W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 6, 2024 – 02:52 PM EST

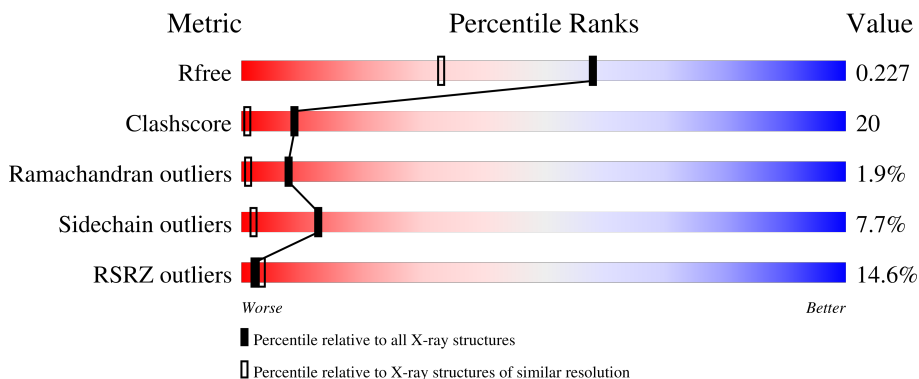|		
PDB ID	:	2F1F
Title	:	Crystal structure of the regulatory subunit of acetohydroxyacid synthase isozyme III from E. coli
Authors	:	Kaplun, A.; Vyazmensky, M.; Barak, Z.; Chipman, D.M.; Shaanan, B.
Deposited on	:	2005-11-14
Resolution	:	1.75 Å(reported)

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 1.75 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	Percentile Ranks	Value
Rfree		0.227
Clashscore		20
Ramachandran outliers		1.9%
Sidechain outliers		7.7%
RSRZ outliers		14.6%

Worse   *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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	164	13% / 74% / 21% / • ••
1	B	164	16% / 63% / 27% / 5% • •

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:

![World Wide Protein Data Bank logo]

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	1PE	A	601	-	-	X	-
4	P33	B	501[A]	-	-	X	-
4	P33	B	501[B]	-	-	X	-

2   Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 2784 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 Acetolactate synthase isozyme III small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	163	Total	C	N	O	S	0	0	0
			1257	785	228	241	3			
1	B	158	Total	C	N	O	S	0	1	0
			1217	760	219	236	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	-	SEE REMARK 999	UNP P00894
B	1	ALA	-	SEE REMARK 999	UNP P00894

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mg	0	0
			2	2		
2	B	4	Total	Mg	0	0
			4	4		

- Molecule 3 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).

1PE

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 16	C 10	O 6	0	0

- Molecule 4 is 3,6,9,12,15,18-HEXAOXAICOSANE-1,20-DIOL (three-letter code: P33) (formula: $C_{14}H_{30}O_8$).

P33
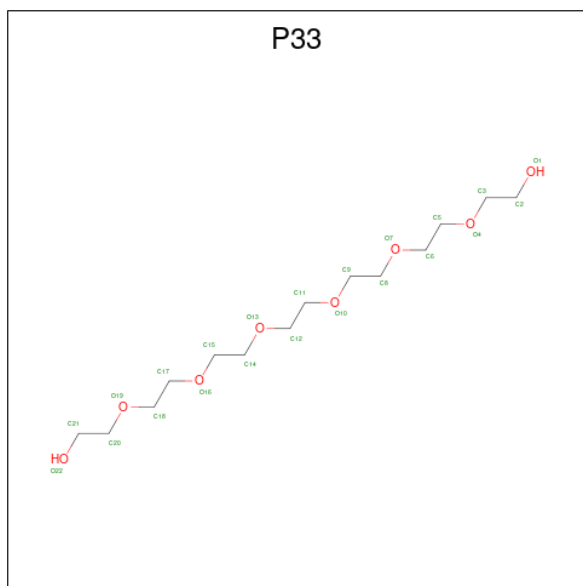
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total 30	C 19	O 11	0	1

