W O R L D W I D E
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wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 17, 2021 – 01:18 AM EDT

PDB ID	:	1R8Q
Title	:	FULL-LENGTH ARF1-GDP-MG IN COMPLEX WITH BREFELDIN A AND A SEC7 DOMAIN
Authors	:	Renault, L.; Guibert, B.; Cherfils, J.
Deposited on	:	2003-10-28
Resolution	:	1.86 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

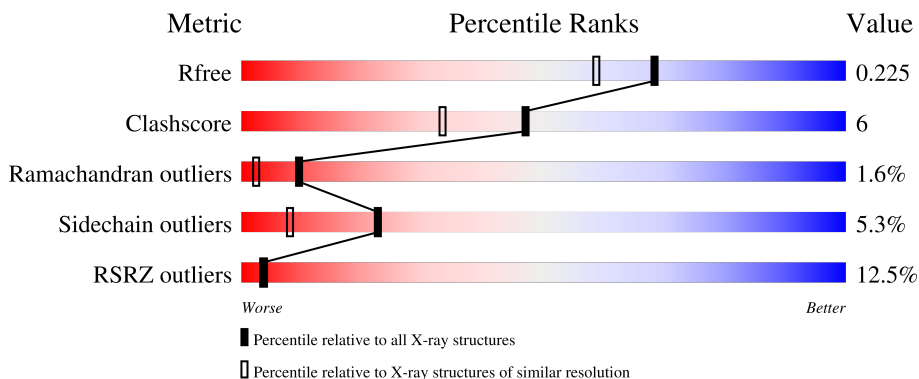|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 1.86 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		0.225
Clashscore		6
Ramachandran outliers		1.6%
Sidechain outliers		5.3%
RSRZ outliers		12.5%

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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	181	15% / 75% 21% ・・・
1	B	181	19% / 78% 14% ・ ・・
2	E	203	9% / 81% 10% ・ 6%
2	F	203	5% / 80% 13% ・・

2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 6487 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 ADP-ribosylation factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	179	Total	C	N	O	S	0	2	0
			1445	920	252	267	6			
1	B	179	Total	C	N	O	S	0	1	0
			1442	918	252	266	6			

- Molecule 2 is a protein called Arno.

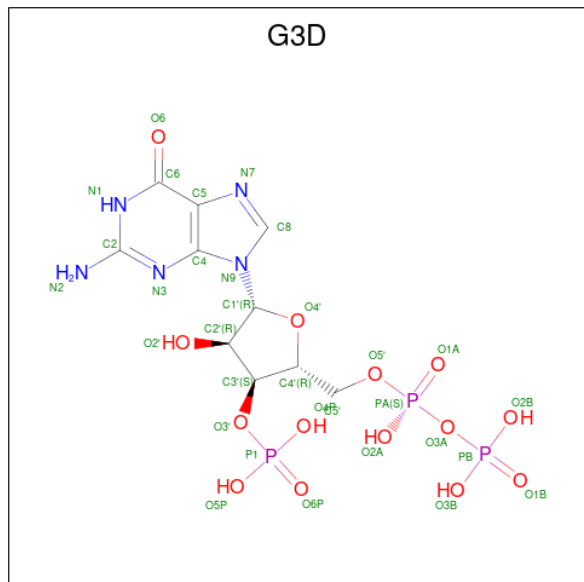| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	191	Total	C	N	O	S	0	1	0
			1559	987	274	287	11			
2	F	194	Total	C	N	O	S	0	2	0
			1589	1003	280	295	11			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	190	TYR	PHE	engineered mutation	UNP Q99418
E	191	SER	ALA	engineered mutation	UNP Q99418
E	198	ASP	SER	engineered mutation	UNP Q99418
E	208	MET	PRO	engineered mutation	UNP Q99418
F	190	TYR	PHE	engineered mutation	UNP Q99418
F	191	SER	ALA	engineered mutation	UNP Q99418
F	198	ASP	SER	engineered mutation	UNP Q99418
F	208	MET	PRO	engineered mutation	UNP Q99418

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is GUANOSINE-3'-MONOPHOSPHATE-5'-DIPHOSPHATE (three-letter code: G3D) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	B	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 5 is 1,6,7,8,9,11A,12,13,14,14A-DECAHYDRO-1,13-DIHYDROXY-6-METHYL -4H-CYCLOPENT[F]OXACYCLOTRIDECIN-4-ONE (three-letter code: AFB) (formula: $C_{16}H_{24}O_4$).
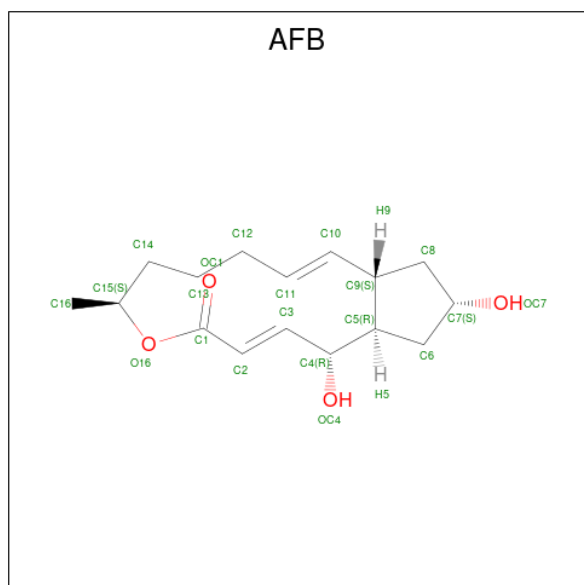
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 20	C 16	O 4	0	0
5	B	1	Total 20	C 16	O 4	0	0

