



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:01 AM UTC

PDB ID : 5BTC / pdb_00005btc
Title : Crystal structure of a topoisomerase II complex
Authors : Blower, T.R.; Williamson, B.H.; Kerns, R.J.; Berger, J.M.
Deposited on : 2015-06-02
Resolution : 2.55 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

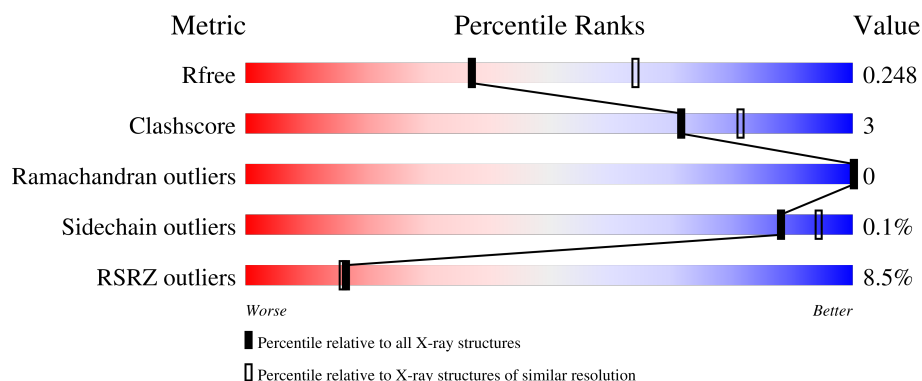
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	503	7% 91% 6%
1	C	503	6% 91% 6%
2	B	253	6% 92% 5%
2	D	253	8% 91% 6%
3	E	24	33% 71% 17% 12%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	H	24	
4	F	24	
4	G	24	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 25950 atoms, of which 12501 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 DNA gyrase subunit A.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	487	Total	C	H	N	O	P	S	0	0	0
			7671	2383	3840	701	733	1	13			
1	C	487	Total	C	H	N	O	P	S	0	0	0
			7671	2383	3840	701	733	1	13			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	90	SER	ALA	engineered mutation	UNP P9WG47
A	501	ILE	-	expression tag	UNP P9WG47
A	502	GLY	-	expression tag	UNP P9WG47
A	503	SER	-	expression tag	UNP P9WG47
A	504	GLY	-	expression tag	UNP P9WG47
C	90	SER	ALA	engineered mutation	UNP P9WG47
C	501	ILE	-	expression tag	UNP P9WG47
C	502	GLY	-	expression tag	UNP P9WG47
C	503	SER	-	expression tag	UNP P9WG47
C	504	GLY	-	expression tag	UNP P9WG47

- Molecule 2 is a protein called DNA gyrase subunit B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	245	Total	C	H	N	O	S	0	0	0
			3906	1217	1974	348	360	7			
2	D	247	Total	C	H	N	O	S	0	0	0
			3930	1224	1984	351	364	7			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	423	SER	-	expression tag	UNP P9WG45
B	424	ASN	-	expression tag	UNP P9WG45

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	425	ALA	-	expression tag	UNP P9WG45
D	423	SER	-	expression tag	UNP P9WG45
D	424	ASN	-	expression tag	UNP P9WG45
D	425	ALA	-	expression tag	UNP P9WG45

- Molecule 3 is a DNA chain called DNA substrate 24-mer GGTCATGAATGACTATGCAC GTAA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	21	Total	C	H	N	O	P	0	21	0
			621	196	211	74	120	20			
3	H	21	Total	C	H	N	O	P	0	21	0
			617	196	207	74	120	20			

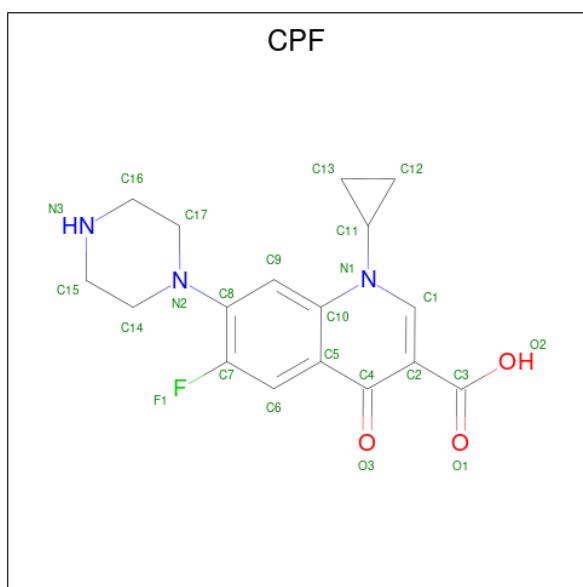
- Molecule 4 is a DNA chain called DNA substrate 24-mer TTACGTGCATAGTCATTCAT GACC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	21	Total	C	H	N	O	P	0	21	0
			618	196	208	74	120	20			
4	G	21	Total	C	H	N	O	P	0	21	0
			613	196	203	74	120	20			

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		

- Molecule 6 is 1-CYCLOPROPYL-6-FLUORO-4-OXO-7-PIPERAZIN-1-YL-1,4-DIHYDRO QUINOLINE-3-CARBOXYLIC ACID (CCD ID: CPF) (formula: C₁₇H₁₈FN₃O₃).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	G	1	Total	C	F	H	N	O	0	0
			41	17	1	17	3	3		
6	G	1	Total	C	F	H	N	O	0	0
			41	17	1	17	3	3		

