



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:53 PM UTC

PDB ID : 8OHV / pdb_00008ohv
Title : Crystal structure of Beta-glucuronidase from Acidobacterium capsulatum in complex with glucuronic acid configured 3-geminal diol iminosugar inhibitor
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Deposited on : 2023-03-21
Resolution : 1.50 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

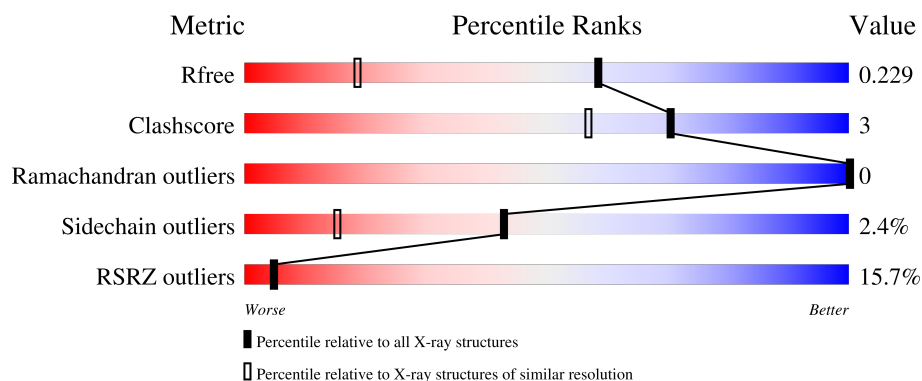
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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}	180053	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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 $\leq 5\%$. 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	475	

2 Entry composition [i](#)

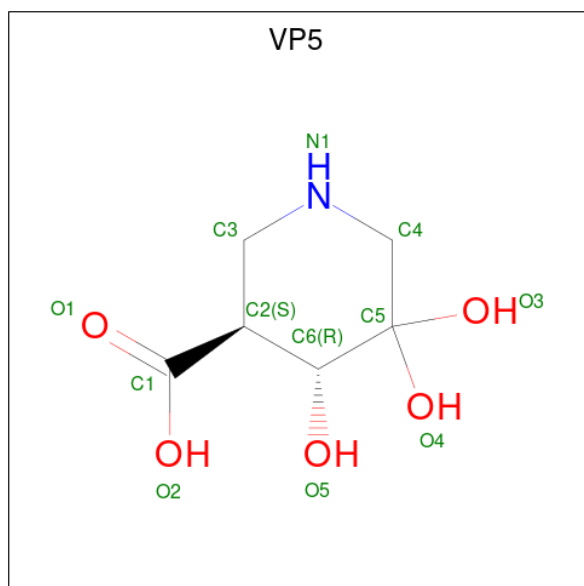
There are 4 unique types of molecules in this entry. The entry contains 3634 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 beta-glucuronidase from *Acidobacterium capsulatum*.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AAA	451	3435	2181	594	651	9	0	3	0

- Molecule 2 is (3 {S},4 {R})-4,5,5-tris(oxidanyl)piperidine-3-carboxylic acid (CCD ID: VP5) (formula: C₆H₁₁NO₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	AAA	1	12	6	1	5	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

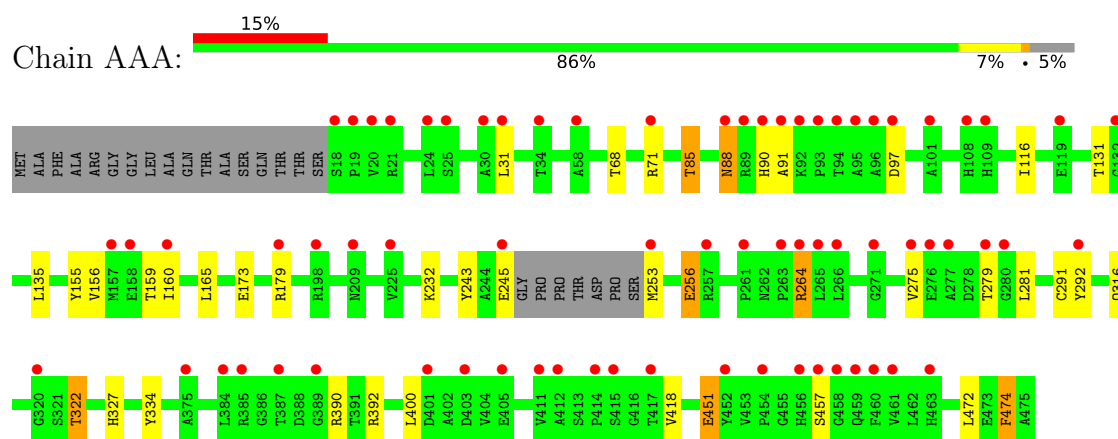
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	182	Total	O	0	0
			182	182		

