



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 11:44 AM UTC

PDB ID : 3L7L / pdb_00003171
Title : Structure of the Wall Teichoic Acid Polymerase TagF, H444N + CDPG (30 minute soak)
Authors : Lovering, A.L.; Strynadka, N.C.J.
Deposited on : 2009-12-28
Resolution : 2.95 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

<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

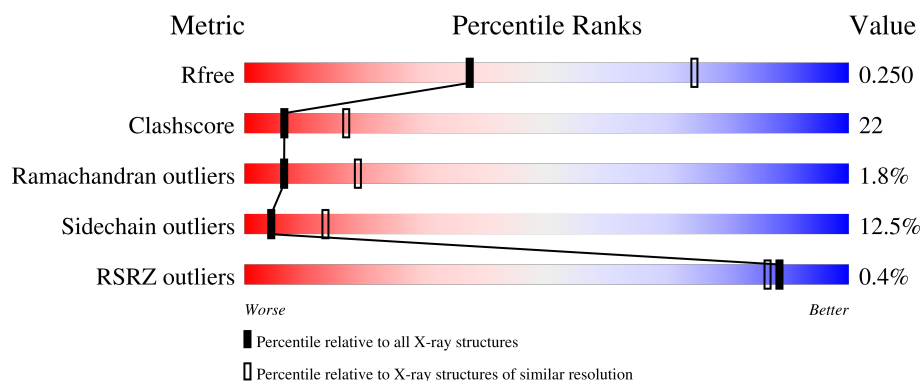
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	729	30% 23% • 44%
1	B	729	31% 20% 5% 44%
1	C	729	32% 21% • 44%
1	D	729	29% 21% • 45%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	B	734	-	-	X	-
3	CL	B	735	-	-	X	-
3	CL	D	732	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13868 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 Teichoic acid biosynthesis protein F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	410	Total	C	N	O	S	0	0	0
			3462	2224	577	650	11			
1	B	411	Total	C	N	O	S	0	0	0
			3467	2227	578	651	11			
1	C	411	Total	C	N	O	S	0	0	0
			3467	2227	578	651	11			
1	D	401	Total	C	N	O	S	0	0	0
			3383	2169	568	635	11			

There are 36 discrepancies between the modelled and reference sequences:

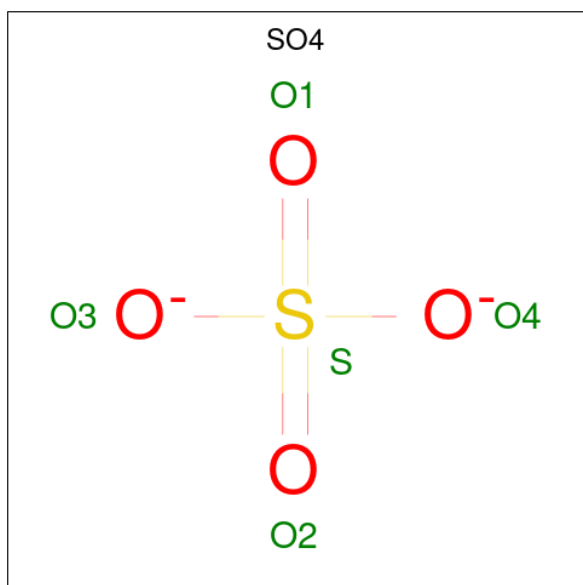
Chain	Residue	Modelled	Actual	Comment	Reference
A	444	ASN	HIS	engineered mutation	UNP Q5HLM5
A	722	LEU	-	expression tag	UNP Q5HLM5
A	723	GLU	-	expression tag	UNP Q5HLM5
A	724	HIS	-	expression tag	UNP Q5HLM5
A	725	HIS	-	expression tag	UNP Q5HLM5
A	726	HIS	-	expression tag	UNP Q5HLM5
A	727	HIS	-	expression tag	UNP Q5HLM5
A	728	HIS	-	expression tag	UNP Q5HLM5
A	729	HIS	-	expression tag	UNP Q5HLM5
B	444	ASN	HIS	engineered mutation	UNP Q5HLM5
B	722	LEU	-	expression tag	UNP Q5HLM5
B	723	GLU	-	expression tag	UNP Q5HLM5
B	724	HIS	-	expression tag	UNP Q5HLM5
B	725	HIS	-	expression tag	UNP Q5HLM5
B	726	HIS	-	expression tag	UNP Q5HLM5
B	727	HIS	-	expression tag	UNP Q5HLM5
B	728	HIS	-	expression tag	UNP Q5HLM5
B	729	HIS	-	expression tag	UNP Q5HLM5
C	444	ASN	HIS	engineered mutation	UNP Q5HLM5
C	722	LEU	-	expression tag	UNP Q5HLM5
C	723	GLU	-	expression tag	UNP Q5HLM5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	724	HIS	-	expression tag	UNP Q5HLM5
C	725	HIS	-	expression tag	UNP Q5HLM5
C	726	HIS	-	expression tag	UNP Q5HLM5
C	727	HIS	-	expression tag	UNP Q5HLM5
C	728	HIS	-	expression tag	UNP Q5HLM5
C	729	HIS	-	expression tag	UNP Q5HLM5
D	444	ASN	HIS	engineered mutation	UNP Q5HLM5
D	722	LEU	-	expression tag	UNP Q5HLM5
D	723	GLU	-	expression tag	UNP Q5HLM5
D	724	HIS	-	expression tag	UNP Q5HLM5
D	725	HIS	-	expression tag	UNP Q5HLM5
D	726	HIS	-	expression tag	UNP Q5HLM5
D	727	HIS	-	expression tag	UNP Q5HLM5
D	728	HIS	-	expression tag	UNP Q5HLM5
D	729	HIS	-	expression tag	UNP Q5HLM5

