



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 05:14 am BST

PDB ID : 2EXA
Title : Crystal structure of penicillin binding protein 4 (dacB) from Escherichia coli, complexed with FAROM
Authors : Kishida, H.; Unzai, S.; Roper, D.I.; Lloyd, A.; Park, S.-Y.; Tame, J.R.H.
Deposited on : 2005-11-08
Resolution : 1.70 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

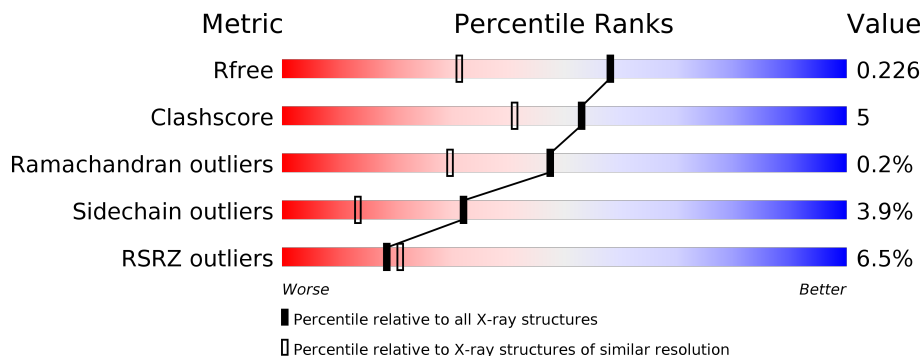
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 on 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	458	

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	DGF	A	501	X	-	-	-

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 3664 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.

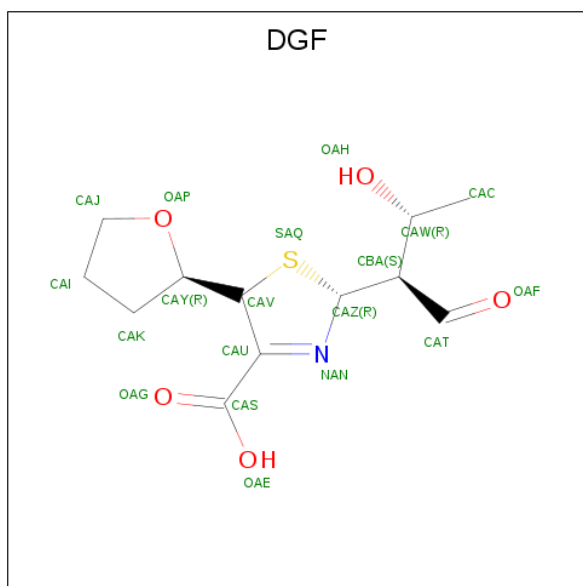
- Molecule 1 is a protein called Penicillin-binding protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	443	3378	2139	593	629	17	0	3	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	MET	-	INITIATING METHIONINE	UNP P24228
A	261	TYR	ASP	ENGINEERED MUTATION	UNP P24228

- Molecule 2 is (2R,5R)-2-[(2S,3R)-3-hydroxy-1-oxobutan-2-yl]-5-[(2R)-tetrahydrofuran-2-yl]-2,5-dihydro-1,3-thiazole-4-carboxylic acid (three-letter code: DGF) (formula: C₁₂H₁₇NO₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	19	12	1	5	1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	261	Total	O	0	0
			261	261		

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	95.63Å 95.63Å 115.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.70 42.77 – 1.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-1.70) 98.5 (42.77-1.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 1.70Å)	Xtrriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.196 , 0.222 0.198 , 0.226	Depositor DCC
R_{free} test set	2967 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	23.6	Xtrriage
Anisotropy	0.024	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 50.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3664	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.28% 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: GOL, DGF

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	0.63	1/3446 (0.0%)	0.84	14/4678 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	439	MET	CB-CG	8.95	1.79	1.51

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	220	ASP	CB-CG-OD2	8.06	125.56	118.30
1	A	138	ASP	CB-CG-OD2	6.73	124.36	118.30
1	A	439	MET	CB-CG-SD	-6.73	92.21	112.40
1	A	100	ASP	CB-CG-OD2	6.43	124.09	118.30
1	A	108	ASP	CB-CG-OD2	6.28	123.95	118.30
1	A	355	ASP	CB-CG-OD2	5.80	123.52	118.30
1	A	396	ASP	CB-CG-OD1	5.77	123.49	118.30
1	A	51	ASP	CB-CG-OD2	5.73	123.46	118.30
1	A	30	LEU	CA-CB-CG	5.65	128.30	115.30
1	A	312	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	146	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	186	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	439	MET	CB-CA-C	5.07	120.54	110.40
1	A	472	ASP	CB-CG-OD2	5.04	122.84	118.30

There are no chirality outliers.

There are no planarity outliers.

