



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 02:40 PM UTC

PDB ID : 8RG1 / pdb_00008rg1
Title : Soluble glucose dehydrogenase from acinetobacter calcoaceticus - wild type pH8
Authors : Lublin, V.; Chavas, L.; Stines-Chaumeil, C.; Kauffmann, B.; Giraud, M.F.; Thompson, A.
Deposited on : 2023-12-13
Resolution : 1.19 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

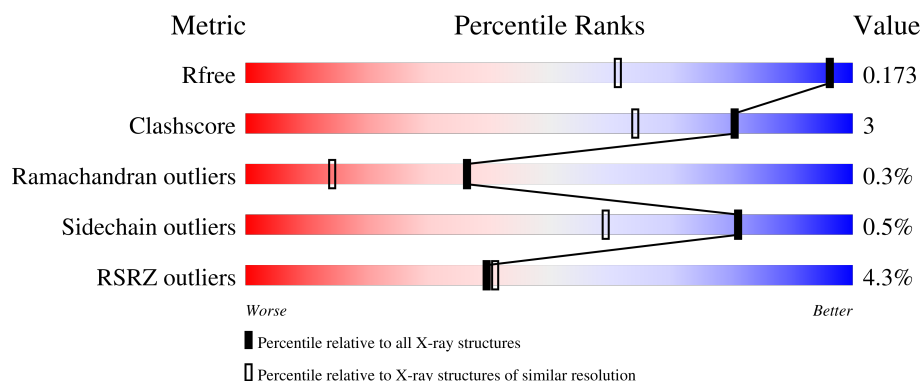
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.19 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	1216 (1.20-1.20)
Clashscore	190562	1265 (1.20-1.20)
Ramachandran outliers	187476	1226 (1.20-1.20)
Sidechain outliers	187428	1226 (1.20-1.20)
RSRZ outliers	180081	1214 (1.20-1.20)

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	A	454	5% 92% 7%
1	B	454	4% 94% 5%

2 Entry composition [i](#)

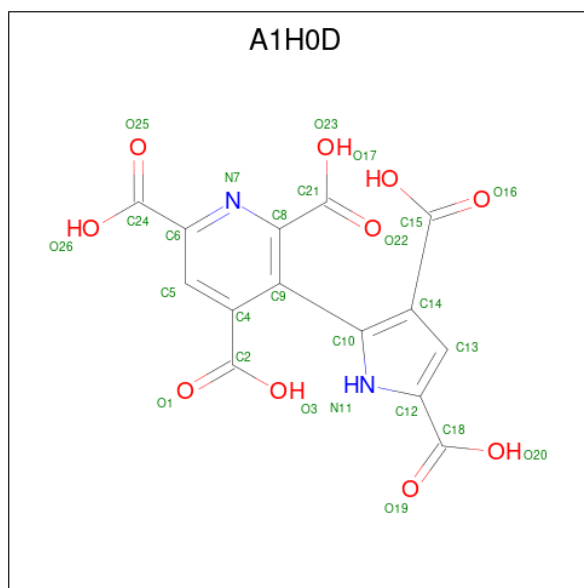
There are 5 unique types of molecules in this entry. The entry contains 15492 atoms, of which 6967 are hydrogens and 0 are deuteriums.

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 Quinoprotein glucose dehydrogenase B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	452	Total	C	H	N	O	S	3	0	0
			7015	2249	3477	600	684	5			
1	B	452	Total	C	H	N	O	S	0	1	0
			7028	2253	3484	601	685	5			

- Molecule 2 is 3-(3,5-dicarboxy-1 {H}-pyrrol-2-yl)pyridine-2,4,6-tricarboxylic acid (CCD ID: A1H0D) (formula: C₁₄H₈N₂O₁₀) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			29	14	3	2	10		
2	B	1	Total	C	H	N	O	0	0
			29	14	3	2	10		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total 3	Ca 3	0	0
3	B	3	Total 3	Ca 3	0	0

- Molecule 4 is LITHIUM ION (CCD ID: LI) (formula: Li).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Li 1	0	0
4	B	1	Total 1	Li 1	0	0