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	130	Total 130	O 130	0	0
5	B	128	Total 128	O 128	0	0

3 Residue-property plots ⓘ

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: Acetolactate synthase isozyme III small subunit
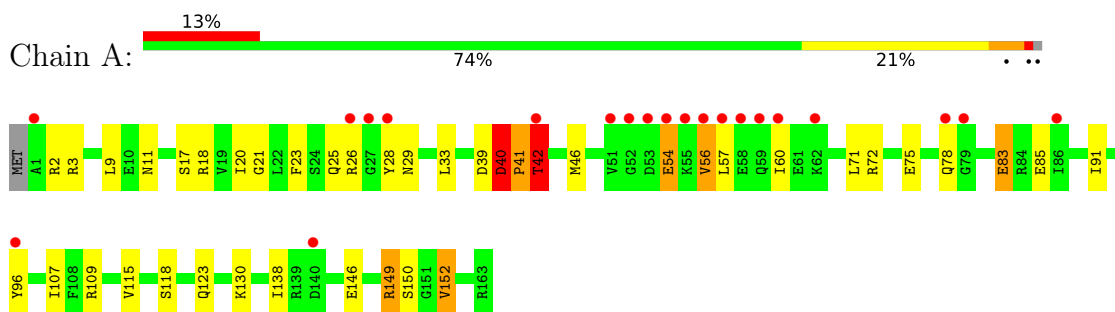
• Molecule 1: Acetolactate synthase isozyme III small subunit
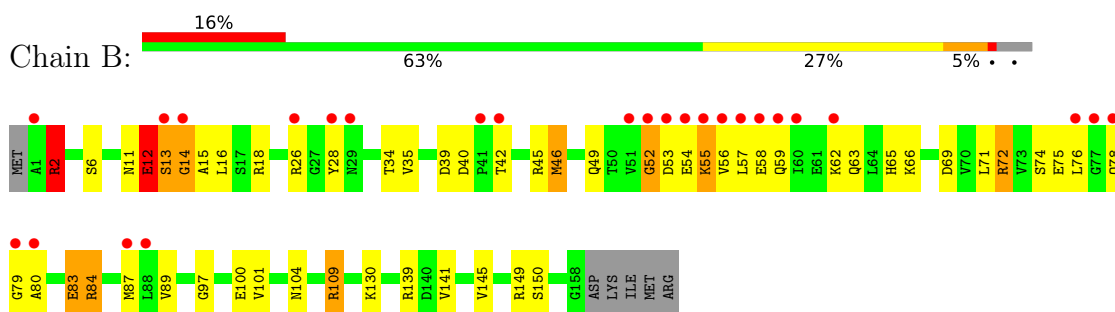
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α, β, γ	98.60Å 98.60Å 80.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.75 38.62 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.3 (20.00-1.75) 99.2 (38.62-1.75)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.69 (at 1.75Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.171 , 0.227 0.172 , 0.227	Depositor DCC
R_{free} test set	1917 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	31.9	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 69.6	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.032 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	2784	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: 1PE, MG, P33

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	1.16	5/1267 (0.4%)	1.10	5/1706 (0.3%)
1	B	1.13	4/1232 (0.3%)	1.08	10/1661 (0.6%)
All	All	1.15	9/2499 (0.4%)	1.09	15/3367 (0.4%)

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
1	B	0	3
All	All	0	5

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	85	GLU	CB-CG	-7.67	1.37	1.52
1	B	104	ASN	CG-OD1	7.54	1.40	1.24
1	A	83	GLU	CB-CG	-7.18	1.38	1.52
1	A	149	ARG	CB-CG	-6.98	1.33	1.52
1	A	152	VAL	CB-CG2	-6.69	1.38	1.52

