-CAB-CAA	2.13	113.40	110.69
2	BBB	301	PVI	OAH-CAG-CAE	-2.05	118.06	121.59

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AAA	301	PVI	CAF-CAE-CAG-OAH
2	AAA	301	PVI	CAF-CAE-CAG-OAI
2	BBB	301	PVI	CAF-CAE-CAG-OAH
2	BBB	301	PVI	CAF-CAE-CAG-OAI
2	BBB	301	PVI	CAD-CAE-CAG-OAH
2	BBB	301	PVI	CAD-CAE-CAG-OAI
2	AAA	301	PVI	CAD-CAE-CAG-OAH
2	AAA	301	PVI	CAD-CAE-CAG-OAI

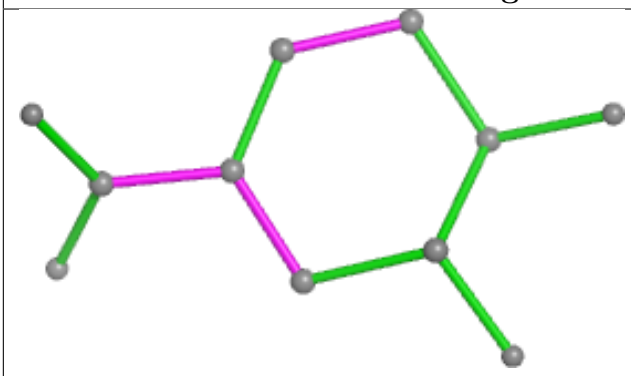
There are no ring outliers.

No monomer is involved in short contacts.

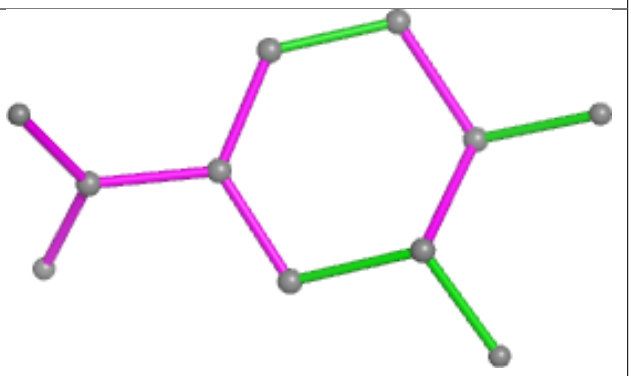
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