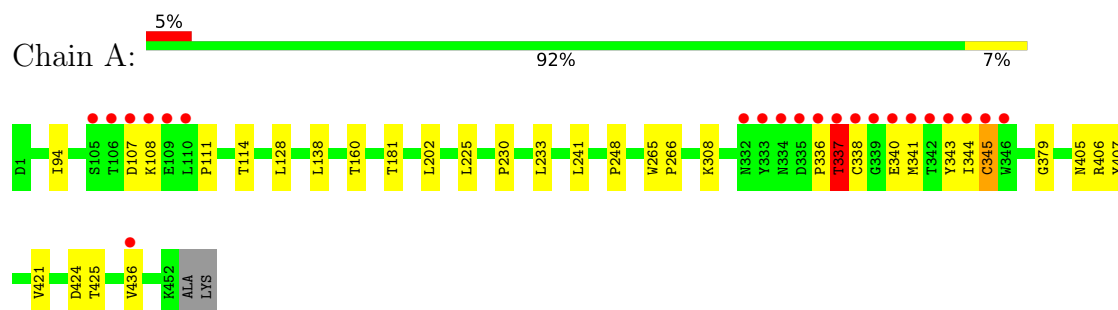
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	696	Total 696	O 696	0	0
5	B	687	Total 687	O 687	0	0

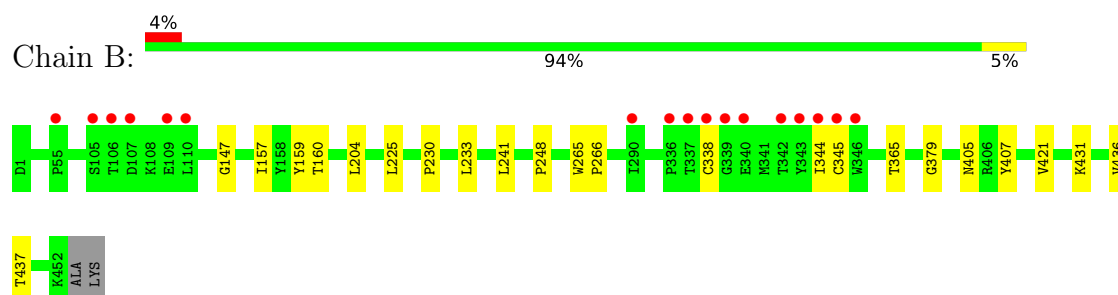
3 Residue-property plots [i](#)

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: Quinoprotein glucose dehydrogenase B



- Molecule 1: Quinoprotein glucose dehydrogenase B



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.35Å 92.51Å 84.71Å 90.00° 105.00° 90.00°	Depositor
Resolution (Å)	42.56 – 1.19 42.56 – 1.19	Depositor EDS
% Data completeness (in resolution range)	69.1 (42.56-1.19) 69.5 (42.56-1.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 1.19Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.148 , 0.173 0.149 , 0.173	Depositor DCC
R_{free} test set	2000 reflections (0.69%)	wwPDB-VP
Wilson B-factor (Å ²)	12.5	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	15492	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.21% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, LI, A1H0D

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	0.58	0/3628	0.62	0/4943
1	B	0.58	0/3637	0.63	0/4955
All	All	0.58	0/7265	0.63	0/9898

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	A	3538	3477	3476	24	1
1	B	3544	3484	3484	11	1
2	A	26	3	0	0	0
2	B	26	3	0	1	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	696	0	0	4	2
5	B	687	0	0	1	1
All	All	8525	6967	6960	36	3