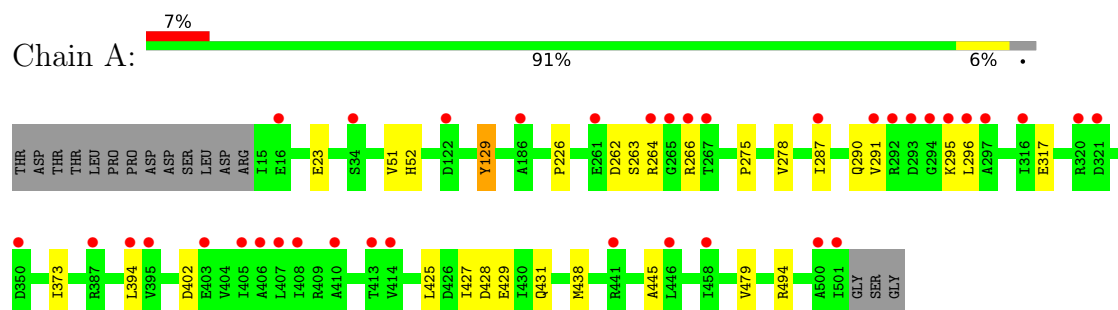
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	76	Total	O	0	0
			76	76		
7	B	31	Total	O	0	0
			31	31		
7	C	65	Total	O	0	0
			65	65		
7	D	26	Total	O	0	0
			26	26		
7	E	2	Total	O	0	0
			2	2		
7	F	8	Total	O	0	0
			8	8		
7	G	8	Total	O	0	0
			8	8		
7	H	1	Total	O	0	0
			1	1		

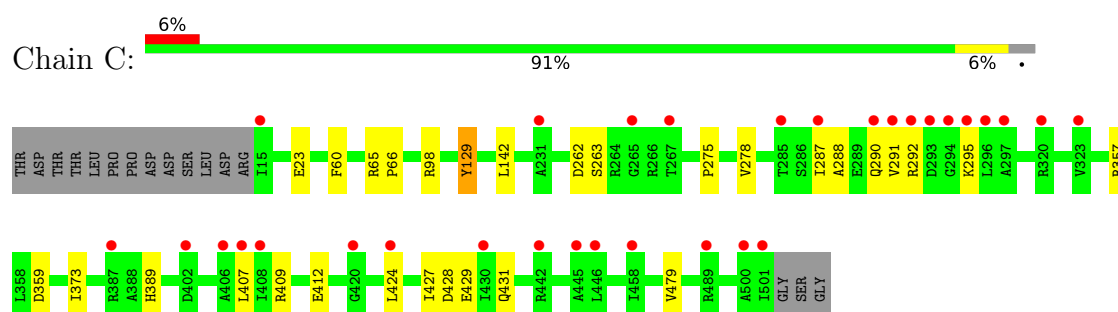
3 Residue-property plots [i](#)

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.

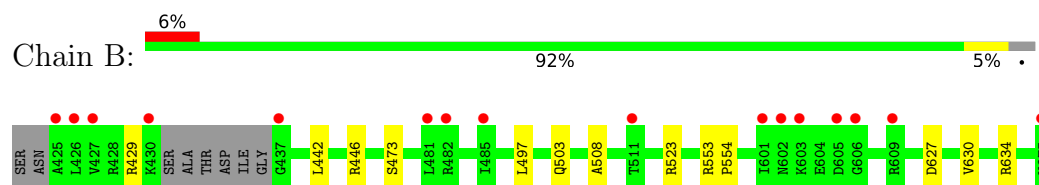
- Molecule 1: DNA gyrase subunit A



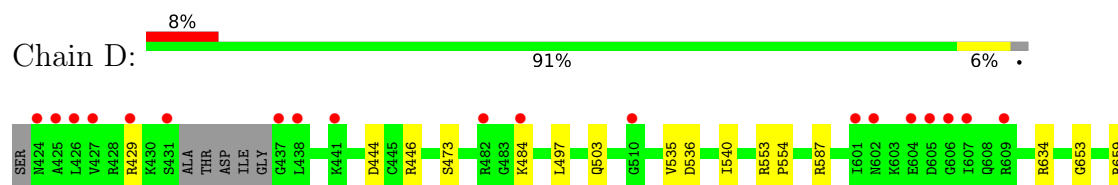
- Molecule 1: DNA gyrase subunit A



- Molecule 2: DNA gyrase subunit B

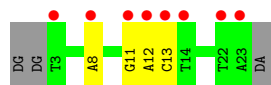


- Molecule 2: DNA gyrase subunit B





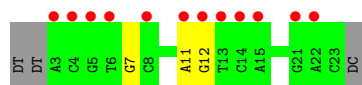
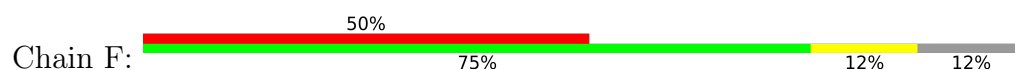
- Molecule 3: DNA substrate 24-mer GGTCATGAATGACTATGCACGTAA



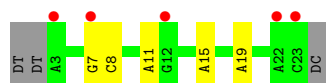
- Molecule 3: DNA substrate 24-mer GGTCATGAATGACTATGCACGTAA



- Molecule 4: DNA substrate 24-mer TTACGTGCATAGTCATTCATGACC



- Molecule 4: DNA substrate 24-mer TTACGTGCATAGTCATTCATGACC



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	108.34Å 82.98Å 129.70Å 90.00° 109.06° 90.00°	Depositor
Resolution (Å)	47.70 – 2.55 47.70 – 2.55	Depositor EDS
% Data completeness (in resolution range)	95.5 (47.70-2.55) 96.0 (47.70-2.55)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.54Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.224 , 0.250 0.230 , 0.248	Depositor DCC
R_{free} test set	3453 reflections (4.10%)	wwPDB-VP
Wilson B-factor (Å ²)	51.0	Xtriage
Anisotropy	0.459	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 60.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	25950	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.37% 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: MG, PTR, CPF