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	1	Total 1	Zn 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	108	Total 108	O 108	0	0
7	E	71	Total 71	O 71	0	0
7	B	73	Total 73	O 73	0	0
7	F	93	Total 93	O 93	0	0

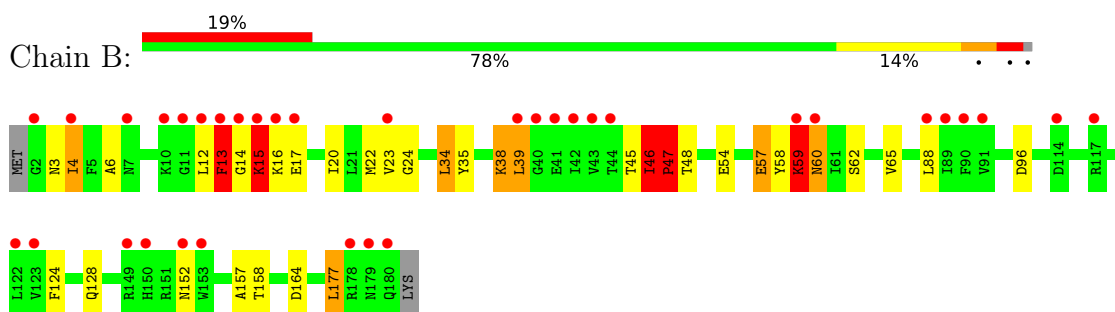# 3 Residue-property plots ⓘ

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.
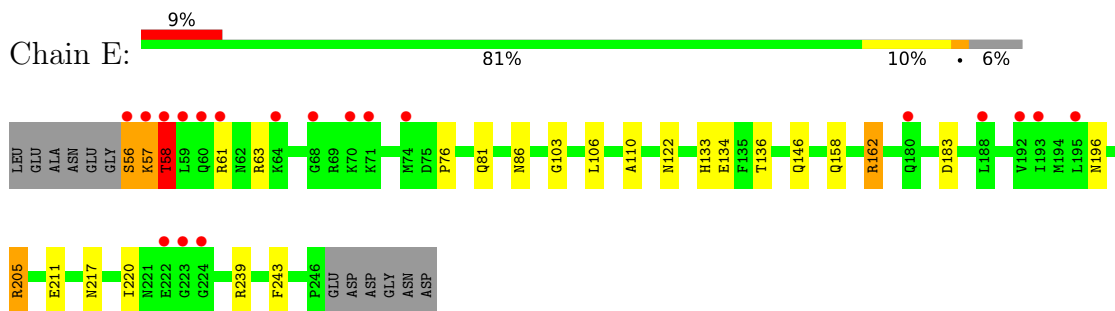
• Molecule 1: ADP-ribosylation factor 1

Chain A:

• Molecule 1: ADP-ribosylation factor 1

Chain B:

• Molecule 2: Arno

Chain E:

• Molecule 2: Arno

Chain F:

LEU GLU ALA ASN GLU GLY S56 K57 M67 D75 T109 R118 V130 H133 E134 V141 Q146 F147 L148 R152 L153 C174 Q180 T184 L188 S189 V192 I193 M194 L195 H200 R205 M208 G209 L210 E211 R212 N217 I220 N221 E222

G223 G224 L234 I238 R239 N240 D248 D249 GLY ASN ASP
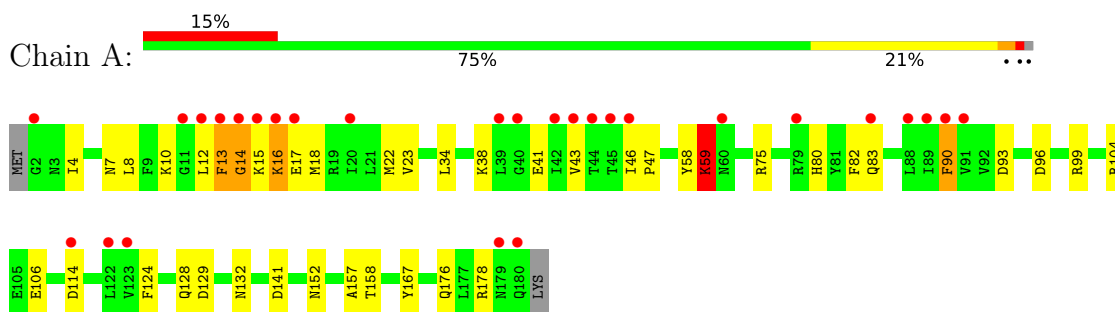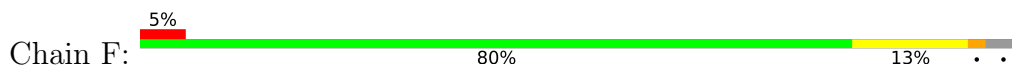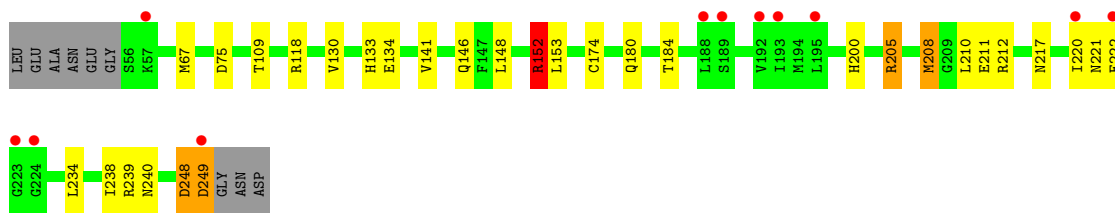
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	69.08Å 109.77Å 118.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.88 – 1.86 23.49 – 1.86	Depositor EDS
% Data completeness (in resolution range)	98.3 (29.88-1.86) 98.3 (23.49-1.86)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.77 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.179 , 0.220 0.189 , 0.225	Depositor DCC
R_{free} test set	3692 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å²)	30.7	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.34 , 51.0	EDS
L-test for twinning [2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6487	wwPDB-VP
Average B, all atoms (Å²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, AFB, ZN, G3D

