



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 22, 2017 – 08:04 PM EDT

PDB ID : 4Z2E
Title : Quinolone(Trovafloxacin)-DNA cleavage complex of gyrase from *S. pneumoniae*
Authors : Laponogov, I.; Veselkov, D.A.; Pan, X.-S.; Selvarajah, J.; Crevel, I.M.-T.; Fisher, L.M.; Sanderson, M.R.
Deposited on : unknown
Resolution : 3.46 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029824
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20029824

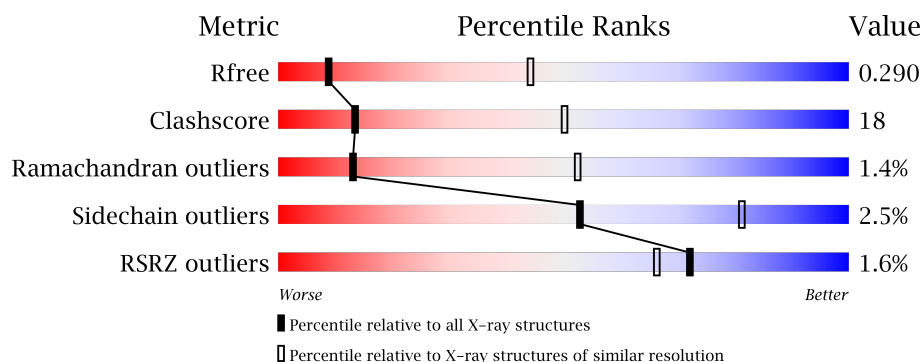
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.46 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.




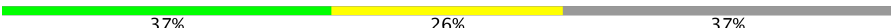

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1135 (3.56-3.36)
Clashscore	112137	1040 (3.52-3.40)
Ramachandran outliers	110173	1009 (3.52-3.40)
Sidechain outliers	110143	1010 (3.52-3.40)
RSRZ outliers	101464	1017 (3.54-3.38)

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. 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	499	
1	B	499	
2	C	269	
2	D	269	
3	E	15	

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Mol	Chain	Length	Quality of chain
3	G	15	 20% 27% 53%
4	F	19	 37% 26% 37%
4	H	19	 21% 37% 42%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 9755 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 gyrase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	485	Total	C	N	O	S	0	0	0
			3340	2082	617	625	16			
1	B	472	Total	C	N	O	S	0	0	0
			3129	1966	564	587	12			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	494	HIS	-	expression tag	UNP Q9R867
A	495	HIS	-	expression tag	UNP Q9R867
A	496	HIS	-	expression tag	UNP Q9R867
A	497	HIS	-	expression tag	UNP Q9R867
A	498	HIS	-	expression tag	UNP Q9R867
A	499	HIS	-	expression tag	UNP Q9R867
B	494	HIS	-	expression tag	UNP Q9R867
B	495	HIS	-	expression tag	UNP Q9R867
B	496	HIS	-	expression tag	UNP Q9R867
B	497	HIS	-	expression tag	UNP Q9R867
B	498	HIS	-	expression tag	UNP Q9R867
B	499	HIS	-	expression tag	UNP Q9R867

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	197	Total	C	N	O	S	0	0	0
			1224	765	223	230	6			
2	D	191	Total	C	N	O	S	0	0	0
			1205	758	218	223	6			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	380	MET	-	initiating methionine	UNP Q59957
C	381	GLY	-	expression tag	UNP Q59957
C	382	HIS	-	expression tag	UNP Q59957
C	383	HIS	-	expression tag	UNP Q59957
C	384	HIS	-	expression tag	UNP Q59957
C	385	HIS	-	expression tag	UNP Q59957
C	386	HIS	-	expression tag	UNP Q59957
C	387	HIS	-	expression tag	UNP Q59957
C	388	HIS	-	expression tag	UNP Q59957
C	389	HIS	-	expression tag	UNP Q59957
C	390	HIS	-	expression tag	UNP Q59957
C	391	HIS	-	expression tag	UNP Q59957
C	392	SER	-	expression tag	UNP Q59957
C	393	SER	-	expression tag	UNP Q59957
C	394	GLY	-	expression tag	UNP Q59957
C	395	HIS	-	expression tag	UNP Q59957
C	396	ILE	-	expression tag	UNP Q59957
C	397	ASP	-	expression tag	UNP Q59957
C	398	ASP	-	expression tag	UNP Q59957
C	399	ASP	-	expression tag	UNP Q59957
C	400	ASP	-	expression tag	UNP Q59957
C	401	LYS	-	expression tag	UNP Q59957
C	402	HIS	-	expression tag	UNP Q59957
C	403	MET	-	expression tag	UNP Q59957
D	380	MET	-	initiating methionine	UNP Q59957
D	381	GLY	-	expression tag	UNP Q59957
D	382	HIS	-	expression tag	UNP Q59957
D	383	HIS	-	expression tag	UNP Q59957
D	384	HIS	-	expression tag	UNP Q59957
D	385	HIS	-	expression tag	UNP Q59957
D	386	HIS	-	expression tag	UNP Q59957
D	387	HIS	-	expression tag	UNP Q59957
D	388	HIS	-	expression tag	UNP Q59957
D	389	HIS	-	expression tag	UNP Q59957
D	390	HIS	-	expression tag	UNP Q59957
D	391	HIS	-	expression tag	UNP Q59957
D	392	SER	-	expression tag	UNP Q59957
D	393	SER	-	expression tag	UNP Q59957
D	394	GLY	-	expression tag	UNP Q59957
D	395	HIS	-	expression tag	UNP Q59957
D	396	ILE	-	expression tag	UNP Q59957
D	397	ASP	-	expression tag	UNP Q59957
D	398	ASP	-	expression tag	UNP Q59957

