W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 18, 2024 – 09:38 PM EDT

PDB ID	:	4KOE
Title	:	Quinolone(Trovafloxacin)-DNA cleavage complex of type IV topoisomerase from S. pneumoniae
Authors	:	Laponogov, I.; Pan, X.-S.; Veselkov, D.A.; Fisher, L.M.; Sanderson, M.R.
Deposited on	:	2013-05-11
Resolution	:	3.02 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
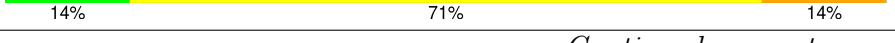*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.02 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.
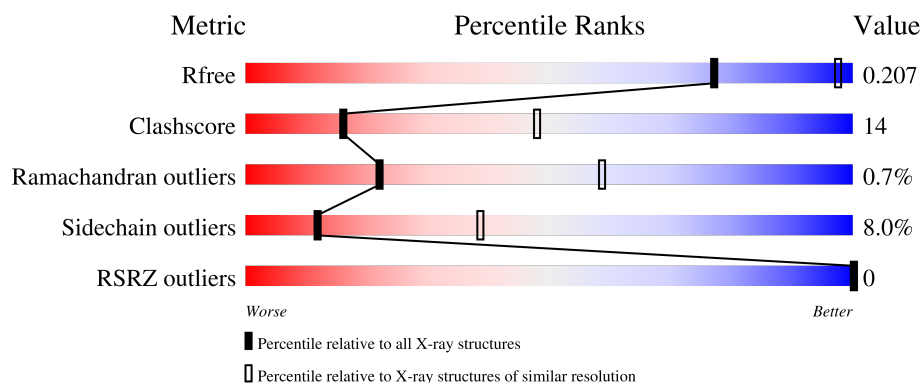
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2399 (3.04-3.00)
Clashscore	141614	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)
RSRZ outliers	127900	2287 (3.04-3.00)

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	496	74% 20% · ·
1	B	496	73% 21% · ·
2	C	268	62% 13% · 22%
2	D	268	57% 18% · 23%
3	E	7	14% 71% 14%

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Mol	Chain	Length	Quality of chain
4	F	11	27% 55% 18%
5	G	7	29% 71%
6	H	11	9% 82% 9%

2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 11133 atoms, of which 28 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 topoisomerase 4 subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	482	Total	C	N	O	S	0	0	0
			3737	2366	647	711	13			
1	B	482	Total	C	N	O	S	0	0	0
			3709	2354	637	705	13			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	257	THR	ILE	ENGINEERED MUTATION	UNP P72525
A	489	LEU	-	EXPRESSION TAG	UNP P72525
A	490	GLU	-	EXPRESSION TAG	UNP P72525
A	491	HIS	-	EXPRESSION TAG	UNP P72525
A	492	HIS	-	EXPRESSION TAG	UNP P72525
A	493	HIS	-	EXPRESSION TAG	UNP P72525
A	494	HIS	-	EXPRESSION TAG	UNP P72525
A	495	HIS	-	EXPRESSION TAG	UNP P72525
A	496	HIS	-	EXPRESSION TAG	UNP P72525
B	257	THR	ILE	ENGINEERED MUTATION	UNP P72525
B	489	LEU	-	EXPRESSION TAG	UNP P72525
B	490	GLU	-	EXPRESSION TAG	UNP P72525
B	491	HIS	-	EXPRESSION TAG	UNP P72525
B	492	HIS	-	EXPRESSION TAG	UNP P72525
B	493	HIS	-	EXPRESSION TAG	UNP P72525
B	494	HIS	-	EXPRESSION TAG	UNP P72525
B	495	HIS	-	EXPRESSION TAG	UNP P72525
B	496	HIS	-	EXPRESSION TAG	UNP P72525

- Molecule 2 is a protein called DNA topoisomerase 4 subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	208	Total	C	N	O	S	0	0	0
			1436	912	252	266	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	207	1427	906	249	266	6	0	0	0