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 (36) 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:344:ILE:HG13	1:A:436:VAL:HG22	1.77	0.66
1:A:308:LYS:HE2	5:A:782:HOH:O	1.97	0.64
2:B:501:A1H0D:O23	5:B:601:HOH:O	2.15	0.63
1:B:265:TRP:CD2	1:B:266:PRO:HA	2.36	0.61
1:A:265:TRP:CD2	1:A:266:PRO:HA	2.37	0.60
1:A:308:LYS:HE3	5:A:1041:HOH:O	2.00	0.60
1:A:94:ILE:HD12	1:A:128:LEU:HD21	1.86	0.57
1:A:343:TYR:CE1	1:A:344:ILE:HD11	2.41	0.56
1:A:108:LYS:HG2	1:A:111:PRO:HB3	1.89	0.55
1:A:338:CYS:SG	1:A:345:CYS:N	2.84	0.49
1:A:425:THR:HG23	5:A:938:HOH:O	2.13	0.49
1:B:233:LEU:HG	1:B:241:LEU:HD11	1.96	0.48
1:A:160:THR:HG23	1:A:233:LEU:HD22	1.96	0.48
1:B:344:ILE:HB	1:B:436:VAL:HG22	1.96	0.48
1:A:233:LEU:HG	1:A:241:LEU:HD11	1.97	0.47
1:A:308:LYS:HE2	1:A:308:LYS:HA	1.95	0.47
1:A:344:ILE:HG13	1:A:436:VAL:CG2	2.43	0.46
1:A:407:TYR:CD1	1:A:421:VAL:HG11	2.51	0.45
1:B:431:LYS:HD3	1:B:437:THR:HB	1.98	0.45
1:B:157:ILE:HG13	1:B:204:LEU:HD23	1.99	0.44
1:A:107:ASP:OD1	1:A:107:ASP:C	2.61	0.44
1:B:160:THR:HB	1:B:230:PRO:HG2	1.99	0.44
1:B:147:GLY:HA2	1:B:159:TYR:CZ	2.54	0.42
1:A:160:THR:HB	1:A:230:PRO:HG2	2.02	0.42
1:B:338:CYS:HB3	1:B:344:ILE:CG2	2.50	0.42
1:A:114:THR:HB	1:A:138:LEU:HB2	2.01	0.42
1:A:344:ILE:CG1	1:A:436:VAL:HG22	2.48	0.42
1:A:379:GLY:HA2	1:A:405:ASN:O	2.19	0.42
1:B:407:TYR:CD1	1:B:421:VAL:HG11	2.54	0.41
1:A:225:LEU:HD12	1:A:225:LEU:C	2.45	0.41
1:A:338:CYS:HB2	1:A:341:MET:O	2.21	0.41
1:A:406:ARG:HB2	1:A:424:ASP:HB2	2.03	0.41
1:B:379:GLY:HA2	1:B:405:ASN:O	2.21	0.41
1:A:336:PRO:O	1:A:337:THR:CB	2.69	0.40
1:A:181:THR:HB	5:A:880:HOH:O	2.22	0.40
1:B:225:LEU:HD12	1:B:225:LEU:C	2.46	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1142:HOH:O	5:B:1075:HOH:O[2_555]	2.06	0.14
1:A:340:GLU:OE2	1:B:365:THR:OG1[2_555]	2.07	0.13
5:A:1015:HOH:O	5:A:1206:HOH:O[2_545]	2.19	0.01

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	450/454 (99%)	435 (97%)	13 (3%)	2 (0%)	30	10
1	B	451/454 (99%)	439 (97%)	11 (2%)	1 (0%)	43	16
All	All	901/908 (99%)	874 (97%)	24 (3%)	3 (0%)	36	14

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	337	THR
1	A	248	PRO
1	B	248	PRO

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	390/391 (100%)	387 (99%)	3 (1%)	73	44
1	B	391/391 (100%)	390 (100%)	1 (0%)	86	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	781/782 (100%)	777 (100%)	4 (0%)	81	59

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	202	LEU
1	A	337	THR
1	A	345	CYS
1	B	345	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	90	ASN
1	A	177	GLN
1	A	295	GLN
1	B	90	ASN
1	B	91	ASN
1	B	255	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](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 8 are 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
2	A1H0D	A	501	3	26,27,27	0.86	1 (3%)	37,40,40	1.35	6 (16%)
2	A1H0D	B	501	3	26,27,27	0.92	1 (3%)	37,40,40	1.29	5 (13%)

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	A1H0D	A	501	3	-	3/24/24/24	0/2/2/2
2	A1H0D	B	501	3	-	1/24/24/24	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	A1H0D	O17-C15	-2.15	1.24	1.30
2	B	501	A1H0D	O20-C18	-2.07	1.24	1.30