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Chain	Residue	Modelled	Actual	Comment	Reference
D	399	ASP	-	expression tag	UNP Q59957
D	400	ASP	-	expression tag	UNP Q59957
D	401	LYS	-	expression tag	UNP Q59957
D	402	HIS	-	expression tag	UNP Q59957
D	403	MET	-	expression tag	UNP Q59957

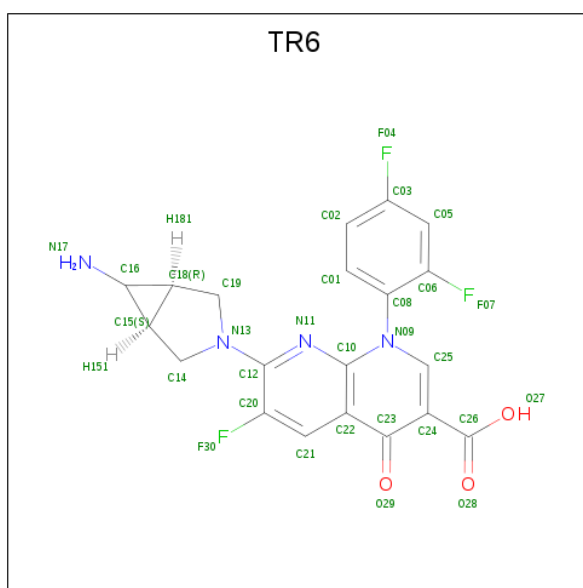
- Molecule 3 is a DNA chain called Symmetrized E-site DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	8	Total	C	N	O	P	0	0	0
			160	79	26	48	7			
3	G	7	Total	C	N	O	P	0	0	0
			141	70	23	42	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	12	Total	C	N	O	P	0	0	0
			243	117	48	67	11			
4	H	11	Total	C	N	O	P	0	0	0
			221	107	43	61	10			

- Molecule 5 is Trovafloxacin (three-letter code: TR6) (formula: $C_{20}H_{15}F_3N_4O_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	F	1	Total	C	F	H	N	O	0	0
			44	20	3	14	4	3		
5	H	1	Total	C	F	H	N	O	0	0
			44	20	3	14	4	3		

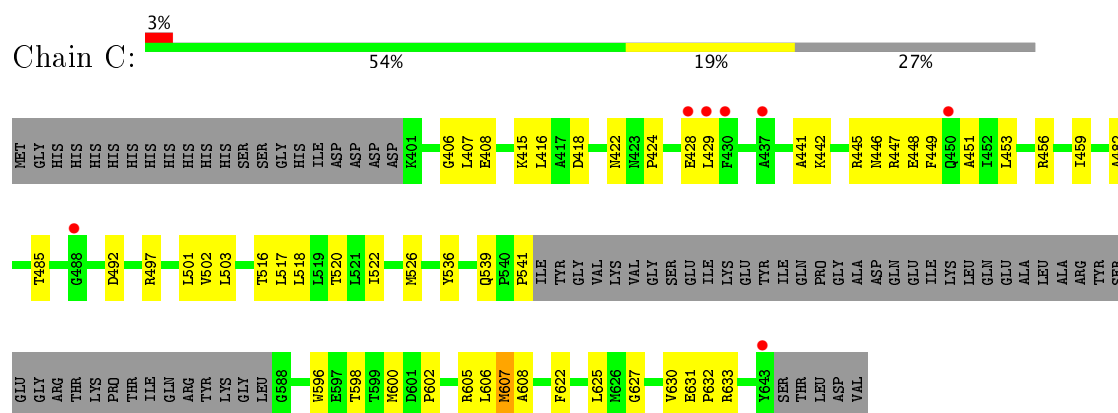
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	1	Total	Mg	0	0
			1	1		
6	F	1	Total	Mg	0	0
			1	1		