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	3378	0	3373	36	0
2	A	19	0	0	2	0
3	A	6	0	8	0	0
4	A	261	0	0	1	0
All	All	3664	0	3381	37	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 (37) 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:439:MET:CB	1:A:439:MET:CG	1.80	1.58
1:A:439:MET:CB	1:A:439:MET:SD	2.53	0.95
2:A:501:MGF:SAQ	2:A:501:MGF:CAC	2.56	0.93
1:A:209:ARG:HH11	1:A:209:ARG:HG2	1.37	0.88
1:A:225:ASP:O	1:A:228:ARG:HD3	1.77	0.84
1:A:209:ARG:CG	1:A:209:ARG:HH11	1.99	0.76
1:A:238:ARG:HD3	1:A:240:GLU:O	1.90	0.71
1:A:30:LEU:HB2	1:A:31:PRO:CD	2.22	0.70
1:A:354:ALA:H	1:A:363:ASN:ND2	1.90	0.68
1:A:472:ASP:OD2	1:A:476:ASN:ND2	2.26	0.64
1:A:57:MET:HB3	1:A:364:LEU:HD22	1.81	0.62
1:A:322:ARG:HH12	1:A:343:GLN:HE22	1.52	0.56
1:A:30:LEU:HB2	1:A:31:PRO:HD3	1.86	0.56
1:A:209:ARG:NH1	1:A:209:ARG:HG2	2.13	0.55
1:A:228:ARG:HH21	1:A:228:ARG:HB2	1.73	0.53
1:A:115:ASP:OD2	1:A:290:LYS:HE3	2.09	0.53
1:A:154:ASN:H	1:A:154:ASN:ND2	2.10	0.50
1:A:308:ASN:HD21	2:A:501:MGF:CAC	2.25	0.49
1:A:134:ASN:HD22	1:A:273:THR:H	1.60	0.48
1:A:199:THR:HB	1:A:228:ARG:HG3	1.95	0.47
1:A:95:GLY:HA2	1:A:127:GLY:O	2.15	0.47
1:A:154:ASN:H	1:A:154:ASN:HD22	1.63	0.46
1:A:61:ALA:HB2	1:A:421:LEU:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:ILE:HB	1:A:461:PRO:HD3	1.97	0.45
1:A:380:HIS:HD2	1:A:383:GLU:OE2	1.99	0.45
1:A:184:PRO:HG3	1:A:237:GLN:HE21	1.81	0.45
1:A:30:LEU:CB	1:A:31:PRO:CD	2.92	0.45
1:A:28:THR:O	1:A:30:LEU:HD23	2.18	0.44
1:A:104:ARG:HA	1:A:138:ASP:HB3	1.99	0.44
1:A:146:ASP:O	1:A:164:PRO:HD2	2.17	0.43
1:A:30:LEU:HD11	1:A:445:LEU:HD21	1.99	0.43
1:A:422:GLN:HG3	1:A:422:GLN:H	1.51	0.43
1:A:438:ARG:HD2	4:A:1161:HOH:O	2.18	0.43
1:A:408:ALA:O	1:A:471:LYS:HD3	2.19	0.42
1:A:421:LEU:HB2	1:A:424:VAL:HB	2.03	0.41
1:A:361:ARG:NH2	1:A:421:LEU:HD21	2.35	0.41
1:A:439:MET:SD	1:A:439:MET:HB3	2.56	0.40

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	439/458 (96%)	430 (98%)	8 (2%)	1 (0%)	47 30

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	THR

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	357/370 (96%)	343 (96%)	14 (4%)	32 13

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	97	LEU
1	A	98	LYS
1	A	125	LYS
1	A	154	ASN
1	A	209	ARG
1	A	228	ARG
1	A	231	LEU
1	A	238	ARG
1	A	364	LEU
1	A	398	SER
1	A	421	LEU
1	A	422	GLN
1	A	459	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	130	GLN
1	A	134	ASN
1	A	154	ASN
1	A	237	GLN
1	A	249	GLN
1	A	277	GLN
1	A	343	GLN
1	A	350	ASN
1	A	363	ASN
1	A	380	HIS
1	A	382	ASN
1	A	385	ASN
1	A	400	GLN
1	A	426	ASN

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Mol	Chain	Res	Type
1	A	475	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	DGF	A	501	1	14,20,20	3.54	6 (42%)	10,28,28	1.19	2 (20%)
3	GOL	A	502	-	5,5,5	0.38	0	5,5,5	0.99	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	DGF	A	501	1	1/1/7/8	2/8/37/37	0/2/2/2
3	GOL	A	502	-	-	2/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	DGF	CAU-NAN	9.88	1.35	1.28
2	A	501	DGF	CAV-SAQ	-7.00	1.72	1.83
2	A	501	DGF	CAS-CAU	2.88	1.56	1.52
2	A	501	DGF	CBA-CAT	2.39	1.54	1.50
2	A	501	DGF	OAP-CAY	2.27	1.48	1.44
2	A	501	DGF	CBA-CAW	2.20	1.56	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	DGF	CAJ-OAP-CAY	-2.31	104.76	108.48
2	A	501	DGF	OAP-CAY-CAK	-2.13	102.58	105.37