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	4/1479 (0.3%)	1.05	7/1999 (0.4%)
1	B	1.06	6/1472 (0.4%)	1.01	3/1989 (0.2%)
2	E	1.05	1/1592 (0.1%)	1.06	7/2142 (0.3%)
2	F	1.05	1/1626 (0.1%)	1.13	10/2188 (0.5%)
All	All	1.08	12/6169 (0.2%)	1.07	27/8318 (0.3%)

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	1
1	B	0	1
All	All	0	2

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	47	PRO	CA-C	8.41	1.69	1.52
1	B	22	MET	SD-CE	-7.22	1.37	1.77
1	A	106	GLU	CD-OE1	6.98	1.33	1.25
1	B	152	ASN	CG-ND2	6.80	1.49	1.32
1	B	152	ASN	CA-C	5.90	1.68	1.52

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	152	ARG	NE-CZ-NH2	-14.73	112.94	120.30
2	F	205	ARG	NE-CZ-NH2	-14.16	113.22	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	162	ARG	NE-CZ-NH2	-13.42	113.59	120.30
2	F	205	ARG	NE-CZ-NH1	11.59	126.10	120.30
2	E	162	ARG	NE-CZ-NH1	11.59	126.09	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	14	GLY	Peptide
1	B	46	ILE	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	1445	0	1444	25	1
1	B	1442	0	1441	20	1
2	E	1559	0	1552	14	0
2	F	1589	0	1576	24	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	32	0	11	0	0
4	B	32	0	11	0	0
5	A	20	0	24	0	0
5	B	20	0	24	0	0
6	E	1	0	0	0	0
7	A	108	0	0	0	0
7	B	73	0	0	0	0
7	E	71	0	0	3	0
7	F	93	0	0	4	0
All	All	6487	0	6083	76	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 6.

The worst 5 of 76 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:ASN:ND2	1:A:176:GLN:OE1	1.78	1.17
2:F:148:LEU:HD22	7:F:305:HOH:O	1.55	1.06
2:F:109[B]:THR:HG23	2:F:152:ARG:NH1	1.72	1.02
1:A:58:TYR:O	1:A:59:LYS:HB2	1.81	0.81
2:F:174:CYS:SG	7:F:317:HOH:O	2.40	0.80

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)
1:A:141:ASP:OD2	1:B:35:TYR:OH[3_555]	2.13	0.07

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	179/181 (99%)	170 (95%)	6 (3%)	3 (2%)	9	2
1	B	178/181 (98%)	167 (94%)	5 (3%)	6 (3%)	3	0
2	E	190/203 (94%)	187 (98%)	1 (0%)	2 (1%)	14	4
2	F	194/203 (96%)	192 (99%)	1 (0%)	1 (0%)	29	15
All	All	741/768 (96%)	716 (97%)	13 (2%)	12 (2%)	9	2

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	PHE
1	A	16	LYS
2	E	57	LYS
2	E	58	THR
1	B	4	ILE

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	155/155 (100%)	146 (94%)	9 (6%)	20	6
1	B	154/155 (99%)	141 (92%)	13 (8%)	11	2
2	E	170/178 (96%)	163 (96%)	7 (4%)	30	13
2	F	174/178 (98%)	169 (97%)	5 (3%)	42	26
All	All	653/666 (98%)	619 (95%)	34 (5%)	22	8

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	177	LEU
2	F	67	MET
2	F	152	ARG
2	E	61	ARG
2	E	58	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	122	ASN
2	F	175	ASN
2	F	133	HIS
2	F	180	GLN
2	E	122	ASN

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.

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5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 3 are 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
5	AFB	B	503	-	21,21,21	2.21	7 (33%)	27,28,28	2.49	12 (44%)
5	AFB	A	403	-	21,21,21	1.97	9 (42%)	27,28,28	2.60	12 (44%)
4	G3D	B	501	3	28,34,34	2.08	10 (35%)	37,54,54	1.85	8 (21%)
4	G3D	A	401	3	28,34,34	1.65	6 (21%)	37,54,54	2.30	13 (35%)

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
5	AFB	B	503	-	-	1/21/33/33	0/2/2/2
5	AFB	A	403	-	-	1/21/33/33	0/2/2/2
4	G3D	B	501	3	-	3/17/37/37	0/3/3/3
4	G3D	A	401	3	-	3/17/37/37	0/3/3/3

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	503	AFB	C4-C3	5.15	1.58	1.50
4	B	501	G3D	P1-O6P	4.83	1.66	1.50
5	A	403	AFB	C4-C3	4.02	1.56	1.50
5	B	503	AFB	C2-C3	3.86	1.41	1.32
4	A	401	G3D	C5'-C4'	3.76	1.63	1.51

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	401	G3D	N3-C2-N1	-6.48	118.57	127.22
5	A	403	AFB	C9-C5-C4	-6.25	106.74	114.76
5	B	503	AFB	C9-C5-C4	-5.81	107.30	114.76
4	A	401	G3D	C2-N3-C4	5.27	121.37	115.36
5	A	403	AFB	C16-C15-C14	-4.83	100.92	113.97

There are no chirality outliers.