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	380	MET	-	EXPRESSION TAG	UNP Q59961
C	381	GLY	-	EXPRESSION TAG	UNP Q59961
C	382	HIS	-	EXPRESSION TAG	UNP Q59961
C	383	HIS	-	EXPRESSION TAG	UNP Q59961
C	384	HIS	-	EXPRESSION TAG	UNP Q59961
C	385	HIS	-	EXPRESSION TAG	UNP Q59961
C	386	HIS	-	EXPRESSION TAG	UNP Q59961
C	387	HIS	-	EXPRESSION TAG	UNP Q59961
C	388	HIS	-	EXPRESSION TAG	UNP Q59961
C	389	HIS	-	EXPRESSION TAG	UNP Q59961
C	390	HIS	-	EXPRESSION TAG	UNP Q59961
C	391	HIS	-	EXPRESSION TAG	UNP Q59961
C	392	SER	-	EXPRESSION TAG	UNP Q59961
C	393	SER	-	EXPRESSION TAG	UNP Q59961
C	394	GLY	-	EXPRESSION TAG	UNP Q59961
C	395	HIS	-	EXPRESSION TAG	UNP Q59961
C	396	ILE	-	EXPRESSION TAG	UNP Q59961
C	397	ASP	-	EXPRESSION TAG	UNP Q59961
C	398	ASP	-	EXPRESSION TAG	UNP Q59961
C	399	ASP	-	EXPRESSION TAG	UNP Q59961
C	400	ASP	-	EXPRESSION TAG	UNP Q59961
C	401	LYS	-	EXPRESSION TAG	UNP Q59961
C	402	HIS	-	EXPRESSION TAG	UNP Q59961
C	403	MET	-	EXPRESSION TAG	UNP Q59961
C	460	ILE	VAL	ENGINEERED MUTATION	UNP Q59961
C	644	ALA	THR	ENGINEERED MUTATION	UNP Q59961
D	380	MET	-	EXPRESSION TAG	UNP Q59961
D	381	GLY	-	EXPRESSION TAG	UNP Q59961
D	382	HIS	-	EXPRESSION TAG	UNP Q59961
D	383	HIS	-	EXPRESSION TAG	UNP Q59961
D	384	HIS	-	EXPRESSION TAG	UNP Q59961
D	385	HIS	-	EXPRESSION TAG	UNP Q59961
D	386	HIS	-	EXPRESSION TAG	UNP Q59961
D	387	HIS	-	EXPRESSION TAG	UNP Q59961
D	388	HIS	-	EXPRESSION TAG	UNP Q59961
D	389	HIS	-	EXPRESSION TAG	UNP Q59961

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Chain	Residue	Modelled	Actual	Comment	Reference
D	390	HIS	-	EXPRESSION TAG	UNP Q59961
D	391	HIS	-	EXPRESSION TAG	UNP Q59961
D	392	SER	-	EXPRESSION TAG	UNP Q59961
D	393	SER	-	EXPRESSION TAG	UNP Q59961
D	394	GLY	-	EXPRESSION TAG	UNP Q59961
D	395	HIS	-	EXPRESSION TAG	UNP Q59961
D	396	ILE	-	EXPRESSION TAG	UNP Q59961
D	397	ASP	-	EXPRESSION TAG	UNP Q59961
D	398	ASP	-	EXPRESSION TAG	UNP Q59961
D	399	ASP	-	EXPRESSION TAG	UNP Q59961
D	400	ASP	-	EXPRESSION TAG	UNP Q59961
D	401	LYS	-	EXPRESSION TAG	UNP Q59961
D	402	HIS	-	EXPRESSION TAG	UNP Q59961
D	403	MET	-	EXPRESSION TAG	UNP Q59961
D	460	ILE	VAL	ENGINEERED MUTATION	UNP Q59961
D	644	ALA	THR	ENGINEERED MUTATION	UNP Q59961

- Molecule 3 is a DNA chain called E-site DNA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	E	7	140	69	27	38	6	0	0	0

- Molecule 4 is a DNA chain called E-site DNA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	F	11	225	108	39	67	11	0	0	0

- Molecule 5 is a DNA chain called E-site DNA3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
5	G	7	139	68	25	40	6	0	0	0

- Molecule 6 is a DNA chain called E-site DNA4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
6	H	11	226	107	43	65	11	0	0	0