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	0.31	0/3872	0.65	0/5243
1	C	0.30	0/3872	0.64	0/5243
2	B	0.29	0/1960	0.60	0/2634
2	D	0.30	0/1974	0.60	0/2653
3	E	0.19	0/458	0.46	0/704
3	H	0.22	0/458	0.49	0/704
4	F	0.19	0/458	0.47	0/704
4	G	0.20	0/458	0.46	0/704
All	All	0.29	0/13510	0.61	0/18589

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 [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	3831	3840	3840	27	0
1	C	3831	3840	3840	22	0
2	B	1932	1974	1973	7	0
2	D	1946	1984	1984	10	0
3	E	410	211	211	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	410	207	207	5	0
4	F	410	208	208	4	0
4	G	410	203	203	5	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	G	48	34	32	2	0
7	A	76	0	0	0	0
7	B	31	0	0	0	0
7	C	65	0	0	0	0
7	D	26	0	0	1	0
7	E	2	0	0	0	0
7	F	8	0	0	0	0
7	G	8	0	0	0	0
7	H	1	0	0	0	0
All	All	13449	12501	12498	68	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 (68) 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:C:129:PTR:O3P	4:G:11[B]:DA:C5'	1.68	1.40
1:C:129:PTR:O3P	3:E:11[A]:DG:C5'	1.88	1.20
1:A:295:LYS:O	1:A:296:LEU:HD12	1.44	1.14
1:C:290:GLN:HG2	1:C:295:LYS:HD2	1.23	1.13
1:A:129:PTR:O1P	3:H:11[B]:DG:C5'	1.98	1.10
1:A:129:PTR:O1P	4:F:11[A]:DA:C5'	2.06	1.03
1:A:295:LYS:C	1:A:296:LEU:HD12	1.93	0.93
2:D:653:GLY:O	2:D:659:ARG:NH2	2.11	0.83
1:C:290:GLN:O	1:C:295:LYS:HB2	1.78	0.83
1:A:290:GLN:HB3	1:A:296:LEU:HD13	1.60	0.81
1:C:98:ARG:NH1	4:F:7[A]:DG:OP1	2.19	0.74
1:C:287:ILE:O	1:C:291:VAL:HG23	1.88	0.72
1:C:288:ALA:O	1:C:292:ARG:HG3	1.92	0.69
1:C:357:ARG:NH1	1:C:359:ASP:OD1	2.25	0.68
2:D:484:LYS:NZ	2:D:536:ASP:O	2.29	0.66
1:A:262:ASP:HB3	1:A:266:ARG:HB2	1.79	0.64
1:A:287:ILE:O	1:A:291:VAL:HG23	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:659:ARG:NH1	4:G:19[B]:DA:OP1	2.40	0.54
2:D:446:ARG:NH2	2:D:473:SER:OG	2.40	0.54
1:C:98:ARG:NH1	3:H:7[B]:DG:OP1	2.41	0.54
2:B:429:ARG:NH1	2:B:442:LEU:O	2.41	0.54
3:E:12[A]:DA:N6	4:F:12[A]:DG:O6	2.43	0.52
1:A:427:ILE:CG2	1:A:431:GLN:HB2	2.39	0.52
1:C:407:LEU:HD11	1:C:424:LEU:HD22	1.93	0.51
2:D:497:LEU:O	2:D:503:GLN:NE2	2.42	0.51
2:B:446:ARG:NH1	2:B:473:SER:OG	2.44	0.49
1:A:51:VAL:HG11	3:E:8[A]:DA:H5'	1.94	0.49
1:C:262:ASP:OD1	1:C:263:SER:N	2.40	0.49
2:D:587:ARG:NH2	7:D:804:HOH:O	2.45	0.49
1:A:52:HIS:NE2	4:G:8[B]:DC:OP1	2.43	0.49
1:C:428:ASP:OD1	1:C:429:GLU:N	2.44	0.48
1:A:262:ASP:CB	1:A:266:ARG:HB2	2.44	0.47
1:A:264:ARG:O	1:A:266:ARG:HG3	2.14	0.47
1:A:23:GLU:OE1	2:B:634:ARG:NH1	2.48	0.47
1:A:295:LYS:C	1:A:296:LEU:CD1	2.78	0.46
1:A:402:ASP:OD1	1:C:409:ARG:NH1	2.48	0.46
1:C:373:ILE:HD12	1:C:479:VAL:HG22	1.98	0.46
2:B:508:ALA:O	2:B:523:ARG:NE	2.44	0.45
4:G:7[B]:DG:N2	3:H:18[B]:DC:O2	2.42	0.45
1:C:389:HIS:O	1:C:431:GLN:NE2	2.43	0.44
1:A:291:VAL:HG22	1:A:296:LEU:HB2	1.99	0.44
1:A:275:PRO:HG2	1:A:278:VAL:HG21	1.99	0.44
1:C:65:ARG:HB3	1:C:66:PRO:HD2	1.99	0.44
1:A:266:ARG:HD3	1:A:317:GLU:OE2	2.18	0.44
1:C:23:GLU:OE1	2:D:634:ARG:NH1	2.51	0.44
2:B:627:ASP:HB3	2:B:630:VAL:HG22	2.00	0.43
1:C:290:GLN:HG2	1:C:295:LYS:CD	2.17	0.43
1:A:262:ASP:OD1	1:A:263:SER:N	2.48	0.42
1:C:60:PHE:HB2	1:C:142:LEU:HD13	2.01	0.42
3:E:13[A]:DC:N4	4:F:11[A]:DA:N6	2.68	0.42
1:A:373:ILE:HD12	1:A:479:VAL:HG22	2.01	0.42
6:G:102:CPF:H171	3:H:15[B]:DA:N3	2.35	0.42
1:A:290:GLN:HB3	1:A:296:LEU:CD1	2.41	0.42
2:D:553:ARG:N	2:D:554:PRO:CD	2.83	0.42
2:B:553:ARG:N	2:B:554:PRO:CD	2.83	0.41
1:C:275:PRO:HG2	1:C:278:VAL:HG21	2.02	0.41
1:A:428:ASP:OD1	1:A:429:GLU:N	2.43	0.41
2:D:429:ARG:HG2	2:D:444:ASP:HB2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:15[B]:DA:N3	6:G:101:CPF:H171	2.36	0.41
1:A:445:ALA:HB3	1:C:412:GLU:HA	2.03	0.41
2:B:497:LEU:O	2:B:503:GLN:NE2	2.53	0.41
1:A:394:LEU:HD22	1:A:438:MET:HE2	2.02	0.41
1:A:226:PRO:O	1:A:494:ARG:NH2	2.53	0.41
2:D:484:LYS:HZ2	2:D:540:ILE:HG13	1.85	0.41
1:A:425:LEU:HB2	1:A:427:ILE:HD11	2.04	0.40
3:H:11[B]:DG:H2"	3:H:12[B]:DA:C8	2.57	0.40
1:A:427:ILE:HG22	1:A:428:ASP:N	2.37	0.40
1:C:427:ILE:CG2	1:C:431:GLN:HB2	2.51	0.40