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	A1H0D	C4-C5-C6	-3.14	117.36	119.93
2	A	501	A1H0D	C8-C9-C10	2.99	125.80	121.21
2	B	501	A1H0D	C8-C9-C10	2.86	125.61	121.21
2	A	501	A1H0D	O16-C15-C14	-2.77	116.93	122.67
2	B	501	A1H0D	C4-C5-C6	-2.75	117.68	119.93
2	B	501	A1H0D	O25-C24-C6	-2.68	115.90	121.30
2	B	501	A1H0D	O16-C15-C14	-2.56	117.36	122.67
2	A	501	A1H0D	C9-C8-C21	2.32	125.82	121.05
2	B	501	A1H0D	O22-C21-C8	-2.18	116.33	120.80
2	A	501	A1H0D	O19-C18-C12	-2.08	116.80	121.01
2	A	501	A1H0D	O25-C24-C6	-2.01	117.25	121.30

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	A1H0D	N11-C12-C18-O20
2	A	501	A1H0D	C13-C12-C18-O19
2	A	501	A1H0D	C13-C12-C18-O20
2	B	501	A1H0D	O3-C2-C4-C5

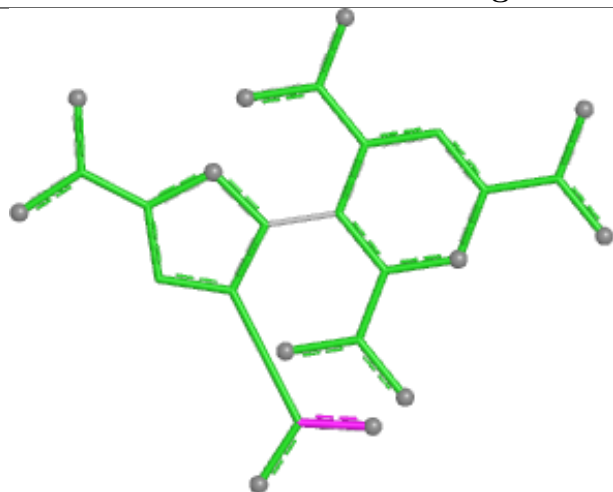
There are no ring outliers.

1 monomer is involved in 1 short contact:

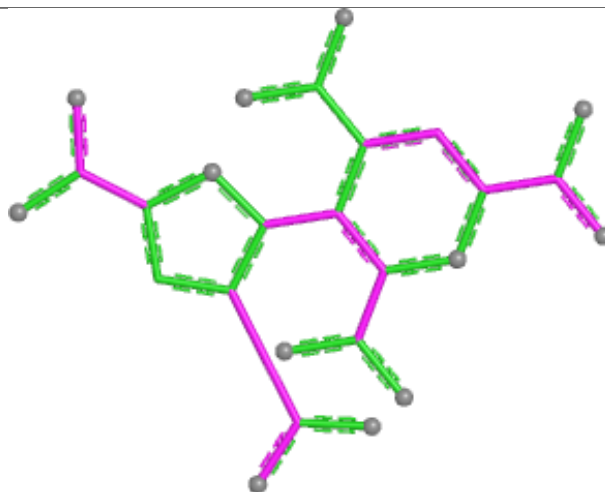
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	A1H0D	1	0

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.