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

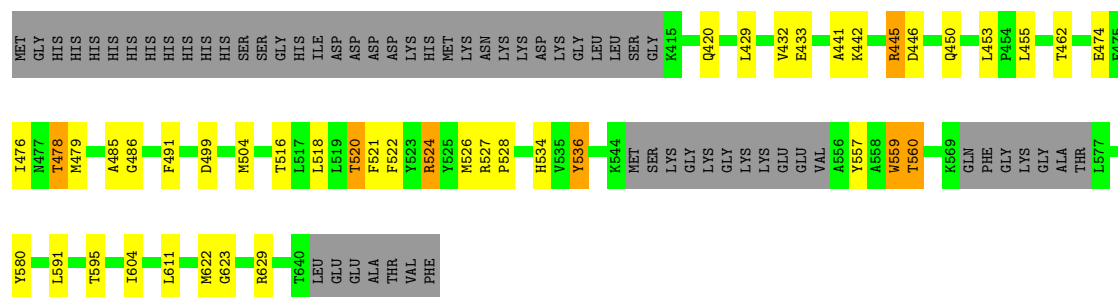| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total 2	Mg 2	0	0
7	B	2	Total 2	Mg 2	0	0
7	C	1	Total 1	Mg 1	0	0
7	D	1	Total 1	Mg 1	0	0

- Molecule 8 is Trovafloxacin (three-letter code: TR6) (formula: $C_{20}H_{15}F_3N_4O_3$).
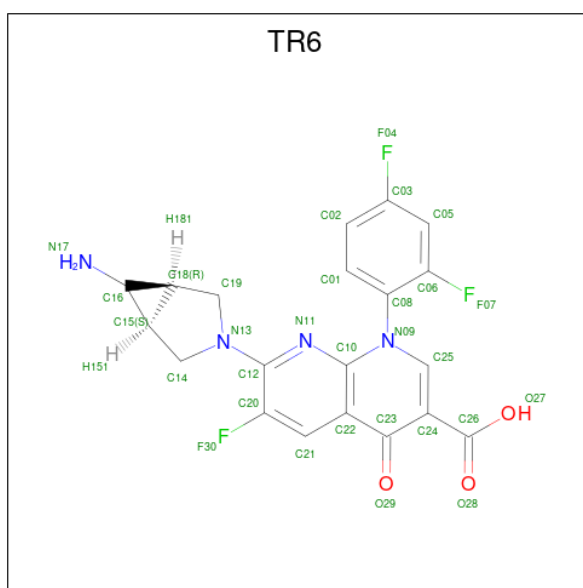
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	F	1	Total 44	C 20	F 3	H 14	N 4	O 3	0	0
8	H	1	Total 44	C 20	F 3	H 14	N 4	O 3	0	0

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: DNA topoisomerase 4 subunit A

Chain A:

- Molecule 1: DNA topoisomerase 4 subunit A

Chain B:

- Molecule 2: DNA topoisomerase 4 subunit B

Chain C:

• **Molecule 2: DNA topoisomerase 4 subunit B**

Chain D:

• **Molecule 3: E-site DNA1**

Chain E:

• **Molecule 4: E-site DNA2**

Chain F:

• **Molecule 5: E-site DNA3**

Chain G:
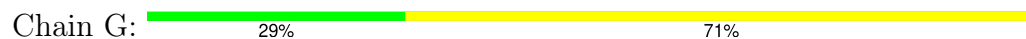
• **Molecule 6: E-site DNA4**

Chain H:
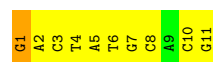
4   Data and refinement statistics   ⓘ

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	158.04Å 158.04Å 210.42Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	62.42 – 3.02 62.42 – 3.02	Depositor EDS
% Data completeness (in resolution range)	99.9 (62.42-3.02) 100.0 (62.42-3.02)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	8.72 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.175 , 0.210 0.172 , 0.207	Depositor DCC
R_{free} test set	3025 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	69.4	Xtriage
Anisotropy	0.591	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 48.0	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11133	wwPDB-VP
Average B, all atoms (Å^2)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.16% 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: TR6, MG

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	0.43	0/3798	0.59	0/5144
1	B	0.44	0/3770	0.61	0/5112
2	C	0.34	0/1462	0.53	0/1999
2	D	0.32	0/1453	0.51	0/1986
3	E	0.69	0/157	1.47	3/241 (1.2%)
4	F	0.79	0/251	1.64	11/385 (2.9%)
5	G	0.81	0/155	1.51	2/238 (0.8%)
6	H	0.78	0/253	1.50	5/388 (1.3%)
All	All	0.44	0/11299	0.71	21/15493 (0.1%)

There are no bond length outliers.