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	464/503 (92%)	443 (96%)	21 (4%)	0	100	100
1	C	484/503 (96%)	467 (96%)	17 (4%)	0	100	100
2	B	241/253 (95%)	233 (97%)	8 (3%)	0	100	100
2	D	243/253 (96%)	233 (96%)	10 (4%)	0	100	100
All	All	1432/1512 (95%)	1376 (96%)	56 (4%)	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	A	407/421 (97%)	407 (100%)	0	100	100
1	C	407/421 (97%)	407 (100%)	0	100	100
2	B	205/211 (97%)	205 (100%)	0	100	100
2	D	207/211 (98%)	206 (100%)	1 (0%)	81	88
All	All	1226/1264 (97%)	1225 (100%)	1 (0%)	88	94

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	535	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	161	GLN
1	A	207	ASN
1	A	277	GLN
1	A	344	ASN
1	A	449	GLN
1	C	207	ASN
1	C	277	GLN
1	C	290	GLN
1	C	449	GLN
1	C	490	HIS
2	D	514	HIS
2	D	525	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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
1	PTR	A	129	1	15,16,17	1.43	1 (6%)	17,22,24	1.05	1 (5%)
1	PTR	C	129	1	15,16,17	1.21	2 (13%)	17,22,24	0.79	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
1	PTR	A	129	1	-	2/10/11/13	0/1/1/1
1	PTR	C	129	1	-	2/10/11/13	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	129	PTR	OH-CZ	-2.79	1.34	1.40
1	C	129	PTR	OH-CZ	-2.46	1.35	1.40
1	C	129	PTR	O-C	2.12	1.28	1.20

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129	PTR	O3P-P-O2P	2.28	116.34	107.80

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	129	PTR	CA-CB-CG-CD1
1	C	129	PTR	CA-CB-CG-CD2
1	A	129	PTR	CA-CB-CG-CD2
1	A	129	PTR	CA-CB-CG-CD1

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	129	PTR	2	0
1	C	129	PTR	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 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
6	CPF	G	102	5	27,27,27	2.63	6 (22%)	40,40,40	2.21	9 (22%)
6	CPF	G	101	5	27,27,27	2.61	6 (22%)	40,40,40	2.19	9 (22%)

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
6	CPF	G	102	5	-	4/12/22/22	0/4/4/4
6	CPF	G	101	5	-	8/12/22/22	0/4/4/4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	101	CPF	C10-N1	9.22	1.51	1.40
6	G	102	CPF	C10-N1	9.14	1.51	1.40
6	G	102	CPF	C1-N1	6.50	1.45	1.34
6	G	101	CPF	C1-N1	6.42	1.45	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	102	CPF	C1-C2	3.72	1.48	1.38
6	G	101	CPF	C1-C2	3.63	1.47	1.38
6	G	101	CPF	C8-N2	2.51	1.46	1.41
6	G	102	CPF	C8-N2	2.48	1.46	1.41
6	G	102	CPF	C2-C3	2.31	1.52	1.48
6	G	102	CPF	C17-N2	-2.23	1.42	1.46
6	G	101	CPF	C2-C3	2.22	1.52	1.48
6	G	101	CPF	C17-N2	-2.16	1.43	1.46