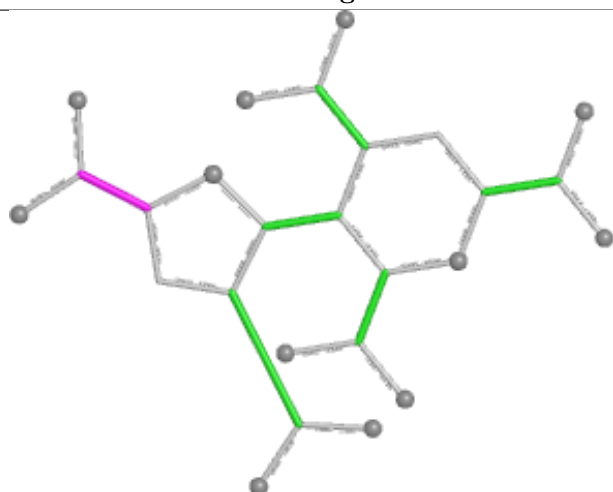
Ligand A1H0D A 501



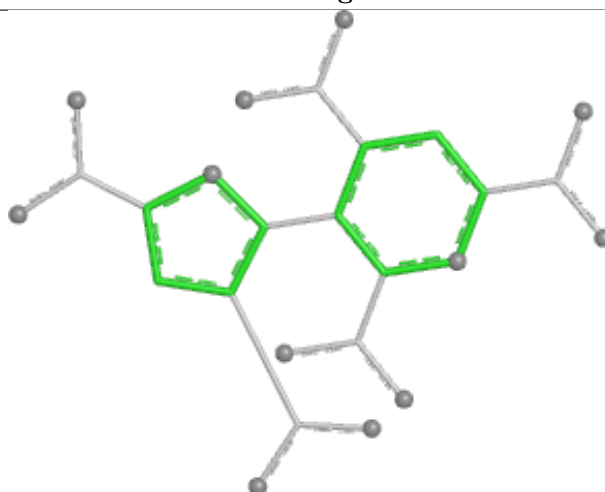
Bond lengths



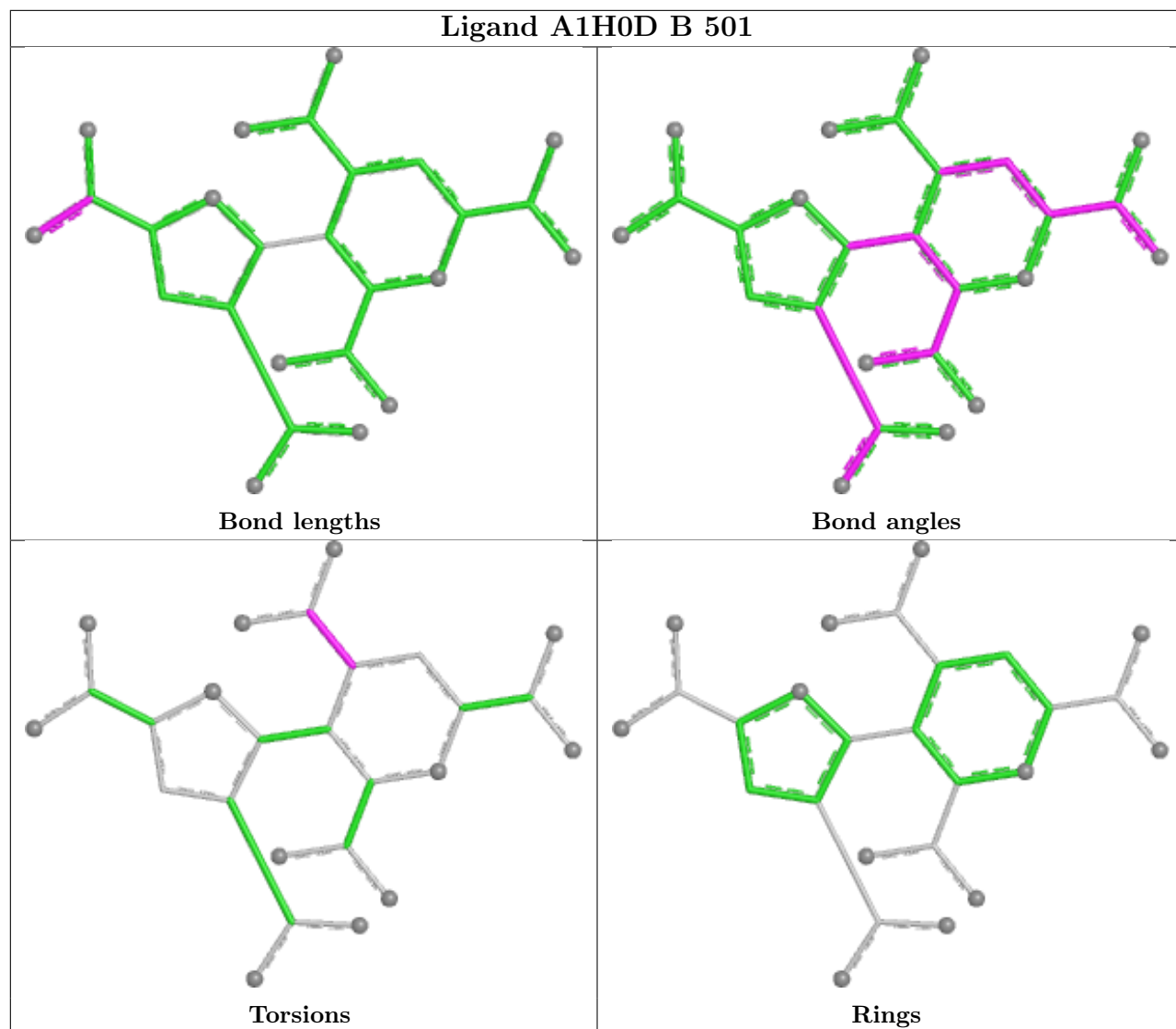
Bond angles



Torsions



Rings



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	A	452/454 (99%)	0.13	22 (4%) 35 37	10, 17, 33, 101	6 (1%)
1	B	452/454 (99%)	-0.09	17 (3%) 44 44	10, 17, 32, 94	3 (0%)
All	All	904/908 (99%)	0.02	39 (4%) 40 41	10, 17, 32, 101	9 (0%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	344	ILE	15.8
1	A	333	TYR	14.9
1	A	343	TYR	14.8
1	A	338	CYS	11.7
1	A	332	ASN	9.8
1	A	342	THR	9.8
1	B	338	CYS	9.0
1	A	337	THR	8.4
1	A	339	GLY	8.1
1	A	336	PRO	7.3
1	A	334	ASN	7.2
1	B	337	THR	7.1
1	B	110	LEU	6.6
1	A	335	ASP	6.0
1	A	341	MET	5.7
1	A	106	THR	5.3
1	B	345	CYS	5.1