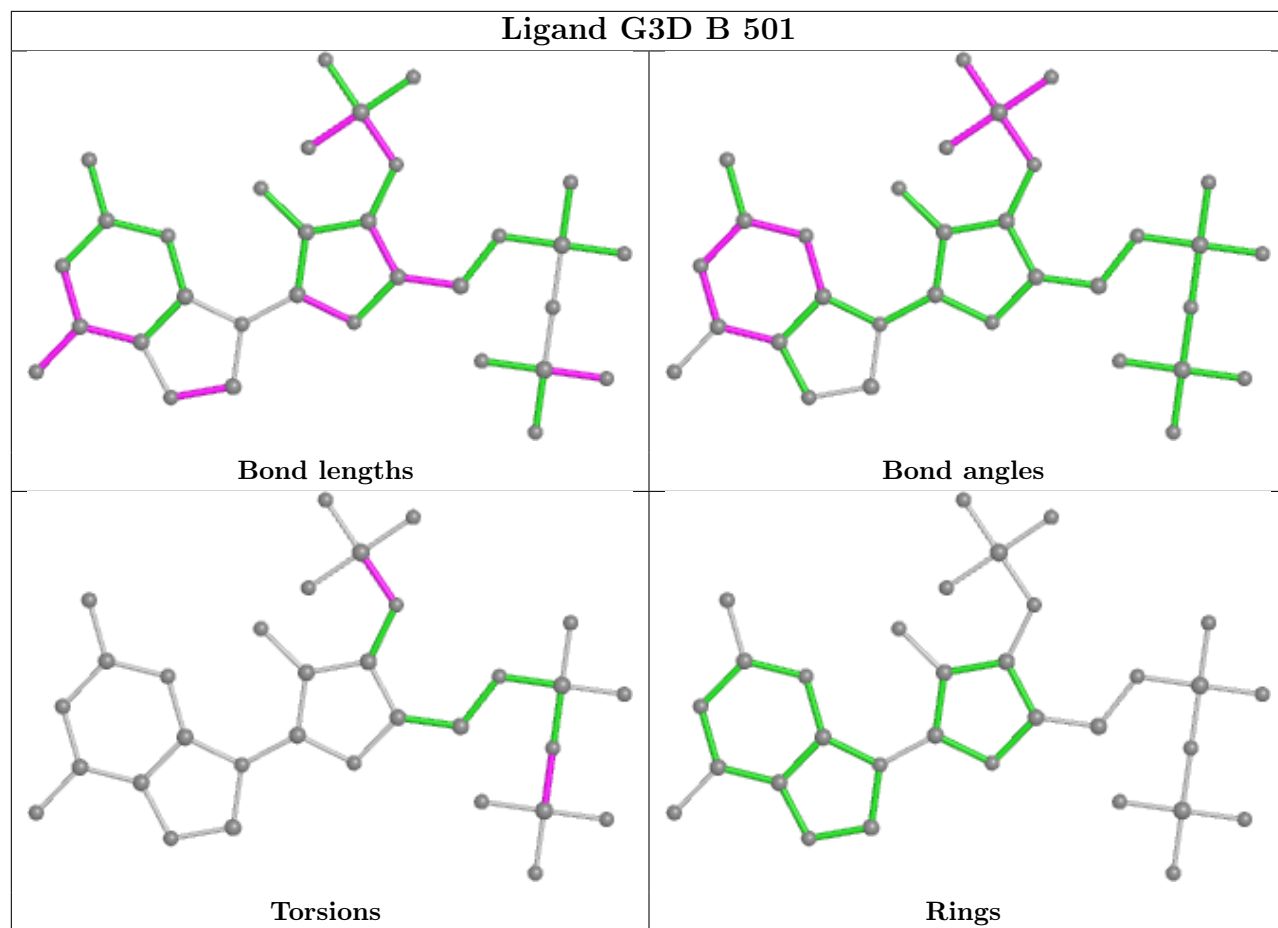5 of 8 torsion outliers are listed below:

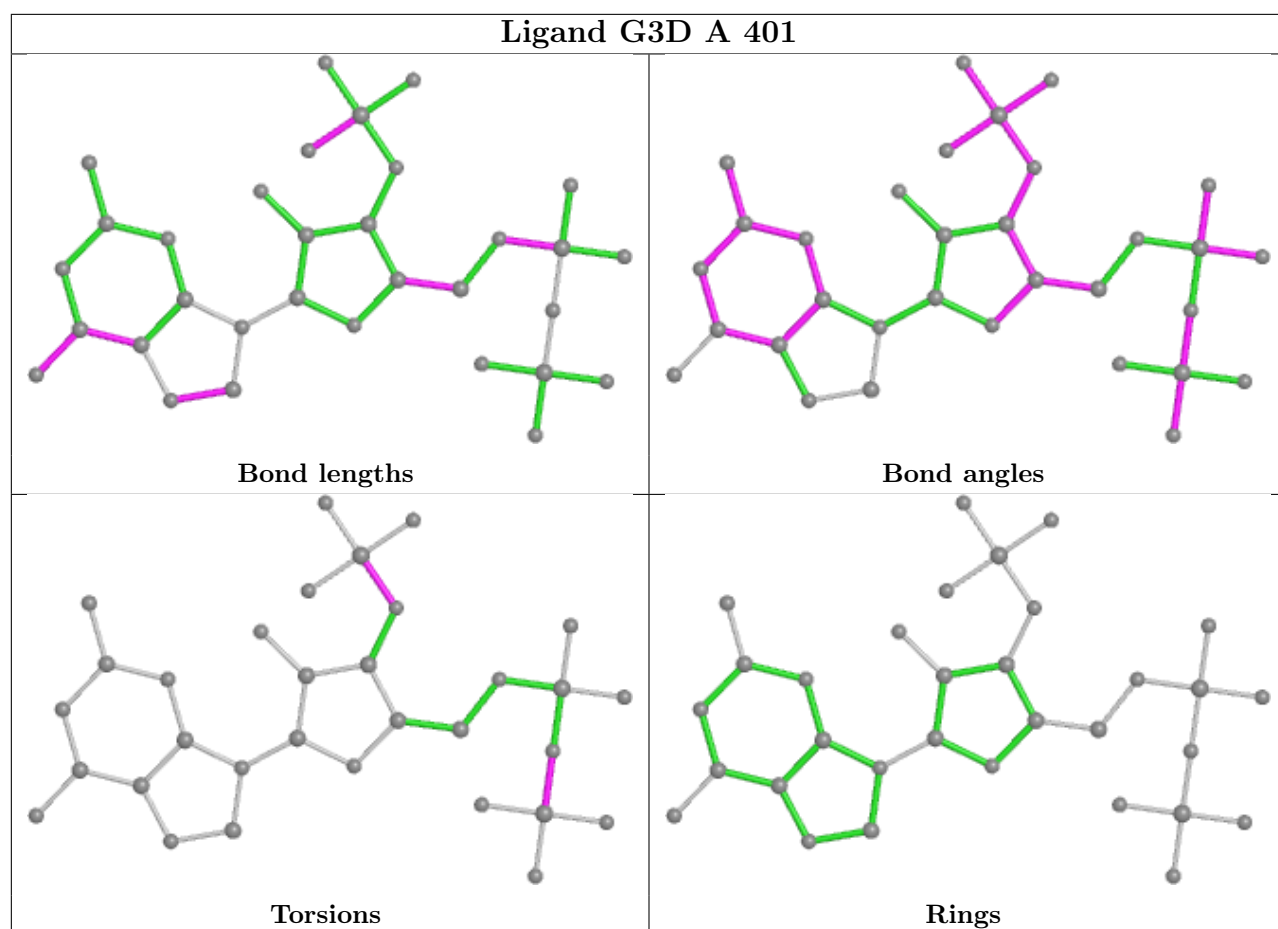| Mol	Chain	Res	Type	Atoms
4	A	401	G3D	PA-O3A-PB-O2B
4	B	501	G3D	PA-O3A-PB-O2B
4	B	501	G3D	C3'-O3'-P1-O6P
5	A	403	AFB	C12-C13-C14-C15
5	B	503	AFB	C12-C13-C14-C15