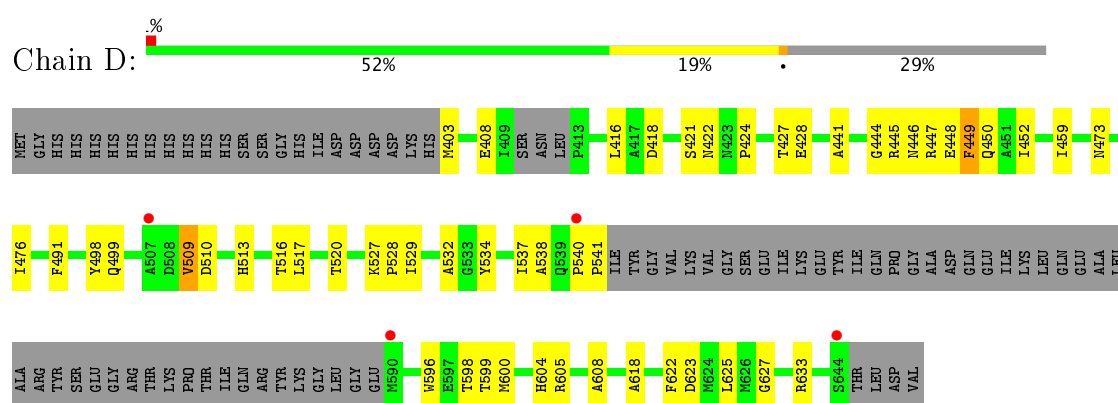
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	O	0	0
			2	2		

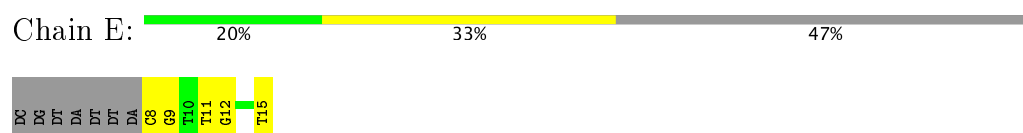
- Molecule 2: DNA gyrase subunit B



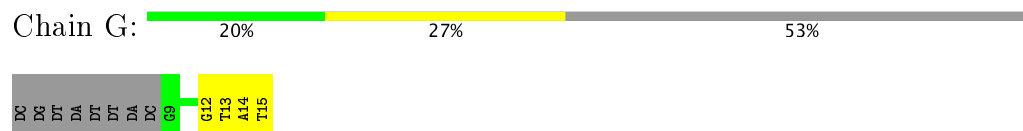
- Molecule 2: DNA gyrase subunit B



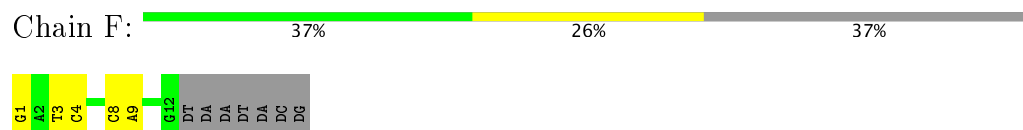
- Molecule 3: Symmetrized E-site DNA



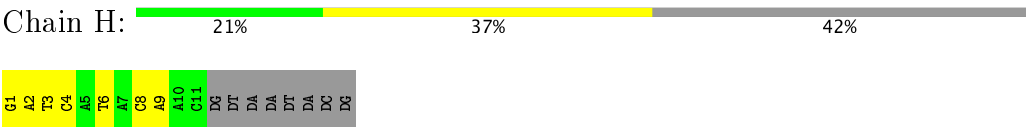
- Molecule 3: Symmetrized E-site DNA



- Molecule 4: Symmetrized E-site DNA



- Molecule 4: Symmetrized E-site DNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	94.19Å 96.62Å 275.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.05 – 3.46 56.04 – 3.37	Depositor EDS
% Data completeness (in resolution range)	99.6 (56.05-3.46) 94.5 (56.04-3.37)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.247 , 0.292 0.247 , 0.290	Depositor DCC
R_{free} test set	1543 reflections (4.81%)	DCC
Wilson B-factor (Å ²)	104.9	Xtriage
Anisotropy	0.635	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 105.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.026 for k,h,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9755	wwPDB-VP
Average B, all atoms (Å ²)	130.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% 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, TR6

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	0.19	0/3394	0.37	0/4637
1	B	0.19	0/3180	0.36	0/4355
2	C	0.19	0/1244	0.36	0/1708
2	D	0.19	0/1225	0.35	0/1676
3	E	0.43	0/178	1.09	0/274
3	G	0.44	0/157	1.10	0/242
4	F	0.45	0/273	0.97	0/419
4	H	0.44	0/248	0.97	1/380 (0.3%)
All	All	0.22	0/9899	0.47	1/13691 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	6	DT	O4'-C4'-C3'	-5.12	102.45	104.50

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	3340	0	2824	119	0
1	B	3129	0	2521	109	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1224	0	908	39	0
2	D	1205	0	906	40	0
3	E	160	0	91	4	0
3	G	141	0	80	5	0
4	F	243	0	136	8	0
4	H	221	0	125	8	0
5	F	30	14	14	3	0
5	H	30	14	14	1	0
6	F	1	0	0	0	0
6	H	1	0	0	0	0
7	A	2	0	0	0	0
All	All	9727	28	7619	307	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 18.