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: beta-glucuronidase from *Acidobacterium capsulatum*



4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	82.04Å 42.61Å 140.14Å 90.00° 99.42° 90.00°	Depositor
Resolution (Å)	40.76 – 1.50 40.76 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.76-1.50) 100.0 (40.76-1.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.199 , 0.223 0.207 , 0.229	Depositor DCC
R_{free} test set	3861 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	17.9	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 29.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3634	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: SO4, VP5

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	1.09	3/3524 (0.1%)	1.26	11/4796 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	173	GLU	N-CA	6.32	1.50	1.46
1	AAA	418	VAL	C-O	5.75	1.30	1.24
1	AAA	327	HIS	CE1-NE2	5.25	1.37	1.32

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	97	ASP	CB-CA-C	7.08	123.32	109.72
1	AAA	451	GLU	CB-CA-C	6.61	122.36	109.33
1	AAA	264	ARG	CG-CD-NE	-6.26	98.22	112.00
1	AAA	256	GLU	CB-CG-CD	5.92	122.66	112.60
1	AAA	97	ASP	CA-CB-CG	5.43	118.03	112.60
1	AAA	322	THR	CA-CB-OG1	5.37	117.66	109.60
1	AAA	131	THR	CA-C-O	-5.32	113.23	119.24
1	AAA	474	PHE	CB-CA-C	5.12	118.15	109.50
1	AAA	68	THR	CA-CB-OG1	-5.04	102.05	109.60
1	AAA	85	THR	CB-CA-C	5.02	118.40	109.72
1	AAA	316	GLN	CA-C-O	-5.01	115.11	120.42

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	3435	0	3294	23	0
2	AAA	12	0	0	0	0
3	AAA	5	0	0	0	0
4	AAA	182	0	0	1	0
All	All	3634	0	3294	23	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 3.

All (23) 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:275:VAL:O	1:AAA:279:THR:HG22	1.60	1.02
1:AAA:156:VAL:HG13	1:AAA:160:ILE:HD12	1.52	0.91
1:AAA:279:THR:HG23	1:AAA:281:LEU:H	1.46	0.81
1:AAA:322:THR:HG23	4:AAA:827:HOH:O	1.84	0.77
1:AAA:135:LEU:CD2	1:AAA:160:ILE:HD13	2.15	0.76
1:AAA:135:LEU:HD22	1:AAA:160:ILE:HD13	1.69	0.74
1:AAA:85:THR:HG22	1:AAA:116:ILE:HG13	1.84	0.60
1:AAA:279:THR:HG23	1:AAA:281:LEU:N	2.17	0.59
1:AAA:155:TYR:CE2	1:AAA:159[B]:THR:HG21	2.37	0.59
1:AAA:253:MET:HG2	1:AAA:291[A]:CYS:SG	2.50	0.51
1:AAA:245:GLU:HB2	1:AAA:253:MET:HE2	1.93	0.50
1:AAA:256:GLU:HG3	1:AAA:400:LEU:HD12	1.93	0.50
1:AAA:390:ARG:HD3	1:AAA:474:PHE:O	2.13	0.49
1:AAA:165:LEU:C	1:AAA:165:LEU:HD13	2.42	0.44
1:AAA:390:ARG:CD	1:AAA:474:PHE:O	2.66	0.44
1:AAA:135:LEU:CD2	1:AAA:160:ILE:CD1	2.93	0.43
1:AAA:31:LEU:HD23	1:AAA:31:LEU:HA	1.83	0.43
1:AAA:90:HIS:O	1:AAA:90:HIS:CG	2.71	0.43
1:AAA:85:THR:CG2	1:AAA:116:ILE:HG13	2.47	0.42
1:AAA:88:ASN:HB3	1:AAA:91:ALA:HB2	2.01	0.42
1:AAA:392:ARG:HA	1:AAA:472:LEU:O	2.20	0.41
1:AAA:88:ASN:HB3	1:AAA:91:ALA:CB	2.51	0.41
1:AAA:243:TYR:H	1:AAA:264:ARG:NH1	2.18	0.41

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	449/475 (94%)	443 (99%)	6 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	339/357 (95%)	331 (98%)	8 (2%)	43	15

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	71	ARG
1	AAA	88	ASN
1	AAA	179	ARG
1	AAA	232	LYS
1	AAA	292	TYR
1	AAA	334	TYR
1	AAA	451	GLU
1	AAA	457	SER

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 ⓘ

2 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	VP5	AAA	601	-	11,12,12	1.24	1 (9%)	13,18,18	1.38	3 (23%)
3	SO4	AAA	602	-	4,4,4	0.50	0	6,6,6	0.18	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
2	VP5	AAA	601	-	-	4/4/21/21	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	601	VP5	C4-N1	2.99	1.49	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AAA	601	VP5	O1-C1-C2	-3.00	115.94	123.01
2	AAA	601	VP5	O2-C1-C2	2.16	119.53	113.93
2	AAA	601	VP5	C5-C6-C2	2.08	112.16	109.78

There are no chirality outliers.