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	501	DGF	CAW

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	DGF	CAU-CAV-CAY-CAK
2	A	501	DGF	CAU-CAV-CAY-OAP
3	A	502	GOL	O1-C1-C2-C3
3	A	502	GOL	O1-C1-C2-O2

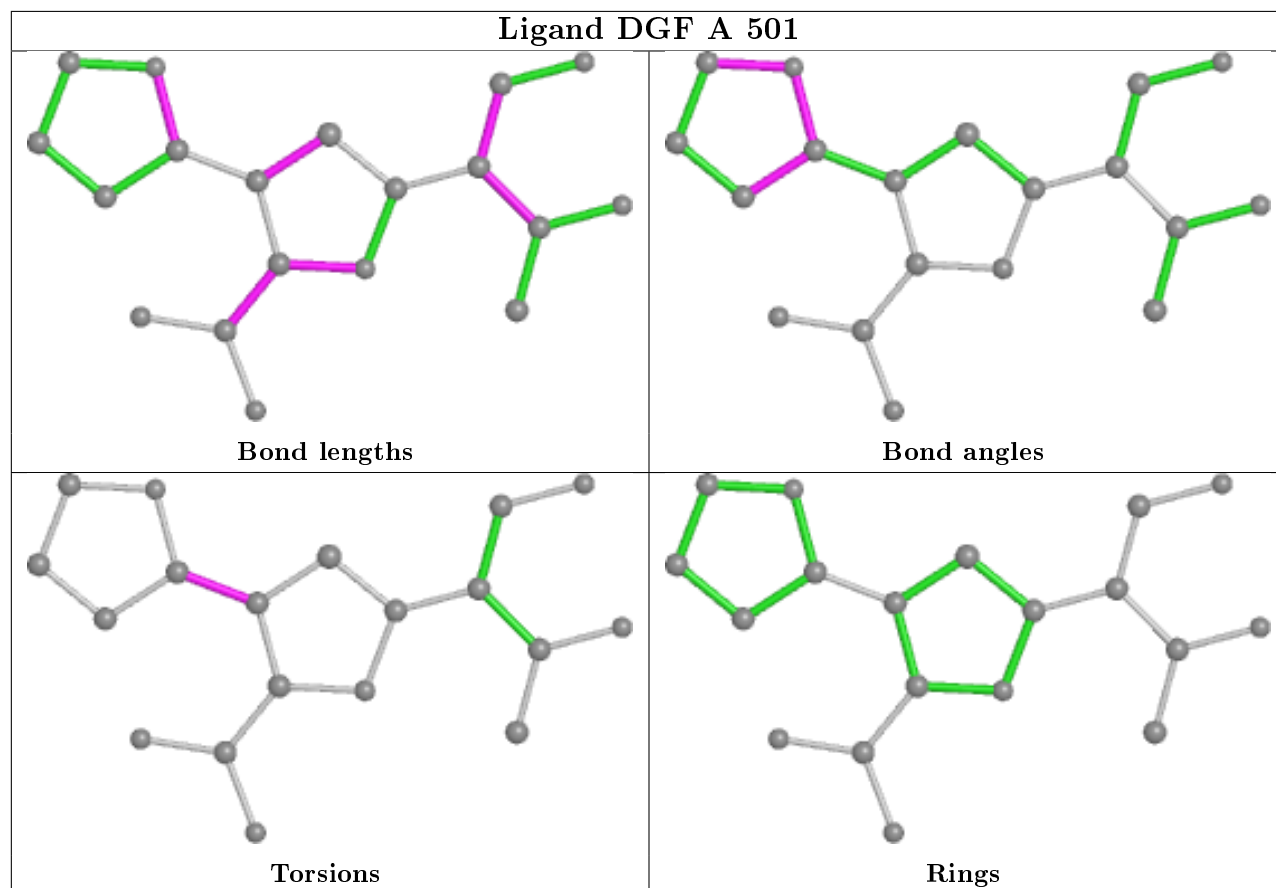
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	DGF	2	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.