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	102	CPF	C13-C11-N1	7.05	130.02	118.87
6	G	101	CPF	C13-C11-N1	6.91	129.80	118.87
6	G	102	CPF	C12-C11-N1	5.90	128.20	118.87
6	G	101	CPF	C12-C11-N1	5.80	128.05	118.87
6	G	101	CPF	F1-C7-C8	4.81	122.96	118.37
6	G	102	CPF	F1-C7-C8	4.53	122.69	118.37
6	G	101	CPF	C2-C1-N1	-3.77	119.91	124.42
6	G	101	CPF	C9-C8-N2	-3.75	117.12	122.59
6	G	102	CPF	C2-C1-N1	-3.75	119.93	124.42
6	G	102	CPF	C9-C8-N2	-3.74	117.15	122.59
6	G	102	CPF	C7-C8-N2	3.56	124.58	120.42
6	G	101	CPF	C7-C8-N2	3.53	124.55	120.42
6	G	101	CPF	C6-C7-C8	-3.43	120.32	123.35
6	G	102	CPF	C5-C4-C2	3.41	119.94	115.64
6	G	101	CPF	C5-C4-C2	3.39	119.92	115.64
6	G	102	CPF	C6-C7-C8	-3.35	120.39	123.35
6	G	102	CPF	O3-C4-C2	-2.10	119.70	123.07
6	G	101	CPF	O3-C4-C2	-2.06	119.77	123.07

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	G	101	CPF	C7-C8-N2-C17
6	G	102	CPF	C7-C8-N2-C17
6	G	101	CPF	C9-C8-N2-C14
6	G	102	CPF	C9-C8-N2-C14
6	G	101	CPF	C7-C8-N2-C14
6	G	102	CPF	C7-C8-N2-C14
6	G	101	CPF	C9-C8-N2-C17

Continued on next page...

Continued from previous page...

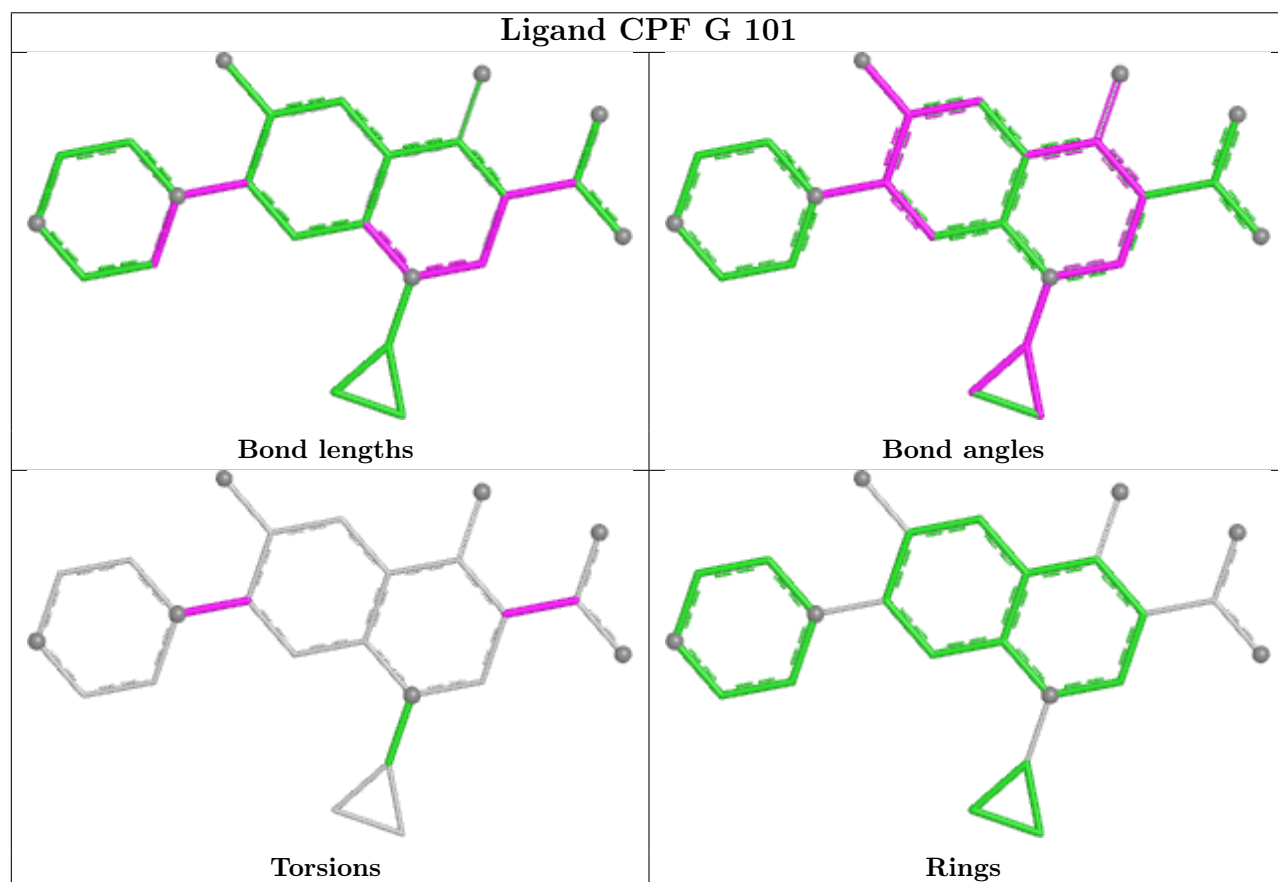
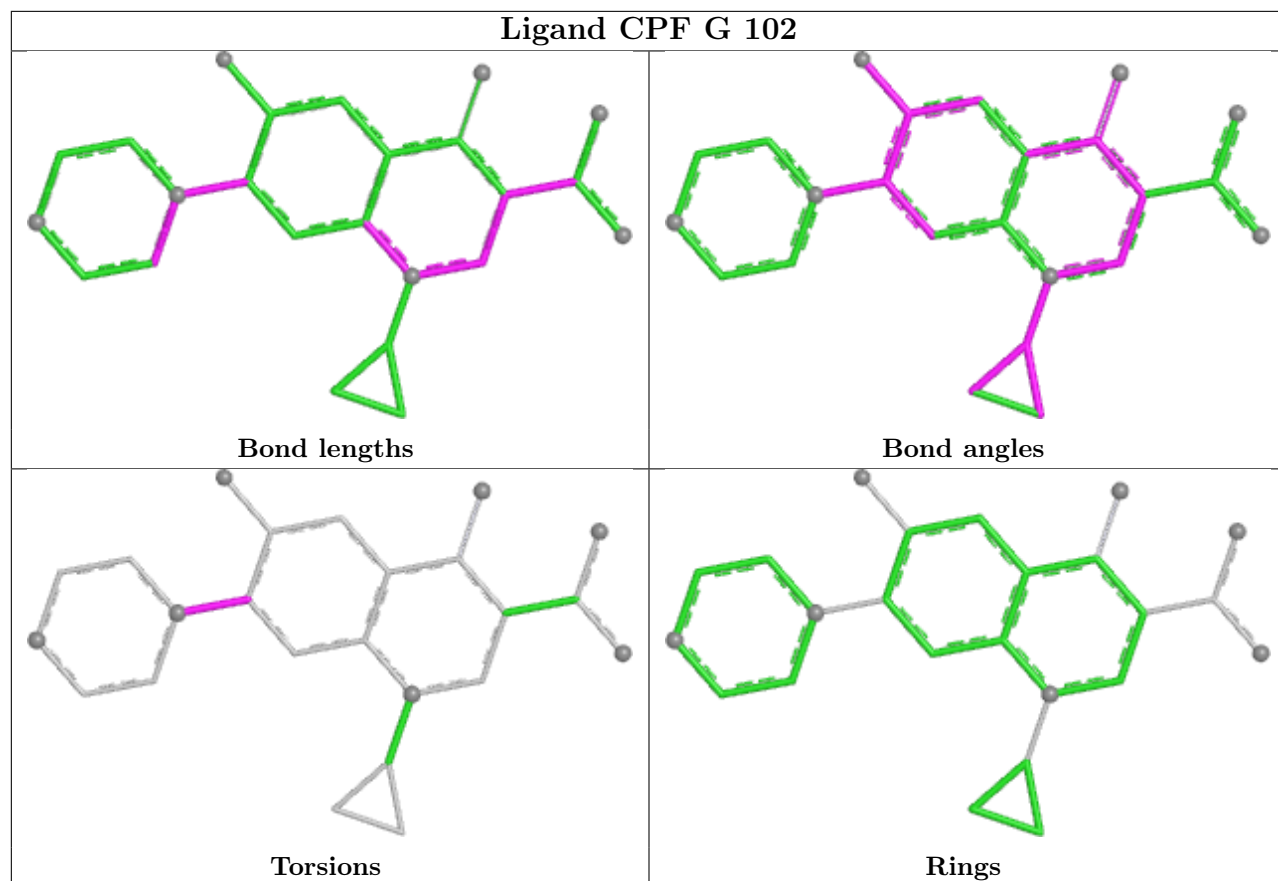
Mol	Chain	Res	Type	Atoms
6	G	102	CPF	C9-C8-N2-C17
6	G	101	CPF	C4-C2-C3-O2
6	G	101	CPF	C4-C2-C3-O1
6	G	101	CPF	C1-C2-C3-O2
6	G	101	CPF	C1-C2-C3-O1