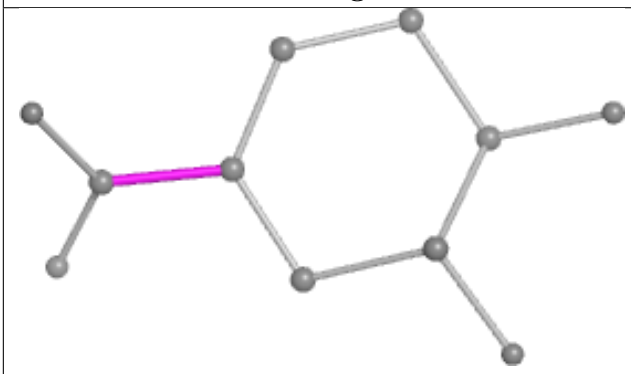
Ligand PVI AAA 301



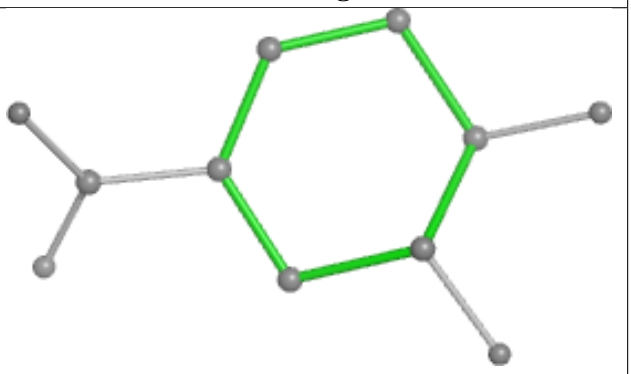
Bond lengths



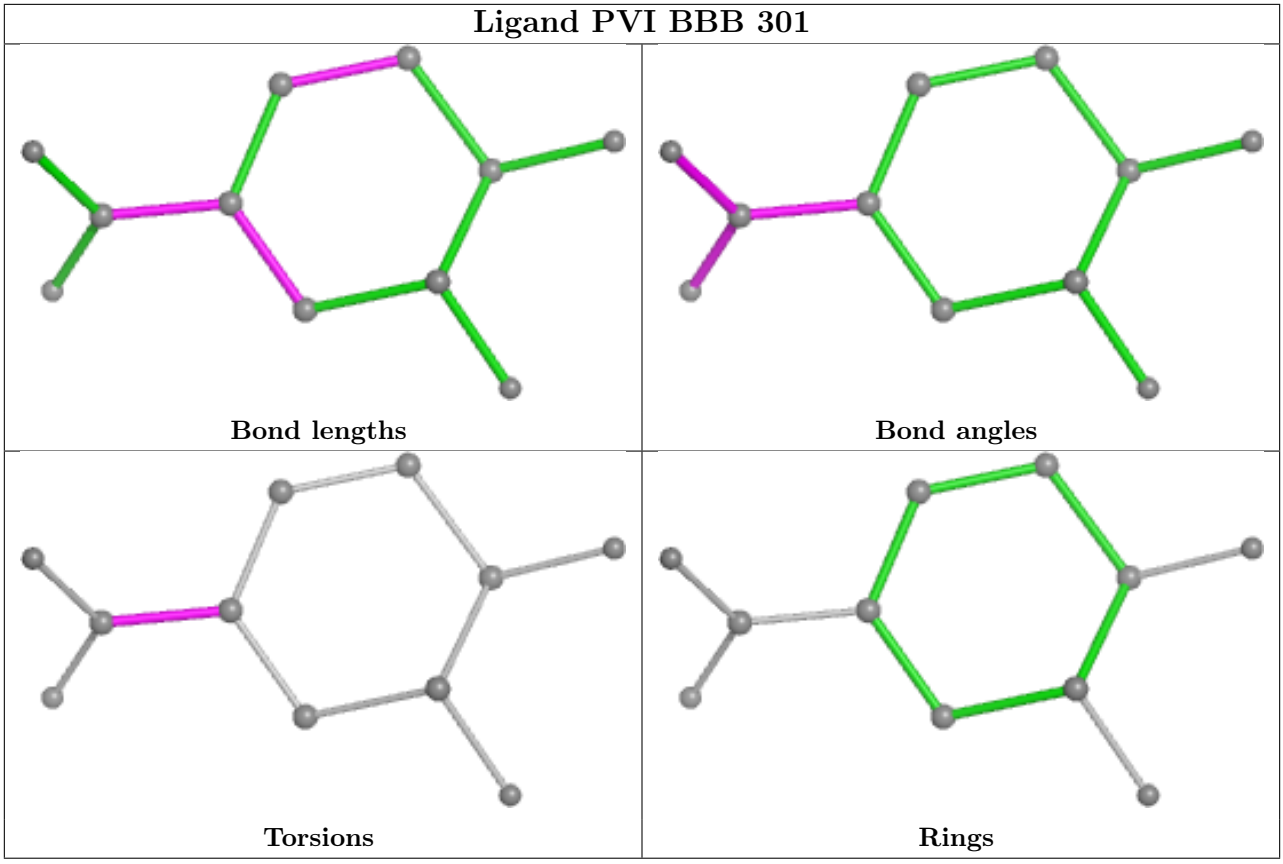
Bond angles



Torsions



Rings



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

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	236/238 (99%)	0.51	16 (6%) 25 27	15, 26, 45, 58	3 (1%)
1	BBB	238/238 (100%)	1.50	71 (29%) 1 1	17, 40, 61, 70	3 (1%)
All	All	474/476 (99%)	1.01	87 (18%) 4 5	15, 33, 57, 70	6 (1%)