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	6	DT	O4'-C4'-C3'	-7.66	101.40	106.00
6	H	2	DA	O4'-C1'-N9	-6.70	103.31	108.00
4	F	1	DA	C1'-O4'-C4'	-6.46	103.64	110.10
6	H	1	DG	O4'-C1'-C2'	-6.38	100.79	105.90
3	E	15	DT	N3-C4-O4	6.23	123.64	119.90

There are no chirality outliers.

There are no planarity outliers.

5.2   Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3737	0	3650	104	0
1	B	3709	0	3617	96	0
2	C	1436	0	1222	40	0
2	D	1427	0	1208	41	0
3	E	140	0	78	7	0
4	F	225	0	126	15	0
5	G	139	0	78	6	0
6	H	226	0	124	21	0
7	A	2	0	0	0	0
7	B	2	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	F	30	14	14	1	0
8	H	30	14	14	1	0
All	All	11105	28	10131	305	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 14.

The worst 5 of 305 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:293:ARG:HH11	1:A:293:ARG:HB3	1.06	1.18
1:A:28:ARG:HG3	1:A:28:ARG:HH11	0.96	1.08
1:B:70:MET:HE1	1:B:78:ASP:HB3	1.32	1.08
1:A:60:ARG:HH11	1:A:60:ARG:HB2	1.16	1.08
1:A:146:ASP:HB3	1:A:148:THR:HG22	1.35	1.08

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	480/496 (97%)	457 (95%)	20 (4%)	3 (1%)	25	62
1	B	480/496 (97%)	449 (94%)	26 (5%)	5 (1%)	15	50
2	C	202/268 (75%)	195 (96%)	6 (3%)	1 (0%)	29	66
2	D	201/268 (75%)	184 (92%)	17 (8%)	0	100	100
All	All	1363/1528 (89%)	1285 (94%)	69 (5%)	9 (1%)	22	59

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	157	ALA
1	B	168	THR
1	A	168	THR
2	C	560	THR
1	A	329	MET

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	379/431 (88%)	349 (92%)	30 (8%)	12	39
1	B	375/431 (87%)	346 (92%)	29 (8%)	13	41
2	C	108/224 (48%)	97 (90%)	11 (10%)	7	27
2	D	107/224 (48%)	99 (92%)	8 (8%)	13	42
All	All	969/1310 (74%)	891 (92%)	78 (8%)	12	39

5 of 78 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	456	GLU
2	D	445	ARG
2	C	420	GLN
2	C	524	ARG
2	D	559	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 8 ligands modelled in this entry, 6 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	$\#|Z| > 2$
8	TR6	H	101	7	33,34,34	2.01	8 (24%)	47,53,53	2.10	13 (27%)
8	TR6	F	101	7	33,34,34	1.99	8 (24%)	47,53,53	2.22	16 (34%)

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
8	TR6	H	101	7	-	2/12/29/29	0/5/5/5
8	TR6	F	101	7	-	5/12/29/29	0/5/5/5

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	101	TR6	C10-N09	-6.53	1.34	1.39
8	F	101	TR6	C10-N09	-5.70	1.35	1.39
8	F	101	TR6	C12-C20	-4.15	1.37	1.42
8	H	101	TR6	C22-C23	-4.05	1.40	1.48
8	H	101	TR6	C12-C20	-3.98	1.37	1.42

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	F	101	TR6	C14-N13-C12	-7.05	103.09	123.60
8	H	101	TR6	C14-N13-C12	-6.03	106.06	123.60
8	H	101	TR6	C19-N13-C12	5.50	139.59	123.60
8	F	101	TR6	C19-N13-C12	4.98	138.09	123.60
8	F	101	TR6	C22-C10-N11	-4.13	120.22	124.06

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	F	101	TR6	C06-C08-N09-C10
8	F	101	TR6	C01-C08-N09-C10
8	H	101	TR6	C01-C08-N09-C10
8	F	101	TR6	C01-C08-N09-C25
8	F	101	TR6	N11-C12-N13-C19

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	H	101	TR6	1	0
8	F	101	TR6	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 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 TR6 H 101