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 AFB B 503

Bond lengths

Bond angles

Torsions

Rings

Ligand AFB A 403

Bond lengths

Bond angles

Torsions

Rings

Ligand G3D B 501

Bond lengths

Bond angles

Torsions

Rings

Ligand G3D A 401

Bond lengths

Bond angles

Torsions

Rings
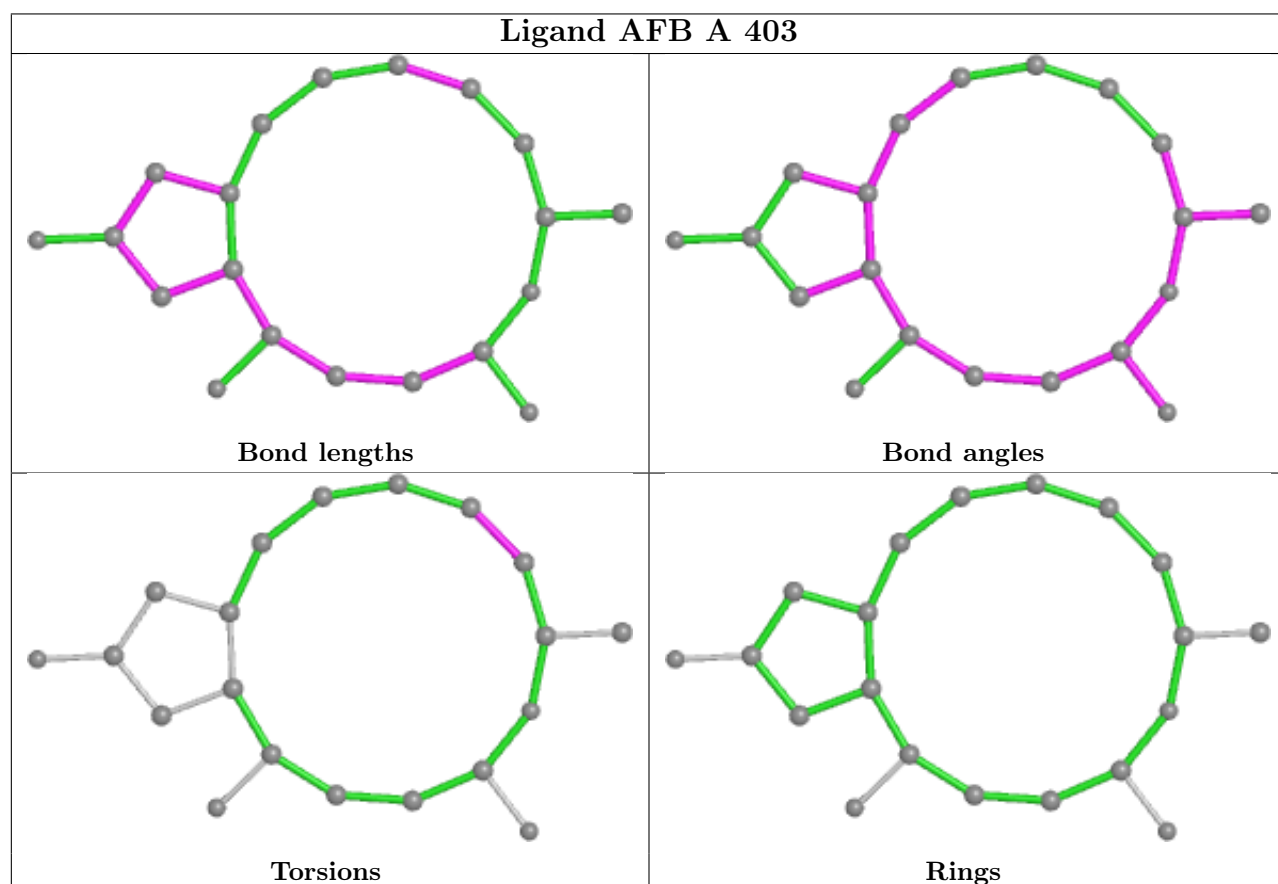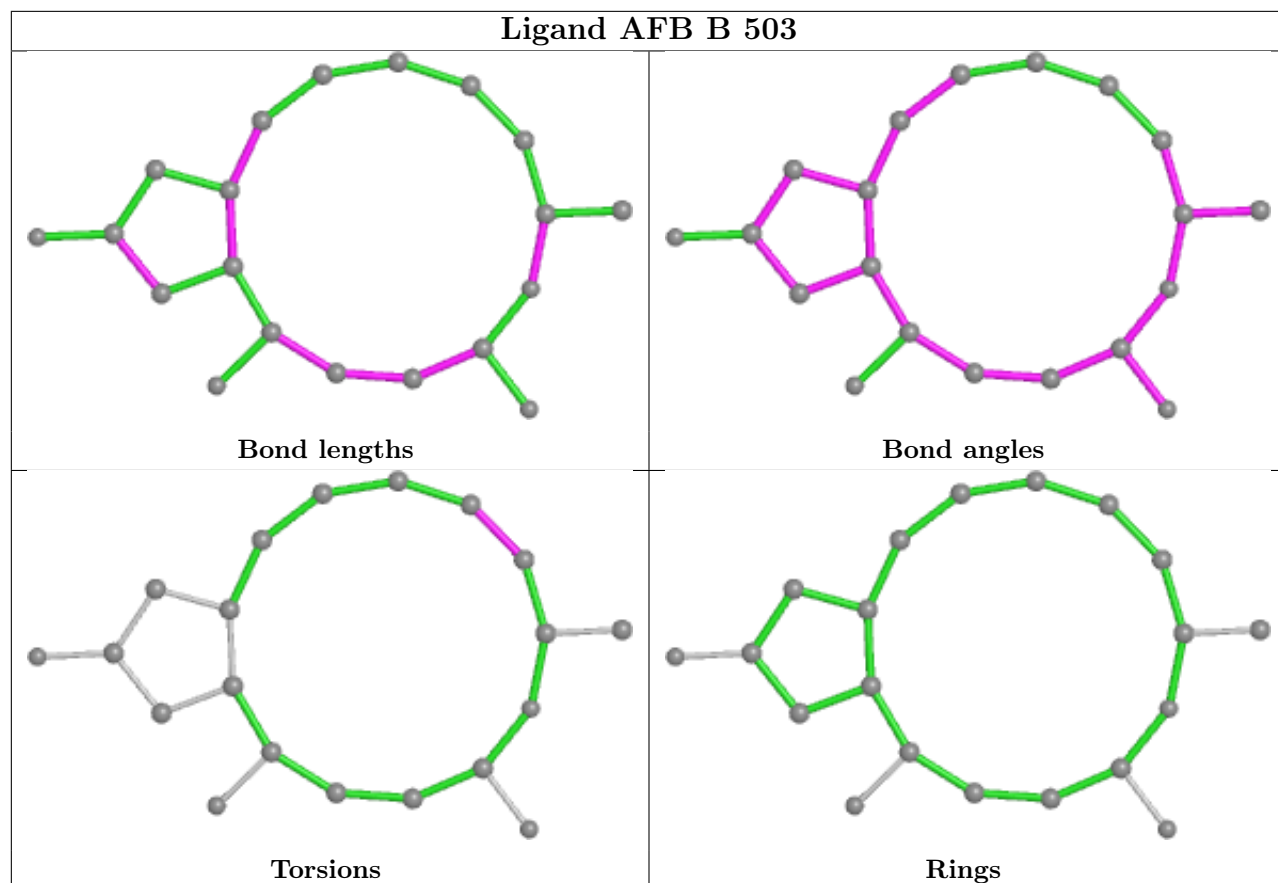
5.7 Other polymers ⓘ