1	A	345	CYS	5.0
1	A	340	GLU	4.5
1	A	107	ASP	4.3
1	B	336	PRO	3.7
1	B	342	THR	3.2
1	B	340	GLU	3.1
1	B	344	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	55	PRO	2.9
1	A	110	LEU	2.8
1	B	343	TYR	2.8
1	A	109	GLU	2.7
1	B	106	THR	2.7
1	A	346	TRP	2.6
1	A	108	LYS	2.6
1	B	339	GLY	2.4
1	B	346	TRP	2.2
1	A	436	VAL	2.2
1	B	290	ILE	2.1
1	B	109	GLU	2.1
1	A	105	SER	2.1
1	B	107	ASP	2.0
1	B	105	SER	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
2	A1H0D	A	501	26/26	0.95	0.08	16,24,29,30	0
4	LI	B	505	1/1	0.96	0.47	3,3,3,3	0
4	LI	A	505	1/1	0.98	0.44	0,0,0,0	0
2	A1H0D	B	501	26/26	0.98	0.04	13,17,22,24	0
3	CA	A	504	1/1	1.00	0.01	10,10,10,10	0
3	CA	B	502	1/1	1.00	0.02	10,10,10,10	0
3	CA	B	503	1/1	1.00	0.01	10,10,10,10	0
3	CA	B	504	1/1	1.00	0.04	11,11,11,11	0