Bond lengths

Bond angles

Torsions

Rings

Ligand TR6 F 101

Bond lengths

Bond angles

Torsions

Rings
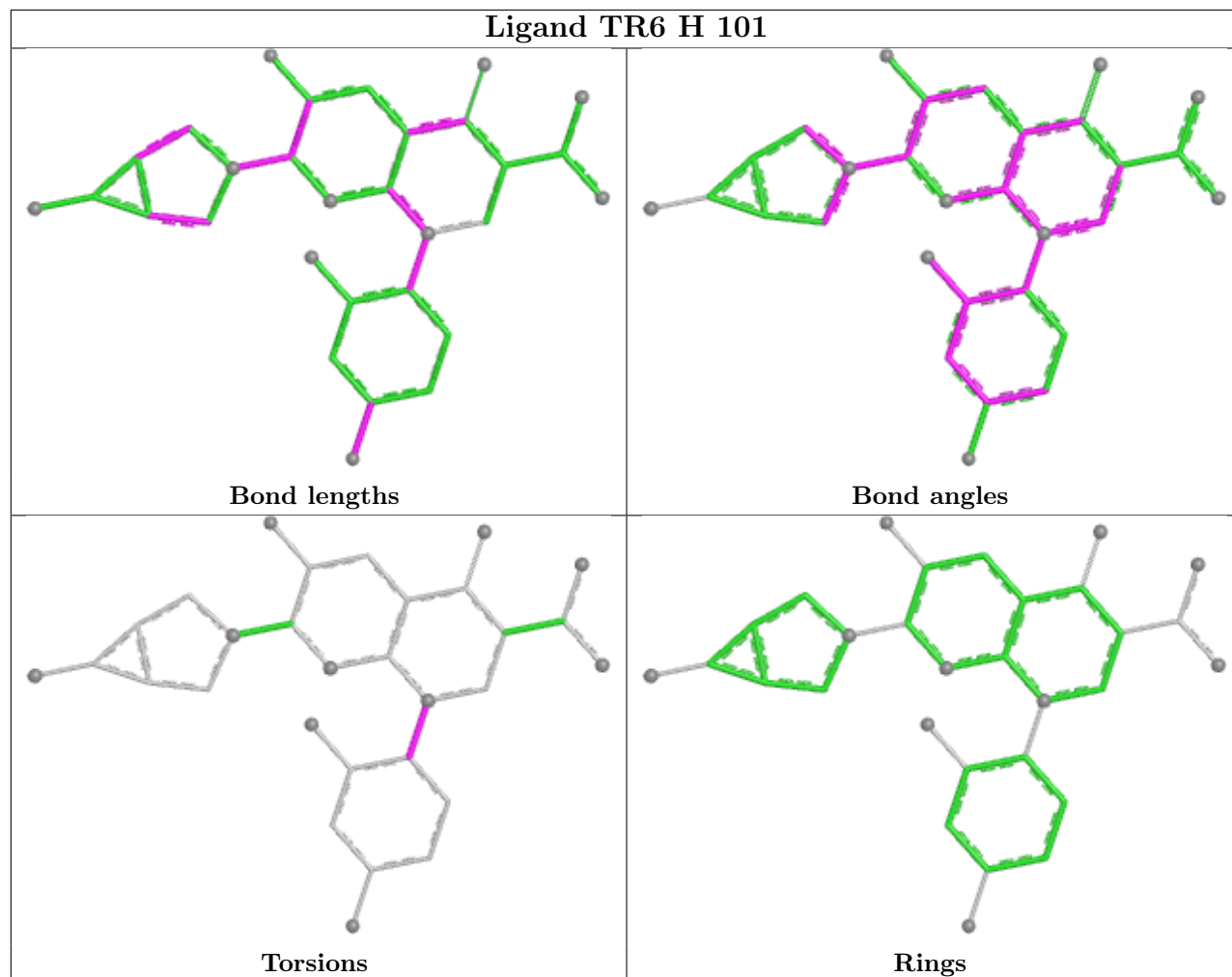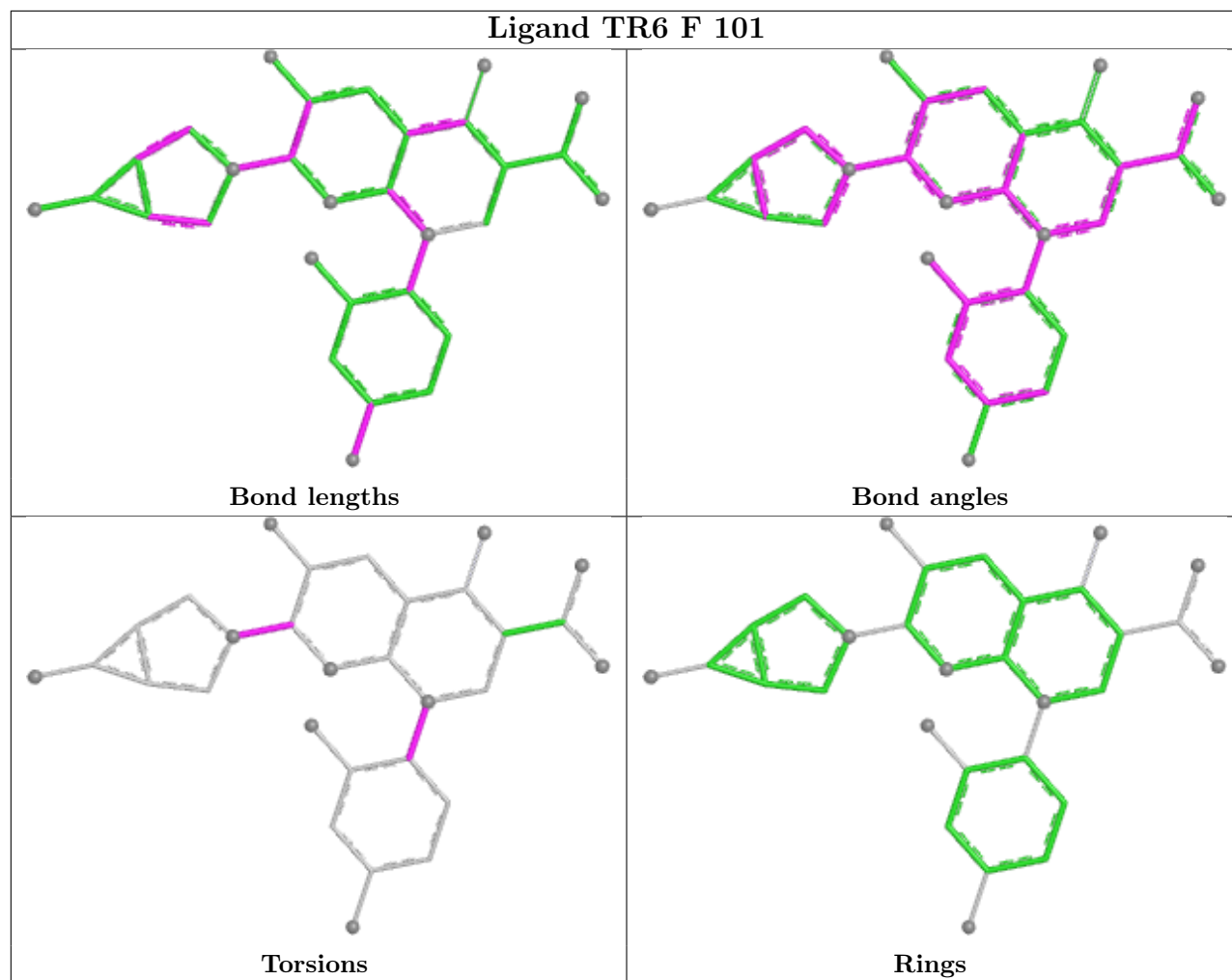
5.7 Other polymers ⓘ