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	443/458 (96%)	0.25	29 (6%) 18 21	18, 27, 45, 69	1 (0%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	459	ARG	7.3
1	A	460	ILE	5.4
1	A	26	TYR	5.2
1	A	182	PRO	4.6
1	A	91	ASN	4.6
1	A	30	LEU	4.2
1	A	209	ARG	4.0
1	A	183	LYS	4.0
1	A	27	ILE	3.9
1	A	210	GLY	3.9
1	A	189	PHE	3.6
1	A	464	ARG	3.4
1	A	239	SER	3.4
1	A	94	ASN	3.3
1	A	32	ALA	3.2
1	A	448	TYR	3.2
1	A	31	PRO	2.7
1	A	449	ALA	2.7
1	A	184	PRO	2.7
1	A	29	GLN	2.6
1	A	98	LYS	2.5
1	A	185	GLY	2.3
1	A	422	GLN	2.3
1	A	179	TYR	2.2
1	A	359	LEU	2.2
1	A	437	GLN	2.2
1	A	205	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	188	ALA	2.1
1	A	287	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](#)

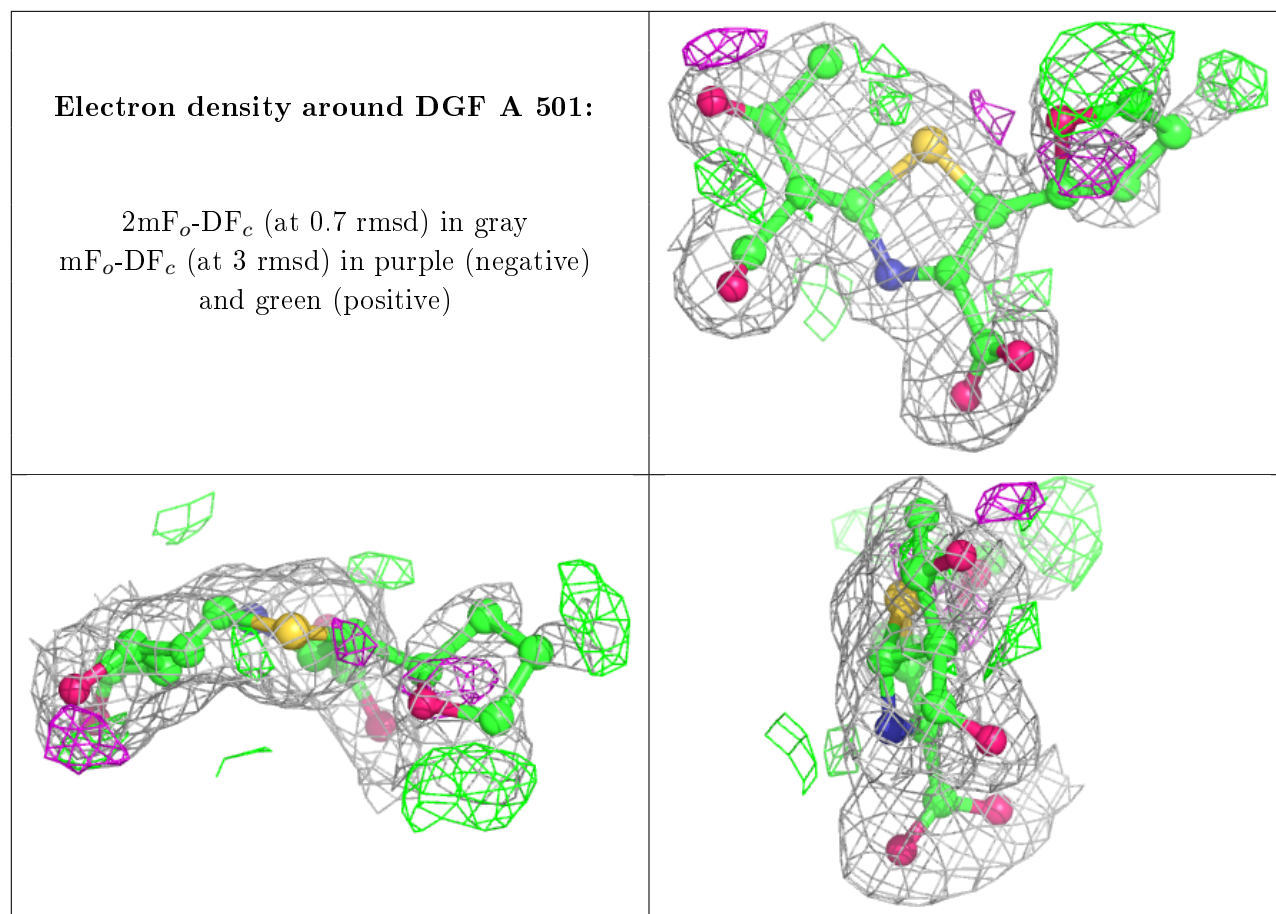
There are no carbohydrates in this entry.

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	DGF	A	501	19/19	0.86	0.15	24,41,52,52	0
3	GOL	A	502	6/6	0.86	0.15	34,40,40,43	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.