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	84	ARG	NE-CZ-NH1	-11.72	114.44	120.30
1	B	84	ARG	NE-CZ-NH2	8.38	124.49	120.30
1	B	2	ARG	NE-CZ-NH1	7.67	124.13	120.30
1	B	87	MET	CA-CB-CG	6.91	125.05	113.30

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WORLDWIDE
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PROTEIN DATA BANK

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	139	ARG	NE-CZ-NH2	-6.25	117.17	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	39	ASP	Peptide
1	A	41	PRO	Peptide
1	B	12	GLU	Peptide
1	B	13	SER	Peptide
1	B	52	GLY	Peptide

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	1257	0	1317	37	0
1	B	1217	0	1269	57	0
2	A	2	0	0	0	0
2	B	4	0	0	0	0
3	A	16	0	22	9	0
4	B	30	0	26	18	0
5	A	130	0	0	11	0
5	B	128	0	0	4	0
All	All	2784	0	2634	106	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 20.

The worst 5 of 106 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:B:40:ASP:OD1	1:B:42:THR:HG22	1.65	0.97
1:B:52:GLY:CA	1:B:53:ASP:HB2	1.97	0.94
1:A:40:ASP:OD2	1:A:40:ASP:O	1.87	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:ARG:HH11	1:B:49:GLN:NE2	1.67	0.91
1:B:109:ARG:CG	1:B:109:ARG:HH11	1.83	0.91

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	A	161/164 (98%)	156 (97%)	1 (1%)	4 (2%)	5	0
1	B	157/164 (96%)	150 (96%)	5 (3%)	2 (1%)	12	2
All	All	318/328 (97%)	306 (96%)	6 (2%)	6 (2%)	8	1

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	ASP
1	B	54	GLU
1	A	26	ARG
1	A	42	THR
1	B	14	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	A	139/140 (99%)	129 (93%)	10 (7%)	14	2
1	B	135/140 (96%)	124 (92%)	11 (8%)	11	1
All	All	274/280 (98%)	253 (92%)	21 (8%)	13	2

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	55	LYS
1	B	74	SER
1	B	109	ARG
1	B	76	LEU
1	B	72	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	B	11	ASN
1	B	49	GLN
1	B	59	GLN

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 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 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	1PE	A	601	-	15,15,15	0.51	0	14,14,14	1.03	0
4	P33	B	501[A]	-	21,21,21	0.79	1 (4%)	20,20,20	1.67	3 (15%)
4	P33	B	501[B]	-	21,21,21	0.80	1 (4%)	20,20,20	1.66	2 (10%)

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	1PE	A	601	-	-	8/13/13/13	-
4	P33	B	501[A]	-	-	13/19/19/19	-
4	P33	B	501[B]	-	-	14/19/19/19	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	501[A]	P33	O16-C15	2.18	1.51	1.42
4	B	501[B]	P33	O16-C15	2.18	1.51	1.42

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	501[A]	P33	O13-C14-C15	5.21	133.88	110.39
4	B	501[B]	P33	O13-C14-C15	5.21	133.88	110.39
4	B	501[A]	P33	C15-O16-C17	3.35	127.81	113.29
4	B	501[B]	P33	C15-O16-C17	3.35	127.81	113.29
4	B	501[A]	P33	C3-O4-C5	2.08	122.30	113.29

There are no chirality outliers.

5 of 35 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	1PE	C13-C23-OH3-C22

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Mol	Chain	Res	Type	Atoms
4	B	501[B]	P33	O4-C5-C6-O7
4	B	501[A]	P33	O13-C14-C15-O16
4	B	501[B]	P33	O13-C14-C15-O16
4	B	501[A]	P33	O7-C8-C9-O10

There are no ring outliers.