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	482/496 (97%)	-0.62	0	100	100	42, 63, 104, 136	0
1	B	482/496 (97%)	-0.62	0	100	100	43, 60, 91, 127	0
2	C	208/268 (77%)	-0.56	0	100	100	68, 98, 145, 187	0
2	D	207/268 (77%)	-0.54	0	100	100	69, 104, 142, 164	0
3	E	7/7 (100%)	-0.29	0	100	100	62, 67, 103, 137	0
4	F	11/11 (100%)	-0.35	0	100	100	68, 89, 127, 132	0
5	G	7/7 (100%)	-0.26	0	100	100	59, 65, 100, 127	0
6	H	11/11 (100%)	-0.40	0	100	100	70, 80, 125, 125	0
All	All	1415/1564 (90%)	-0.59	0	100	100	42, 69, 127, 187	0

There are no RSRZ outliers to report.

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($\mathring{A}^2$)	Q<0.9
7	MG	B	501	1/1	0.74	0.12	90,90,90,90	0
7	MG	D	701	1/1	0.85	0.41	58,58,58,58	0
7	MG	A	501	1/1	0.89	0.07	81,81,81,81	0
7	MG	A	502	1/1	0.89	0.43	74,74,74,74	0
7	MG	C	701	1/1	0.90	0.49	59,59,59,59	0
7	MG	B	502	1/1	0.95	0.55	73,73,73,73	0
8	TR6	F	101	30/30	0.95	0.23	66,83,105,120	0
8	TR6	H	101	30/30	0.95	0.22	61,77,92,110	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.
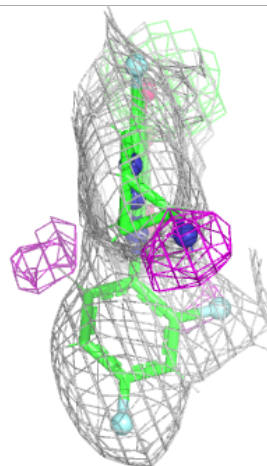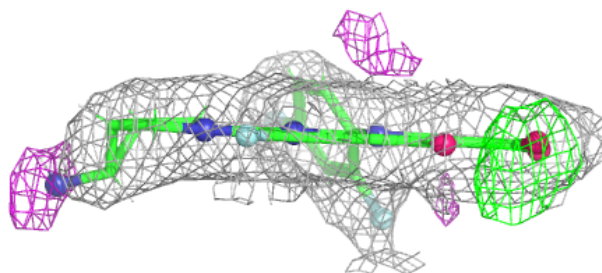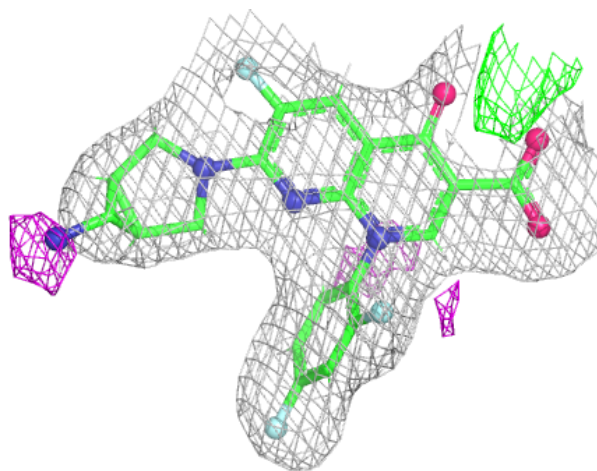
Electron density around TR6 F 101:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
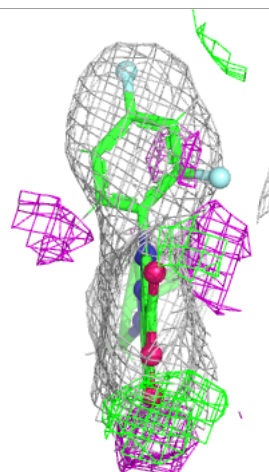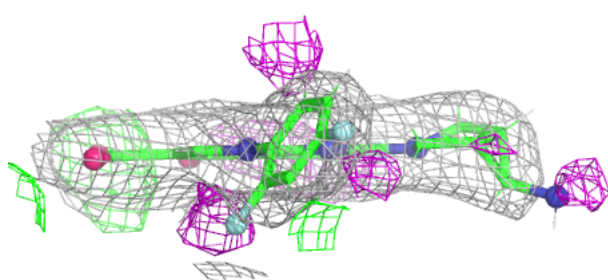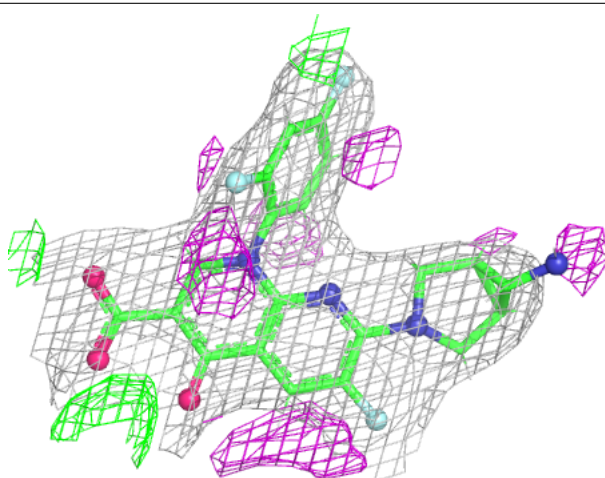
Electron density around TR6 H 101:

$2mF_o$-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 (i)

There are no such residues in this entry.