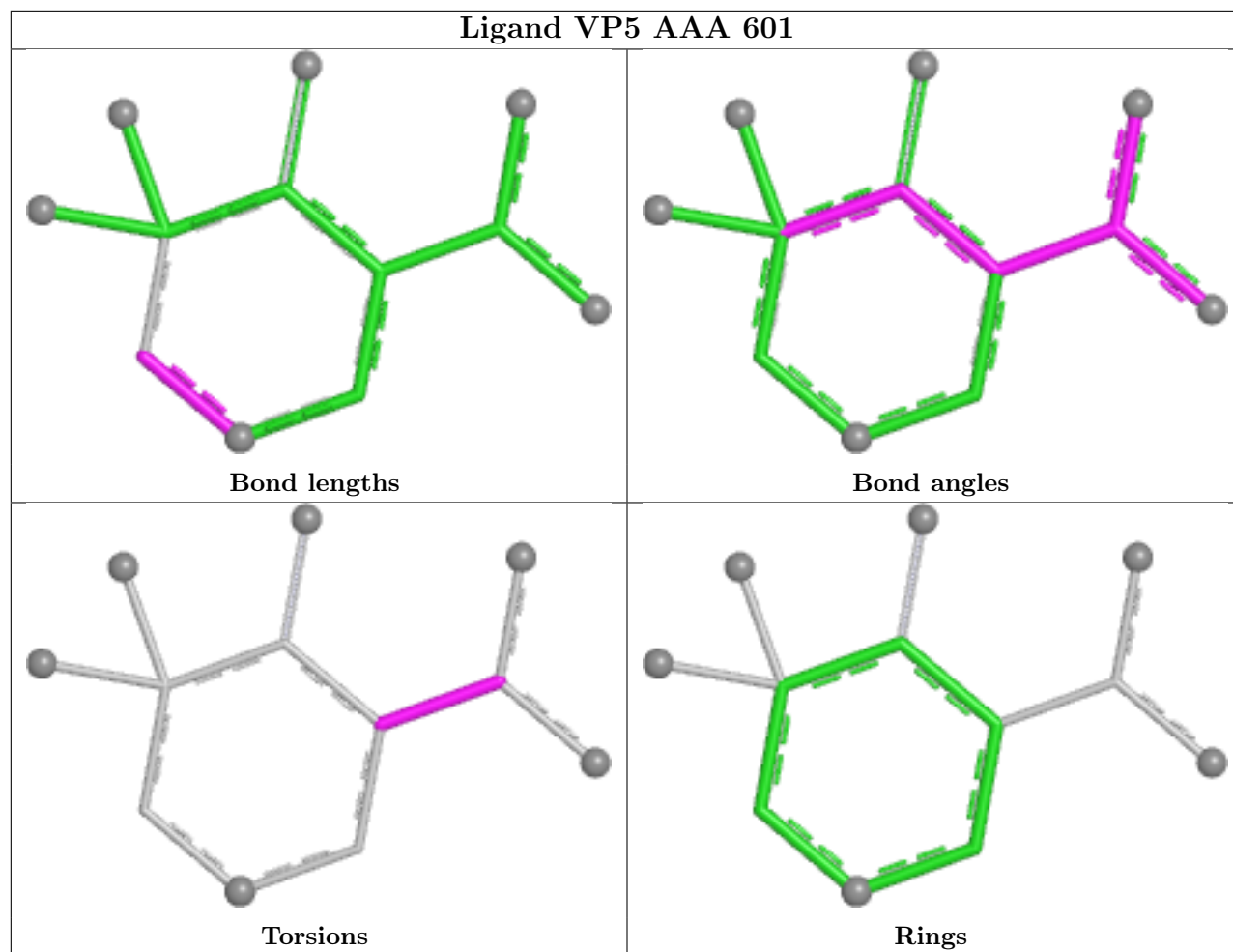
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AAA	601	VP5	O2-C1-C2-C3
2	AAA	601	VP5	O1-C1-C2-C6
2	AAA	601	VP5	O2-C1-C2-C6
2	AAA	601	VP5	O1-C1-C2-C3

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 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](#)

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, 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	AAA	451/475 (94%)	0.78	71 (15%) 5 5	10, 21, 41, 57	7 (1%)