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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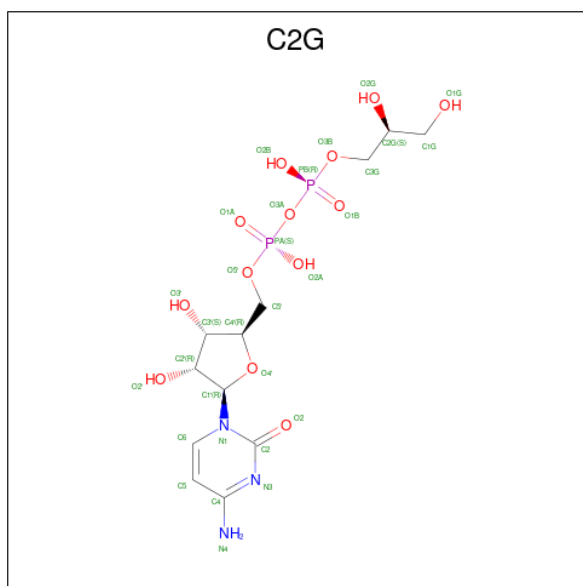
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

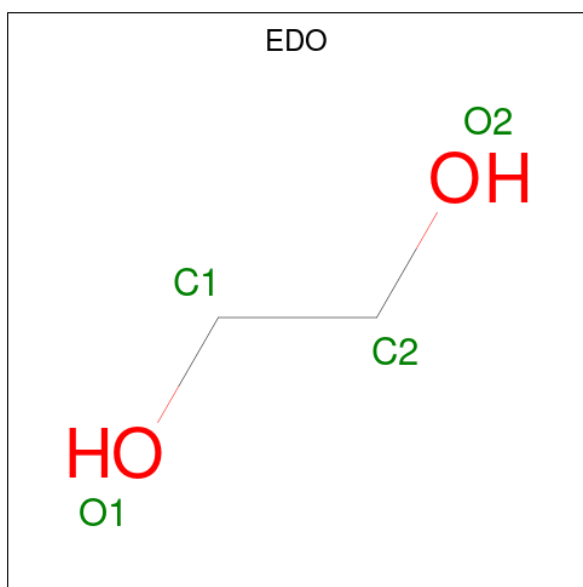
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	8	Total	Cl	0	0
			8	8		
3	B	5	Total	Cl	0	0
			5	5		
3	C	5	Total	Cl	0	0
			5	5		
3	D	3	Total	Cl	0	0
			3	3		

- Molecule 4 is [CYTIDINE-5'-PHOSPHATE] GLYCERYLPHOSPHORIC ACID ESTER (CCD ID: C2G) (formula: C₁₂H₂₁N₃O₁₃P₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	N	O	P	0
			30	12	3	13	2	0