The worst 5 of 307 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:234:GLY:HA2	1:A:331:MET:HE2	1.56	0.88
2:D:403:MET:HA	2:D:421:SER:HA	1.61	0.83
1:B:90:MET:HG2	1:B:96:TYR:HE2	1.45	0.80
1:A:74:LYS:HD3	1:B:66:ARG:HH21	1.50	0.77
2:D:520:THR:HG22	2:D:622:PHE:CD2	2.21	0.76

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	483/499 (97%)	449 (93%)	30 (6%)	4 (1%)	22 65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	466/499 (93%)	431 (92%)	26 (6%)	9 (2%)	9	46
2	C	193/269 (72%)	166 (86%)	25 (13%)	2 (1%)	18	60
2	D	185/269 (69%)	165 (89%)	16 (9%)	4 (2%)	8	43
All	All	1327/1536 (86%)	1211 (91%)	97 (7%)	19 (1%)	13	52

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	447	ARG
1	B	29	ALA
1	B	286	ILE
1	B	289	VAL
1	A	30	ARG

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	257/433 (59%)	252 (98%)	5 (2%)	62	85
1	B	215/433 (50%)	209 (97%)	6 (3%)	49	79
2	C	66/226 (29%)	64 (97%)	2 (3%)	46	78
2	D	66/226 (29%)	64 (97%)	2 (3%)	46	78
All	All	604/1318 (46%)	589 (98%)	15 (2%)	53	81

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	607	MET
1	B	66	ARG
1	B	438	GLN
2	C	456	ARG
1	B	381	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	118	GLN
1	B	404	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 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$
5	TR6	F	101	6	29,34,34	1.63	7 (24%)	28,53,53	2.11	8 (28%)
5	TR6	H	101	6	29,34,34	1.63	7 (24%)	28,53,53	2.31	9 (32%)

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	TR6	F	101	6	-	0/7/29/29	0/4/5/5
5	TR6	H	101	6	-	0/7/29/29	0/4/5/5

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	101	TR6	C12-C20	-2.45	1.39	1.42
5	F	101	TR6	F04-C03	-2.43	1.30	1.36
5	H	101	TR6	C14-C15	-2.40	1.50	1.53
5	H	101	TR6	F04-C03	-2.39	1.30	1.36
5	H	101	TR6	C12-C20	-2.35	1.39	1.42

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	101	TR6	C21-C20-C12	-3.72	119.16	121.73
5	F	101	TR6	C21-C20-C12	-3.65	119.21	121.73
5	F	101	TR6	C25-C24-C23	-2.78	118.69	119.99
5	F	101	TR6	C02-C03-C05	-2.68	119.78	123.29
5	H	101	TR6	C02-C03-C05	-2.63	119.84	123.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	101	TR6	3	0
5	H	101	TR6	1	0

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	485/499 (97%)	-0.24	2 (0%) 92 89	76, 117, 151, 190	0
1	B	472/499 (94%)	-0.21	9 (1%) 67 61	80, 125, 175, 206	0
2	C	197/269 (73%)	-0.05	7 (3%) 43 39	99, 144, 183, 197	0
2	D	191/269 (71%)	-0.15	4 (2%) 64 58	103, 142, 185, 199	0
3	E	8/15 (53%)	0.01	0 100 100	116, 123, 188, 205	0
3	G	7/15 (46%)	-0.06	0 100 100	115, 118, 164, 181	0
4	F	12/19 (63%)	-0.03	0 100 100	124, 144, 171, 197	0
4	H	11/19 (57%)	-0.25	0 100 100	112, 136, 166, 194	0
All	All	1383/1604 (86%)	-0.18	22 (1%) 72 66	76, 127, 177, 206	0

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	643	TYR	3.4
1	B	82	SER	3.3
2	C	437	ALA	2.9
1	B	81	SER	2.8
1	B	256	ILE	2.8

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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
5	TR6	H	101	30/30	0.83	0.30	0.91	136,191,236,244	0
5	TR6	F	101	30/30	0.76	0.31	0.39	213,253,296,309	0
6	MG	F	102	1/1	0.83	0.77	-	201,201,201,201	0
6	MG	H	102	1/1	0.58	0.39	-	148,148,148,148	0

6.5 Other polymers [i](#)

There are no such residues in this entry.