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	102	CPF	1	0
6	G	101	CPF	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.



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	486/503 (96%)	0.52	37 (7%) 20 19	36, 65, 131, 194	0
1	C	486/503 (96%)	0.56	31 (6%) 25 24	37, 67, 133, 184	0
2	B	245/253 (96%)	0.68	16 (6%) 25 24	46, 75, 115, 159	0
2	D	247/253 (97%)	0.71	21 (8%) 16 16	48, 72, 121, 152	0
3	E	21/24 (87%)	2.32	8 (38%) 1 0	25, 49, 117, 162	21 (100%)
3	H	21/24 (87%)	0.71	1 (4%) 35 35	9, 28, 74, 116	21 (100%)
4	F	21/24 (87%)	2.36	12 (57%) 0 0	37, 53, 115, 138	21 (100%)
4	G	21/24 (87%)	1.30	5 (23%) 2 1	16, 29, 81, 105	21 (100%)
All	All	1548/1608 (96%)	0.65	131 (8%) 16 16	9, 69, 129, 194	84 (5%)

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	12[A]	DA	7.9
3	E	11[A]	DG	6.7
4	G	12[B]	DG	6.2
2	D	606	GLY	5.4
1	A	501	ILE	5.3
3	E	13[A]	DC	5.2
2	D	426	LEU	5.2
1	A	265	GLY	4.9
1	A	500	ALA	4.9
1	A	293	ASP	4.8
1	C	501	ILE	4.8
1	C	500	ALA	4.7
2	B	426	LEU	4.7
4	F	11[A]	DA	4.7
4	F	13[A]	DT	4.6
2	B	601	ILE	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	431	SER	4.5
2	D	484	LYS	4.3
4	F	12[A]	DG	4.3
4	G	23[B]	DC	4.2
1	C	424	LEU	4.1
4	G	7[B]	DG	4.1
3	E	14[A]	DT	4.1
3	E	22[A]	DT	3.7
2	B	437	GLY	3.6
2	D	601	ILE	3.5
2	D	605	ASP	3.5
1	C	407	LEU	3.5
3	H	3[B]	DT	3.4
4	F	15[A]	DA	3.3
1	A	414	VAL	3.3
2	B	427	VAL	3.3
1	A	407	LEU	3.3
2	B	430	LYS	3.3
2	B	605	ASP	3.2
2	D	607	ILE	3.2
3	E	8[A]	DA	3.2
1	C	296	LEU	3.1
1	A	297	ALA	3.1
2	D	437	GLY	3.1
4	F	6[A]	DT	3.1
1	A	408	ILE	3.1
1	C	293	ASP	3.0
4	F	21[A]	DG	3.0
1	A	122	ASP	3.0
4	F	5[A]	DG	3.0
2	B	425	ALA	3.0
1	A	394	LEU	2.9
4	F	22[A]	DA	2.9
1	A	296	LEU	2.9
1	A	405	ILE	2.9
2	D	675	VAL	2.9
1	A	410	ALA	2.8
2	B	675	VAL	2.8
1	C	285	THR	2.8
3	E	23[A]	DA	2.8
4	F	8[A]	DC	2.8
2	D	425	ALA	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	482	ARG	2.7
4	F	3[A]	DA	2.7
1	A	406	ALA	2.7
1	A	295	LYS	2.7
1	A	320	ARG	2.7
1	A	294	GLY	2.6
2	B	481	LEU	2.6
4	F	4[A]	DC	2.6
1	A	266	ARG	2.6
1	A	441	ARG	2.6
1	C	287	ILE	2.6
2	D	602	ASN	2.6
1	A	34	SER	2.6
1	C	442	ARG	2.5
1	C	320	ARG	2.5
2	D	429	ARG	2.5
1	C	265	GLY	2.5
1	A	458	ILE	2.5
1	A	186	ALA	2.5
1	A	413	THR	2.5
1	C	387	ARG	2.5
1	A	287	ILE	2.5
4	F	14[A]	DC	2.4
1	A	446	LEU	2.4
1	C	297	ALA	2.4
1	C	489	ARG	2.4
2	B	602	ASN	2.4
1	A	267	THR	2.4
1	C	267	THR	2.4
2	B	606	GLY	2.4
2	D	664	THR	2.4
1	C	290	GLN	2.4
4	G	22[B]	DA	2.4
2	D	424	ASN	2.4
1	C	291	VAL	2.3
1	C	323	VAL	2.3
1	C	420	GLY	2.3
1	C	295	LYS	2.3
2	D	609	ARG	2.3
1	C	458	ILE	2.3
1	A	291	VAL	2.3
1	C	292	ARG	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	403	GLU	2.2
1	C	231	ALA	2.2
2	B	511	THR	2.2
1	C	15	ILE	2.2
2	B	485	ILE	2.2
2	D	427	VAL	2.2
1	C	408	ILE	2.2
1	A	16	GLU	2.2
2	D	604	GLU	2.2
2	B	609	ARG	2.2
2	D	441	LYS	2.2
1	A	264	ARG	2.1
1	A	321	ASP	2.1
1	A	350	ASP	2.1
2	B	603	LYS	2.1
1	C	445	ALA	2.1
1	C	294	GLY	2.1
1	C	430	ILE	2.1
1	C	402	ASP	2.1
2	D	510	GLY	2.1
1	A	387	ARG	2.1
1	A	261	GLU	2.1
1	C	446	LEU	2.1
3	E	3[A]	DT	2.1
1	A	395	VAL	2.0
1	C	406	ALA	2.0
2	D	482	ARG	2.0
2	D	438	LEU	2.0
1	A	316	ILE	2.0
1	A	292	ARG	2.0
4	G	3[B]	DA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	PTR	A	129	16/17	0.91	0.13	46,53,109,115	0
1	PTR	C	129	16/17	0.91	0.12	50,61,103,104	0

6.3 Carbohydrates [i](#)

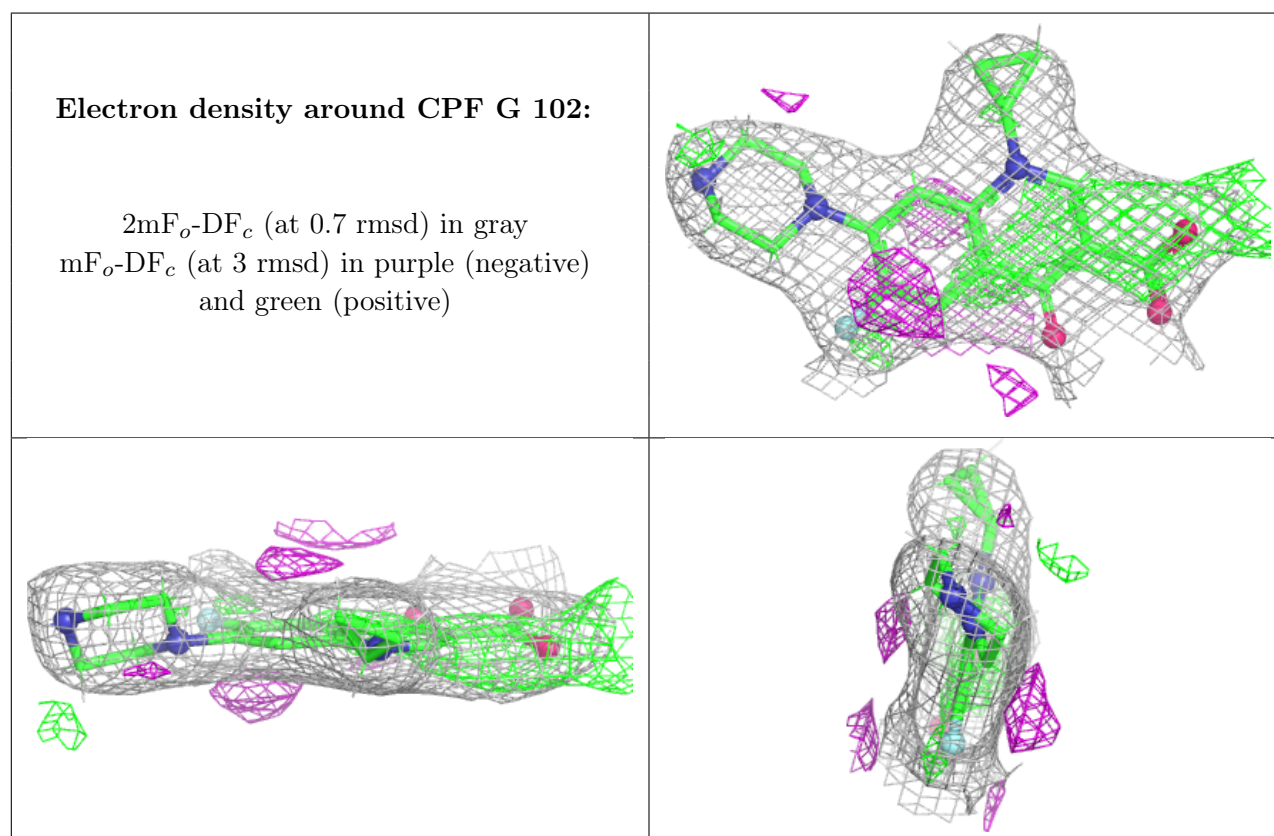
There are no oligosaccharides in this entry.