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(Å^2)	Q<0.9
1	A	179/181 (98%)	0.74	28 (15%)	2	2	16, 24, 57, 74	0
1	B	179/181 (98%)	0.98	35 (19%)	1	1	17, 29, 61, 75	0
2	E	191/203 (94%)	0.53	19 (9%)	7	7	19, 29, 43, 61	0
2	F	194/203 (95%)	0.26	11 (5%)	23	23	15, 24, 45, 60	0
All	All	743/768 (96%)	0.62	93 (12%)	3	4	15, 27, 54, 75	0

The worst 5 of 93 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	13	PHE	11.9
1	B	40	GLY	11.5
1	B	13	PHE	10.9
1	B	2	GLY	9.5
1	A	2	GLY	8.9

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

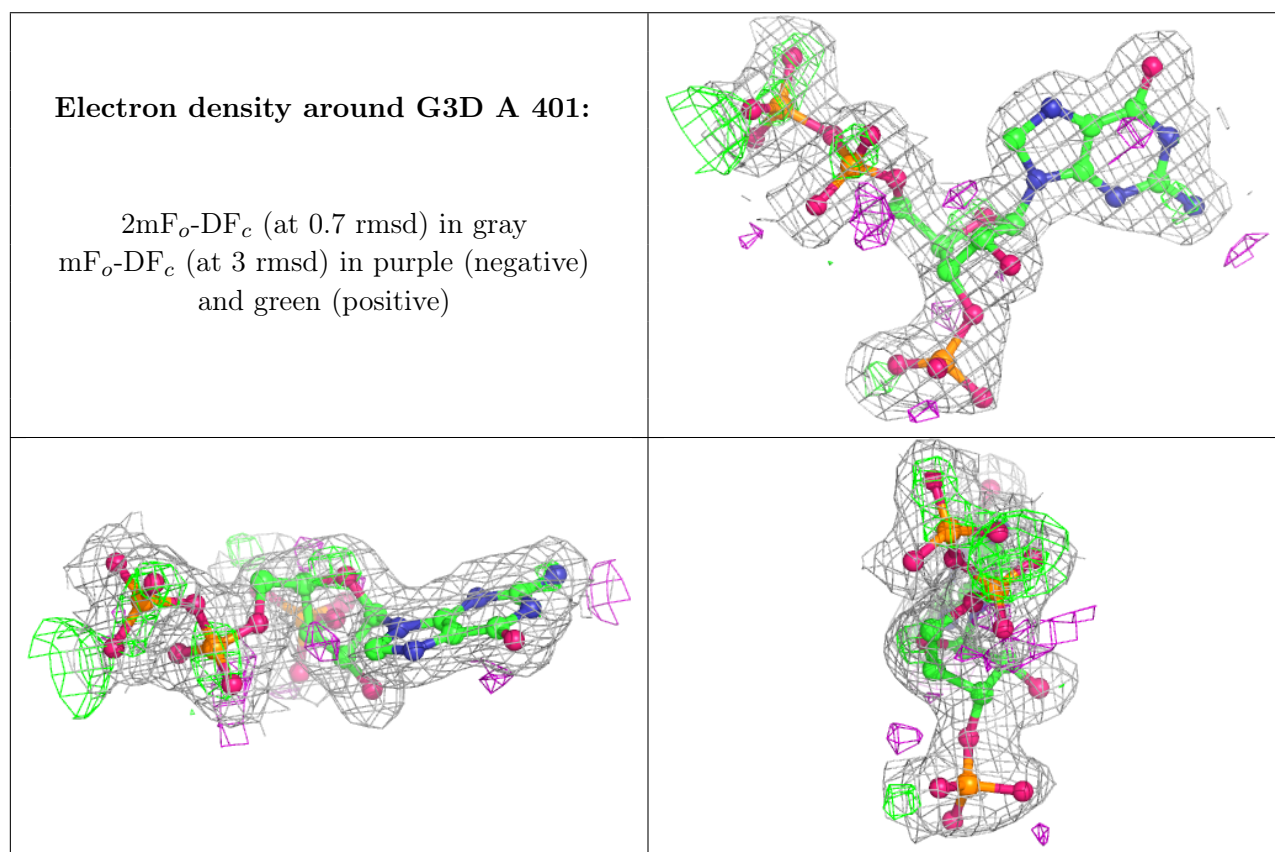There are no non-standard protein/DNA/RNA residues in this entry.

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.
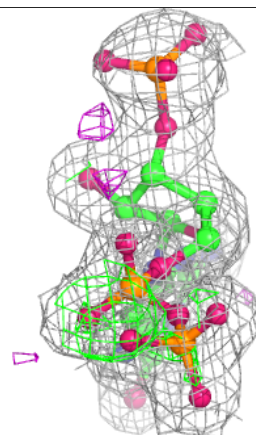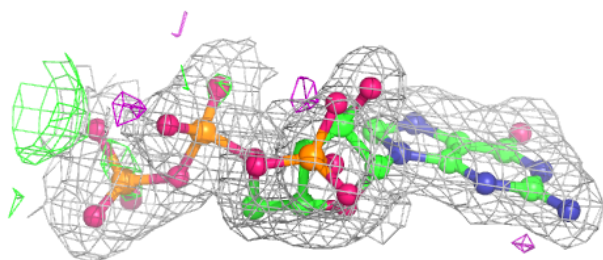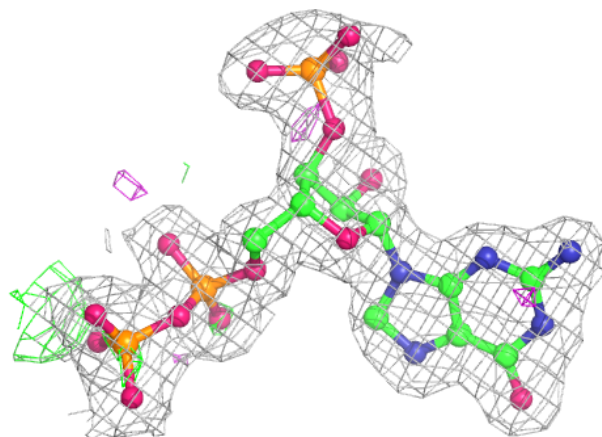
WORLDWIDE
wwPDB
PROTEIN DATA BANK