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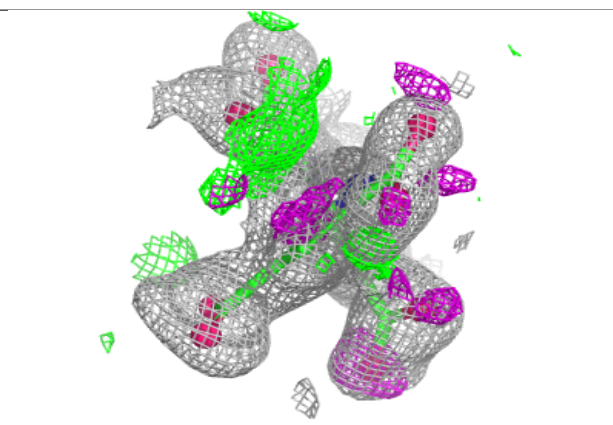
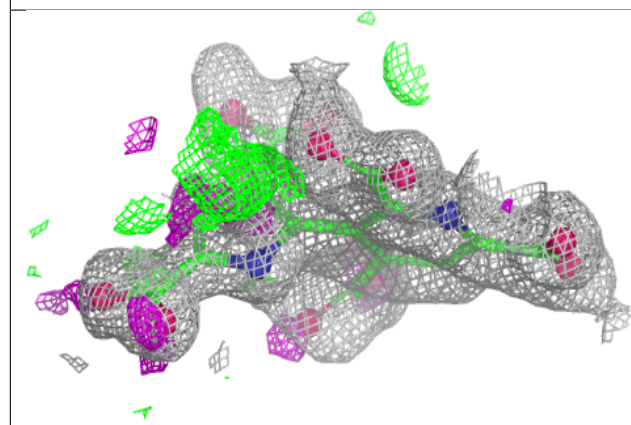
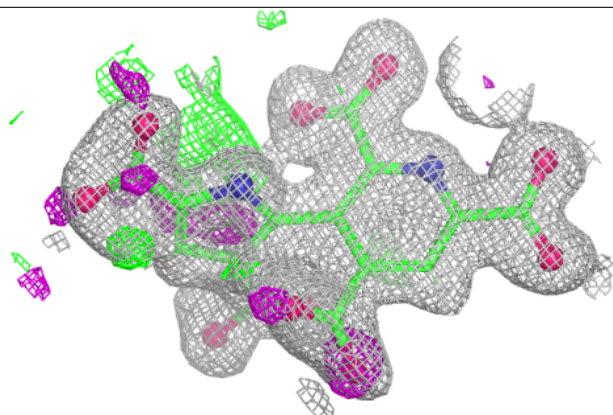
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CA	A	502	1/1	1.00	0.01	9,9,9,9	0
3	CA	A	503	1/1	1.00	0.04	13,13,13,13	0

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.

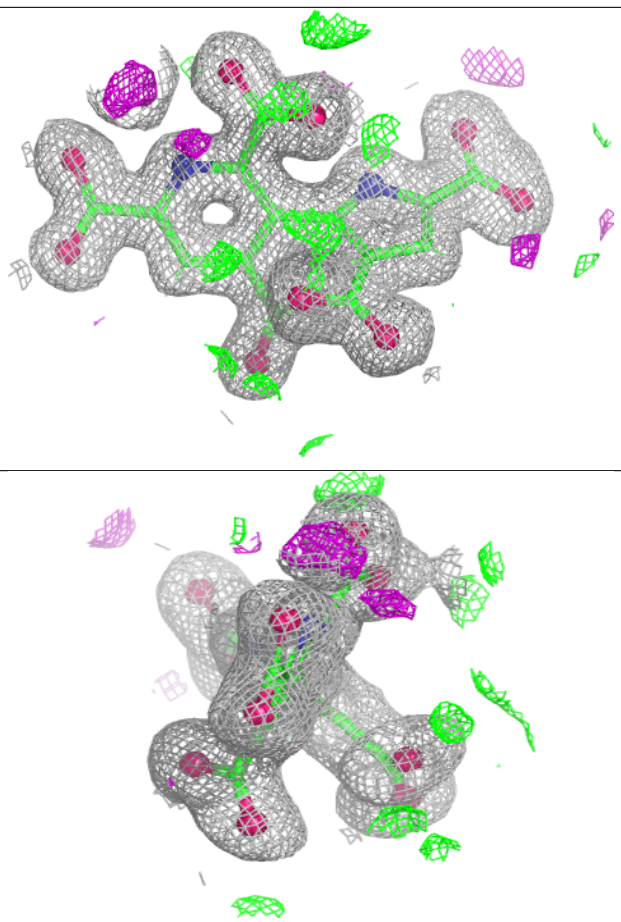
Electron density around A1H0D A 501:

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 A1H0D B 501:

$2mF_o-DF_c$ (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.