3 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	1PE	9	0
4	B	501[A]	P33	9	0
4	B	501[B]	P33	9	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 P33 B 501 (A)

Bond lengths — Bond angles — Torsions — Rings

Ligand P33 B 501 (B)

Bond lengths — Bond angles — Torsions — Rings
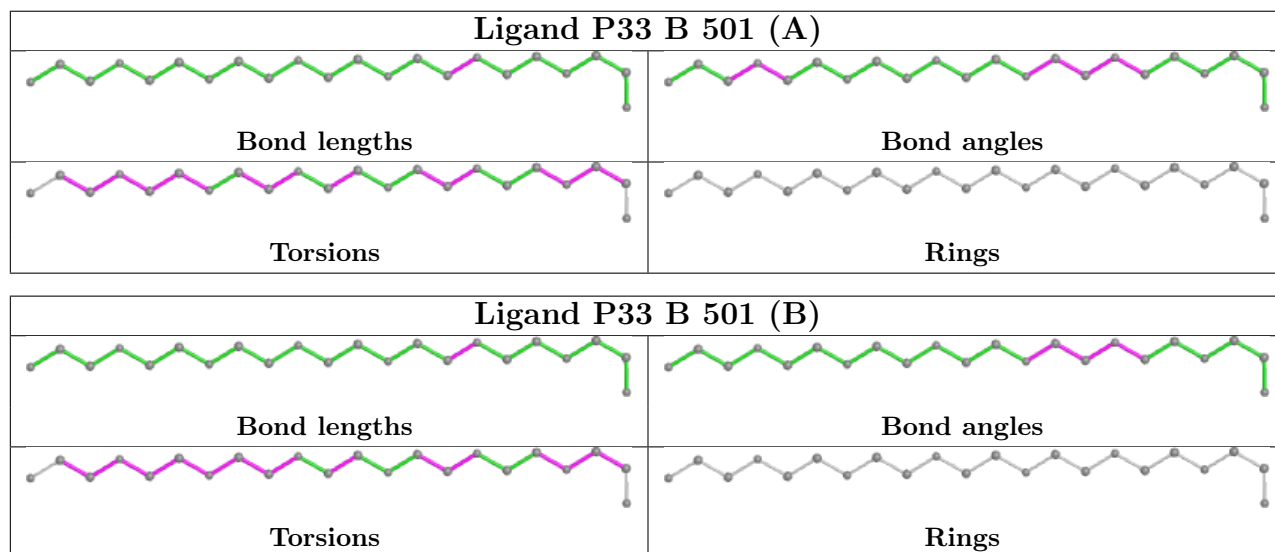
5.7 Other polymers ⓘ

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, 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(Å²)	Q<0.9
1	A	163/164 (99%)	0.82	21 (12%)	3	5	24, 36, 64, 82	0
1	B	158/164 (96%)	0.89	26 (16%)	1	2	23, 39, 74, 84	1 (0%)
All	All	321/328 (97%)	0.86	47 (14%)	2	3	23, 37, 71, 84	1 (0%)

The worst 5 of 47 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	57	LEU	8.1
1	A	56	VAL	7.5
1	A	55	LYS	6.9
1	B	52	GLY	6.4
1	A	1	ALA	6.4