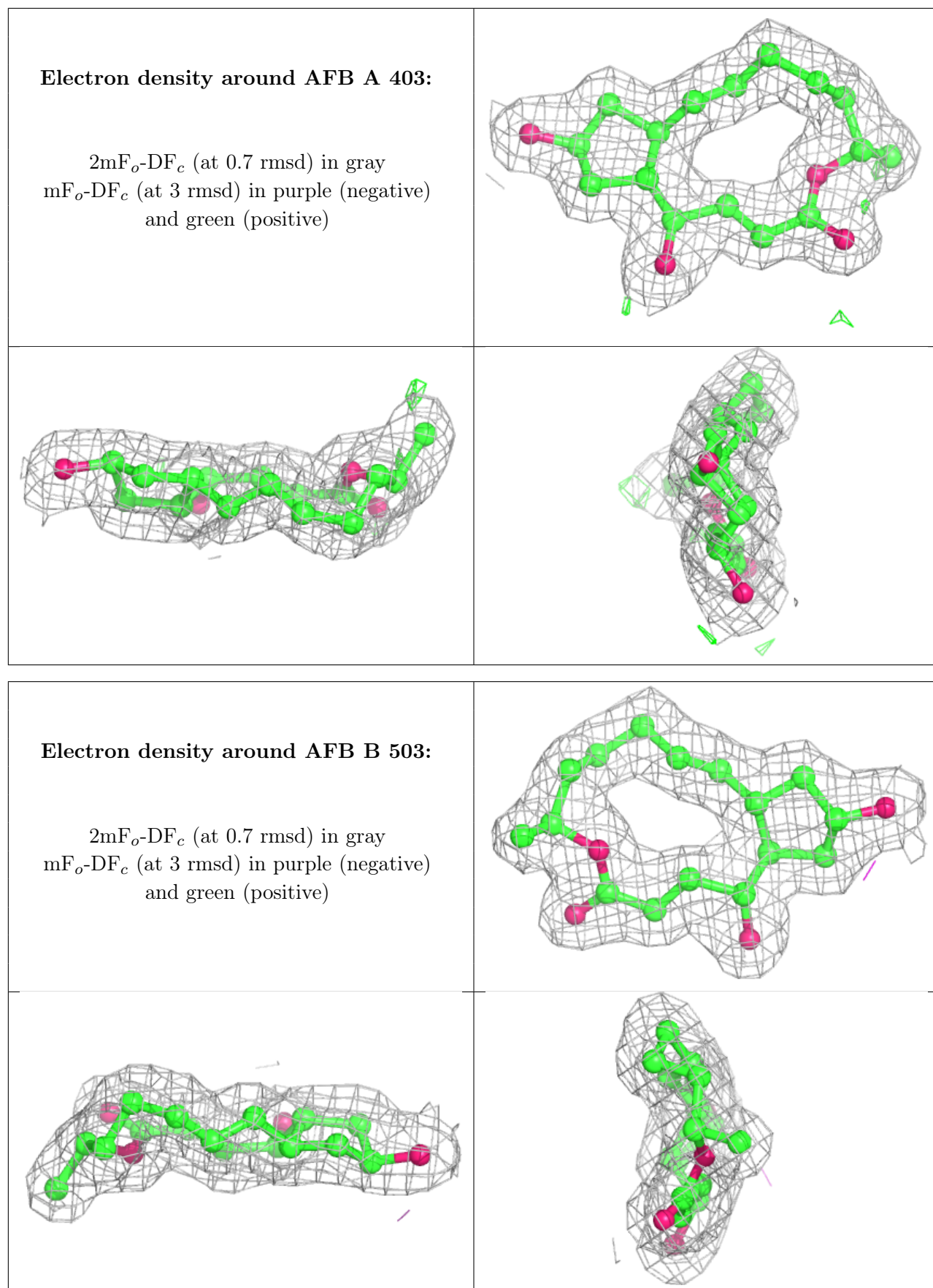| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	G3D	A	401	32/32	0.95	0.12	22,26,47,50	0
4	G3D	B	501	32/32	0.97	0.10	23,27,51,56	0
5	AFB	A	403	20/20	0.97	0.09	21,26,30,33	0
5	AFB	B	503	20/20	0.97	0.08	20,24,28,29	0
3	MG	A	402	1/1	0.99	0.32	8,8,8,8	0
3	MG	B	502	1/1	0.99	0.23	6,6,6,6	0
6	ZN	E	601	1/1	0.99	0.03	34,34,34,34	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 G3D A 401:

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

Electron density around G3D 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)

Electron density around AFB A 403:

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

Electron density around AFB B 503:

$2mF_o$-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.