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	457	SER	7.7
1	AAA	280	GLY	5.3
1	AAA	95	ALA	5.0
1	AAA	264	ARG	4.8
1	AAA	94	THR	4.5
1	AAA	456	HIS	4.4
1	AAA	375	ALA	3.9
1	AAA	93	PRO	3.9
1	AAA	263	PRO	3.6
1	AAA	415	SER	3.5
1	AAA	21	ARG	3.5
1	AAA	97	ASP	3.4
1	AAA	414	PRO	3.4
1	AAA	90	HIS	3.4
1	AAA	387	THR	3.4
1	AAA	96	ALA	3.3
1	AAA	109	HIS	3.3
1	AAA	265	LEU	3.2
1	AAA	411	VAL	3.2
1	AAA	412	ALA	3.2
1	AAA	454	PRO	3.2
1	AAA	108	HIS	3.2
1	AAA	31	LEU	3.1
1	AAA	89	ARG	3.1
1	AAA	266	LEU	3.1
1	AAA	91	ALA	3.1
1	AAA	459	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	AAA	261	PRO	2.9
1	AAA	34	THR	2.9
1	AAA	463	HIS	2.9
1	AAA	198	ARG	2.8
1	AAA	389	GLY	2.8
1	AAA	277	ALA	2.8
1	AAA	385	ARG	2.8
1	AAA	279	THR	2.8
1	AAA	88	ASN	2.7
1	AAA	92	LYS	2.7
1	AAA	292	TYR	2.7
1	AAA	275	VAL	2.7
1	AAA	401	ASP	2.7
1	AAA	101	ALA	2.6
1	AAA	18	SER	2.6
1	AAA	225	VAL	2.6
1	AAA	452	TYR	2.5
1	AAA	160	ILE	2.5
1	AAA	461	VAL	2.5
1	AAA	245	GLU	2.4
1	AAA	179	ARG	2.4
1	AAA	158	GLU	2.4
1	AAA	132	GLY	2.4
1	AAA	384	LEU	2.4
1	AAA	460	PHE	2.4
1	AAA	405	GLU	2.3
1	AAA	458	GLY	2.3
1	AAA	58	ALA	2.3
1	AAA	271	GLY	2.3
1	AAA	157	MET	2.2
1	AAA	276	GLU	2.2
1	AAA	403	ASP	2.2
1	AAA	417	THR	2.1
1	AAA	253	MET	2.1
1	AAA	71	ARG	2.1
1	AAA	24	LEU	2.1
1	AAA	320	GLY	2.1
1	AAA	19	PRO	2.1
1	AAA	25	SER	2.1
1	AAA	119	GLU	2.0
1	AAA	209	ASN	2.0
1	AAA	257	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	AAA	30	ALA	2.0
1	AAA	20	VAL	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

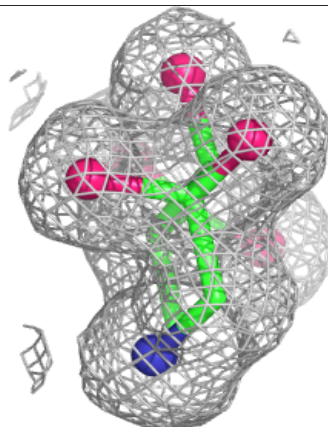
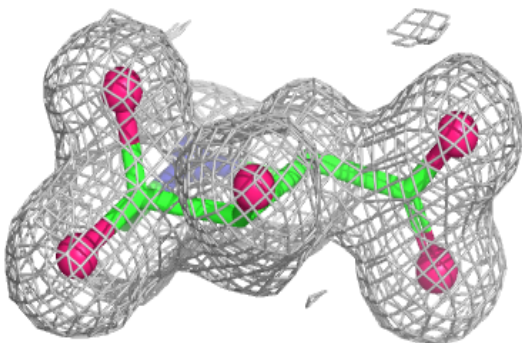
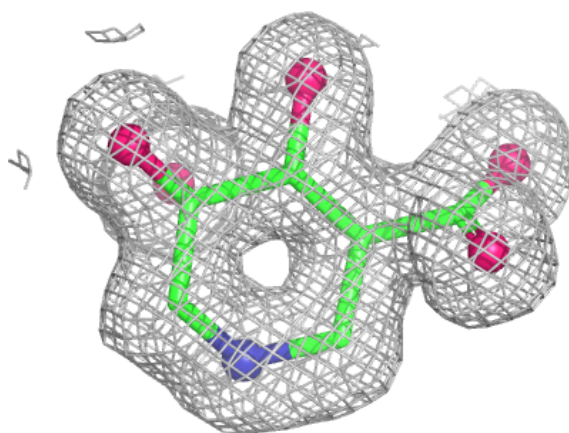
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	AAA	602	5/5	0.89	0.11	30,32,34,37	0
2	VP5	AAA	601	12/12	0.96	0.06	16,16,17,18	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 VP5 AAA 601:

$2mF_o-DF_c$ (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.