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	53	ILE	5.0
1	BBB	20	LEU	4.4
1	BBB	73	LEU	4.4
1	BBB	88	LEU	4.0
1	BBB	146	PHE	4.0
1	BBB	58	VAL	3.9
1	AAA	14	LEU	3.8
1	BBB	56	LEU	3.7
1	BBB	46	VAL	3.7
1	AAA	15	TYR	3.6
1	AAA	58	VAL	3.5
1	BBB	54	THR	3.5
1	BBB	217	ILE	3.5
1	BBB	55	LYS	3.4
1	BBB	220	PRO	3.3
1	BBB	17	GLU	3.3
1	BBB	228	VAL	3.3
1	BBB	63	PHE	3.2
1	BBB	233	ALA	3.2
1	BBB	237	LEU	3.1
1	AAA	43	ASN	3.1
1	AAA	3	HIS	3.1
1	BBB	49	VAL	3.1
1	BBB	200	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	BBB	34	LEU	2.9
1	BBB	45	THR	2.9
1	BBB	218	GLY	2.9
1	BBB	29	ASP	2.8
1	BBB	30	ALA	2.8
1	BBB	98	ILE	2.8
1	BBB	15	TYR	2.8
1	AAA	135	PHE	2.8
1	BBB	235	VAL	2.8
1	BBB	3	HIS	2.7
1	BBB	66	LEU	2.7
1	BBB	44	VAL	2.7
1	BBB	93	ALA	2.6
1	BBB	1	MET	2.6
1	AAA	219	GLU	2.5
1	BBB	92	LEU	2.5
1	BBB	109	ILE	2.5
1	BBB	19	THR	2.5
1	BBB	222	ALA	2.5
1	BBB	224	GLY	2.5
1	BBB	229	THR	2.5
1	BBB	80	PHE	2.4
1	BBB	21	ILE	2.4
1	BBB	97	GLY	2.4
1	BBB	99	ASP	2.4
1	AAA	220	PRO	2.4
1	AAA	235	VAL	2.4
1	BBB	59	MET	2.4
1	BBB	28	ILE	2.3
1	AAA	222	ALA	2.3
1	BBB	50	ALA	2.3
1	BBB	6	VAL	2.3
1	BBB	86	LEU	2.3
1	BBB	24	ILE	2.3
1	BBB	117	ILE	2.3
1	BBB	226	ILE	2.3
1	BBB	232	LYS	2.3
1	AAA	184	THR	2.3
1	AAA	83	ASP	2.3
1	BBB	207	VAL	2.3
1	BBB	16	ILE	2.2
1	BBB	124	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	BBB	61	ASP	2.2
1	BBB	84	LEU	2.2
1	BBB	135	PHE	2.2
1	BBB	2	THR	2.2
1	BBB	119	THR	2.2
1	BBB	57	LYS	2.2
1	BBB	83	ASP	2.1
1	BBB	111	ILE	2.1
1	BBB	72	LYS	2.1
1	BBB	225	GLN	2.1
1	BBB	89	ILE	2.1
1	BBB	101	ILE	2.1
1	AAA	19	THR	2.1
1	BBB	95	ILE	2.1
1	AAA	221	GLN	2.1
1	AAA	61	ASP	2.1
1	BBB	14	LEU	2.1
1	BBB	128	VAL	2.0
1	BBB	236	THR	2.0
1	AAA	22	GLN	2.0
1	BBB	47	ASN	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^{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
3	SO4	BBB	302	5/5	0.70	0.13	73,74,75,80	0
3	SO4	AAA	302	5/5	0.80	0.10	63,69,72,73	0

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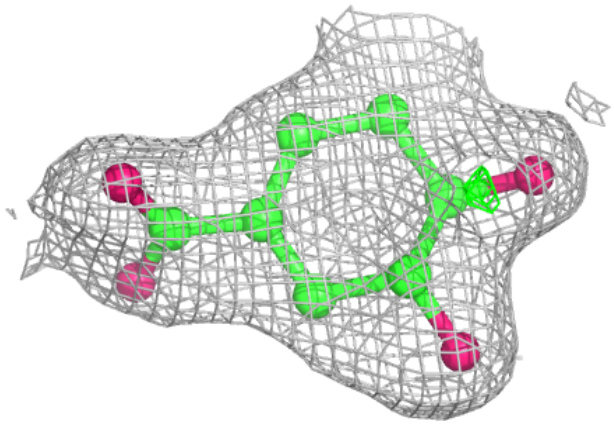
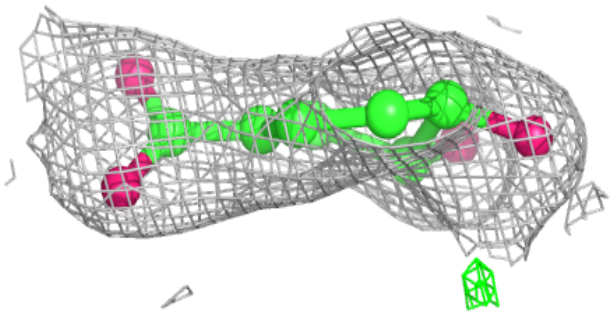
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PVI	BBB	301	11/12	0.88	0.11	38,42,47,49	0
2	PVI	AAA	301	11/12	0.93	0.08	24,27,29,30	0
4	CL	AAA	303	1/1	0.94	0.10	35,35,35,35	0