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C O 4 2 2	0	0

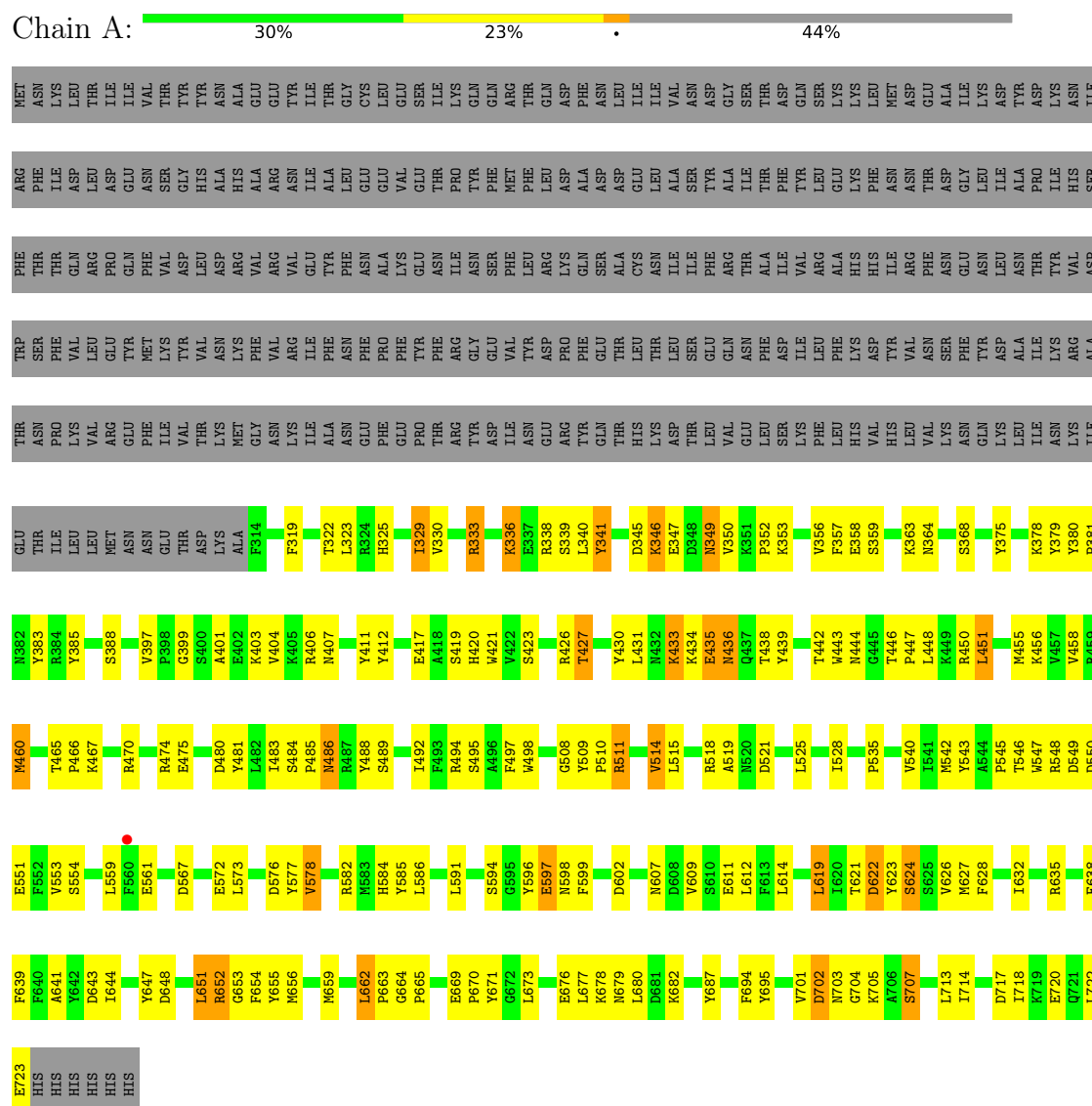
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total O 2 2	0	0
6	D	2	Total O 2 2	0	0