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

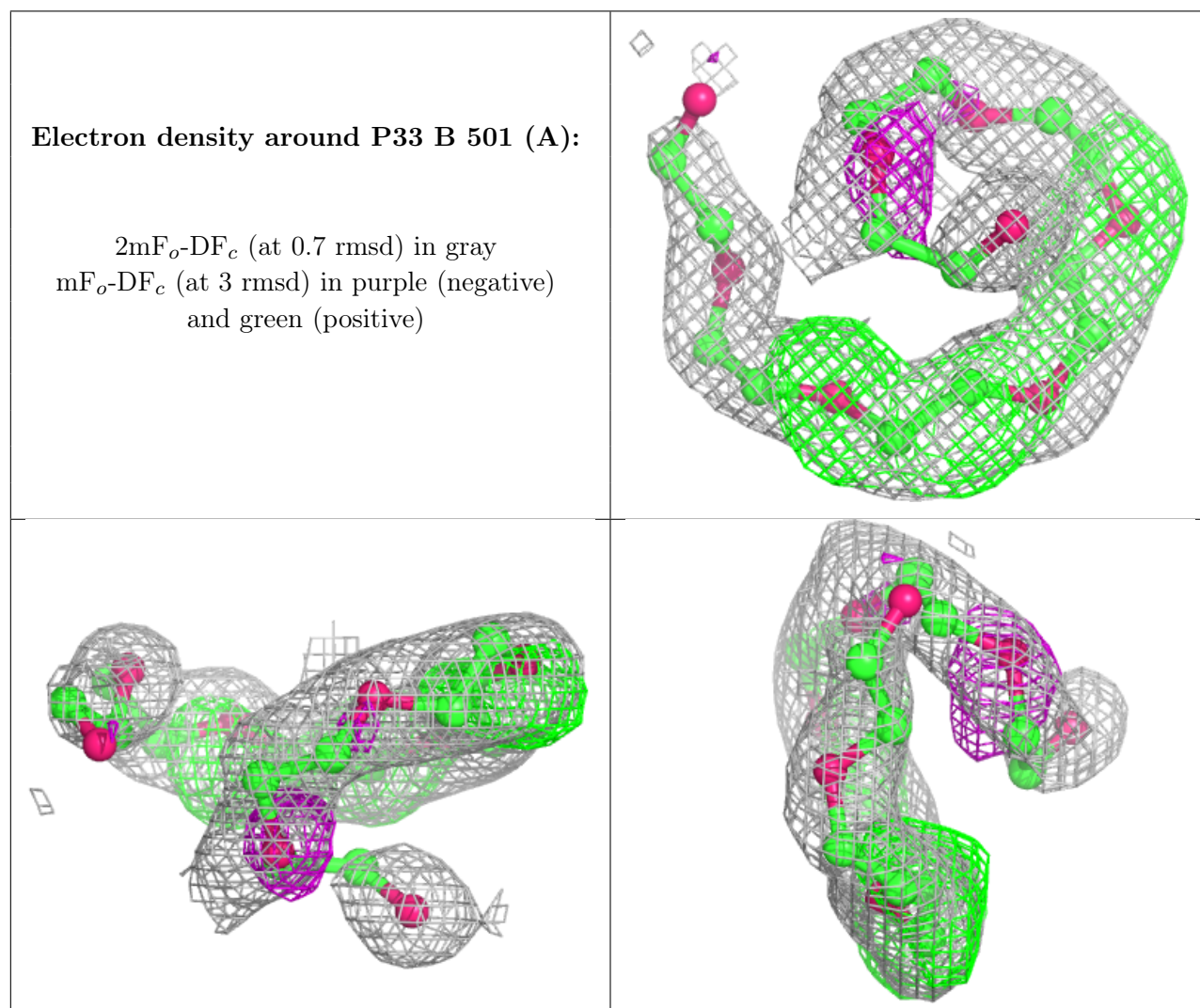There are no non-standard protein/DNA/RNA residues in this entry.