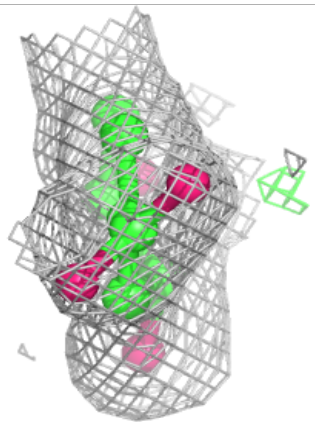
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PVI BBB 301:

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

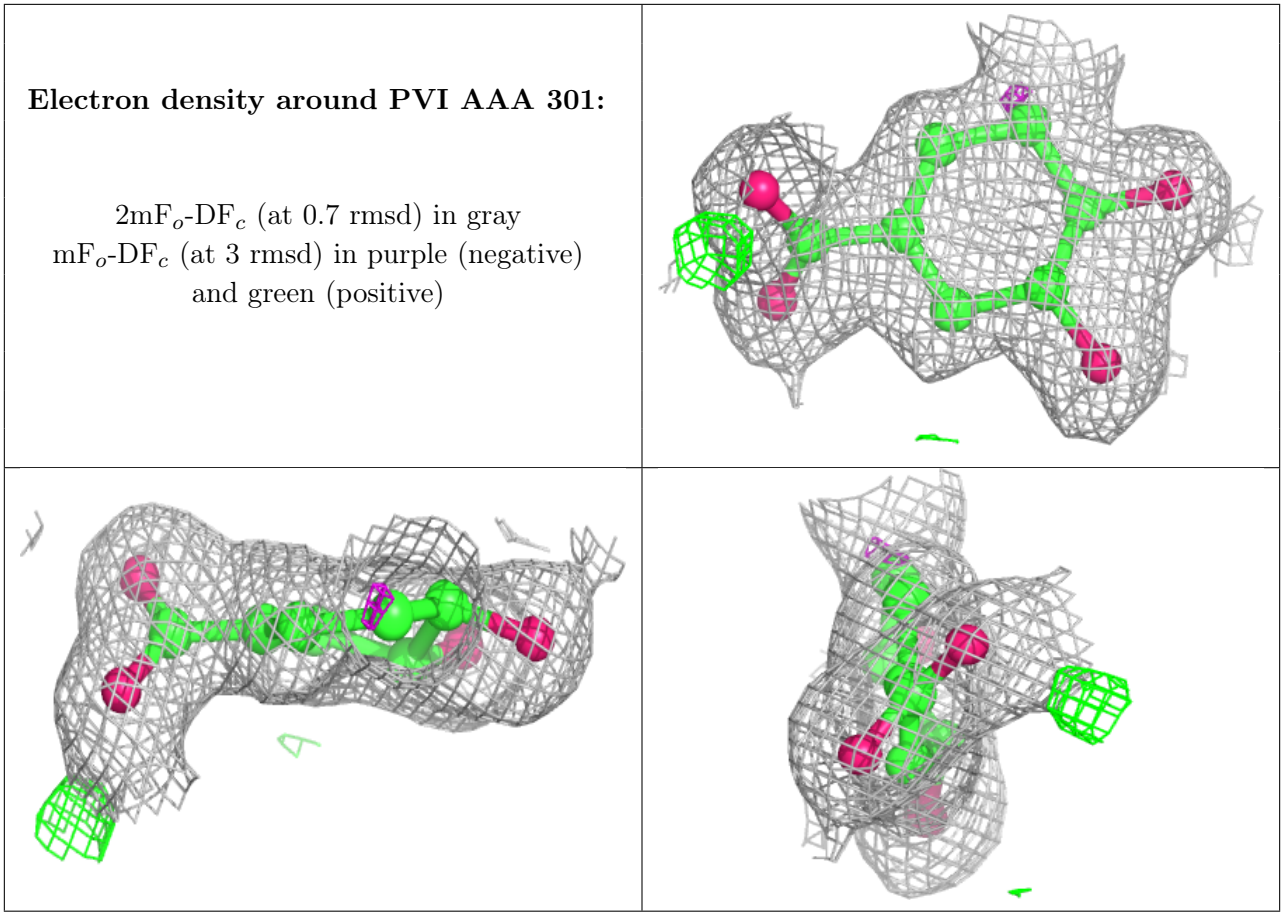






Electron density around PVI AAA 301:

$2mF_o$-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

There are no such residues in this entry.