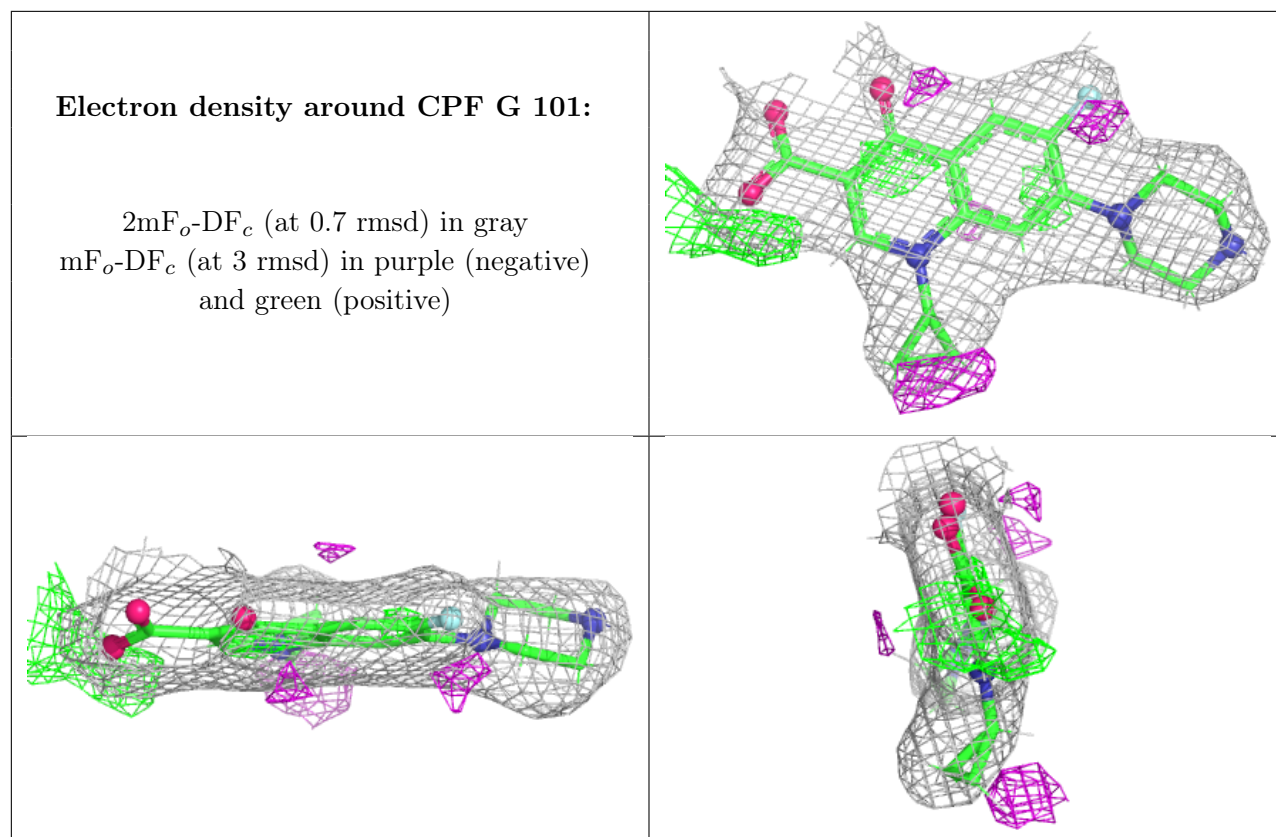
6.4 Ligands [i](#)

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
6	CPF	G	102	24/24	0.89	0.23	73,84,101,105	0
6	CPF	G	101	24/24	0.91	0.16	51,64,92,101	0
5	MG	D	701	1/1	0.95	0.07	47,47,47,47	0
5	MG	A	601	1/1	0.96	0.07	58,58,58,58	0
5	MG	B	701	1/1	0.97	0.04	39,39,39,39	0
5	MG	C	601	1/1	0.98	0.04	42,42,42,42	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.