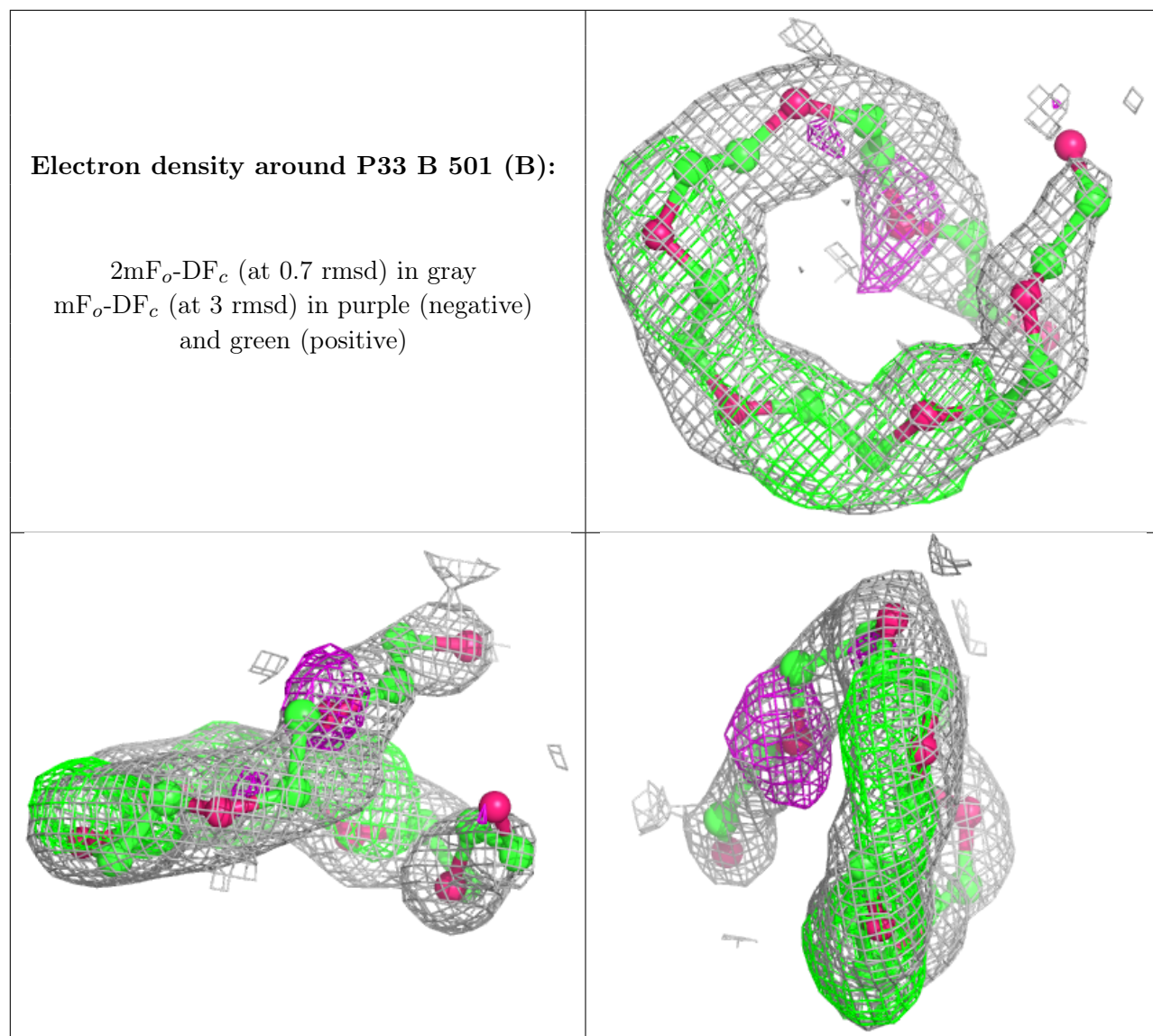## 6.3 Carbohydrates ⓘ

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, 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(Å²)	Q<0.9
4	P33	B	501[A]	22/22	0.69	0.40	14,30,42,44	22
4	P33	B	501[B]	22/22	0.69	0.40	14,36,48,49	22
2	MG	B	810	1/1	0.73	0.31	101,101,101,101	1
2	MG	B	805	1/1	0.82	0.06	66,66,66,66	1
2	MG	A	802	1/1	0.82	0.08	67,67,67,67	0
2	MG	B	902	1/1	0.90	0.15	54,54,54,54	0
2	MG	B	901	1/1	0.95	0.18	38,38,38,38	1
3	1PE	A	601	16/16	0.95	0.13	31,46,52,54	1
2	MG	A	801	1/1	0.97	0.10	36,36,36,36	1

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 P33 B 501 (A):

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

Electron density around P33 B 501 (B):

$2mF_o$-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.