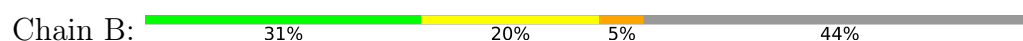
3 Residue-property plots

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: Teichoic acid biosynthesis protein F



• Molecule 1: Teichoic acid biosynthesis protein F



[illegible]

- Molecule 1: Teichoic acid biosynthesis protein F

Chain C:  32% 21% . 44%

P381	GLU	THR	THR	TPP	PHE	ARG	MET
N382	THR	ASN	THR	SER	THR	PHE	ASN
N383	ILE	PRO	THR	PHE	THR	ILE	LYS
R384	LEU	LYS	GLN	VAL	GLN	ASP	THR
R385	LEU	VAL	ARG	LEU	THR	LEU	THR
R386	MET	ARG	GLU	GLU	PRO	ASP	ILE
N387	ASN	GLU	THR	TYP	GLN	GLU	ILE
R388	ASN	PHE	PHE	MET	PHE	VAL	VAL
F389	GLU	ILE	LYS	LYS	VAL	SER	THR
	THR	VAL	VAL	TYP	ASP	GLY	THR
P392	ASP	THR	LYS	ASN	ASP	HIS	TYP
	LYS	LYS	ASN	LYS	ASP	ALA	ASN
A401	A313	MET	MET	LYS	ARG	HIS	ALA
E402	F314	GLY	GLY	PHE	VAL	ARG	GLU
K403	K315	ASN	ASN	VAL	ARG	ALA	GLU
	V316	LYS	LYS	ARG	VAL	ASN	TYP
E410	N317	ILE	ILE	ILE	ILE	ILE	ILE
Y411		ALA	PHE	PHE	TYP	ALA	THR
Y412	K321	ASN	ASN	ASN	PHE	LEU	GLY
	T322	GLU	PHE	PHE	LEU	GLU	CYS
E417	R323	PHE	PRO	PRO	ALA	GLU	LEU
	R324	GLU	GLU	PHE	LYS	VAL	LEU
H420	H325	PRO	PRO	TYP	GLU	GLU	SER
	V326	THR	THR	PHE	ASN	THR	ILE
		ARG	ARG	ARG	ILE	PRO	LYS
R426	T329	TYP	TYP	GLY	ILE	TYP	GLN
L429	V330	ASP	ASP	GLU	SER	PHE	GLN
Y430	L331	ILE	ILE	VAL	ASN	MET	ARG
	R332	ASN	ASN	TYP	LEU	PHE	THR
K434	R338	GLU	GLU	ASP	ARG	LEU	GLN
E435	S339	ARG	ARG	PRO	LYS	ASP	ASP
M436	S339	TYP	TYP	PHE	GLN	ALA	PHE
Q437	L340	GLN	GLN	GLU	SER	ASN	ASN
T438	Y341	THR	THR	THR	THR	ALA	ASP
Y439		HIS	HIS	LEU	CYS	GLU	ILE
I440	T344	LYS	LYS	THR	ASN	LEU	ILE
Q441	D345	ASP	ASP	LEU	ILE	ALA	VAL
T442	K346	THR	THR	SER	ILE	SER	ASN
W443	E347	LEU	GLU	GLU	PHE	TYP	ASP
N444	D348	VAL	GLN	GLN	ARG	ALA	GLY
G445	N349	GLU	GLU	ASN	THR	ILE	SER
T446	V350	LEU	LEU	PHE	ALA	THR	THR
F447	K351	SER	SER	ASP	ILE	PHE	ASP
L448	P352	LYS	LYS	ILE	VAL	TYP	THR
K449	K353	PHE	LEU	PHE	ARG	GLU	SER
R450		LEU	LEU	PHE	ALA	GLU	LYS
L451	V356	HIS	HIS	LYS	HIS	LYS	LYS
A452		VAL	HIS	ASP	HIS	PHE	LEU
M453	Y365	HIS	VAL	TYP	ILE	ASN	MET
	S366	LEU	LEU	VAL	ASN	ASN	ASP
V457	D367	VAL	VAL	ASN	PHE	THR	GLU
W458	S368	LYS	LYS	PHE	ARG	ASP	ALA
R459	P369	ASN	ASN	SER	GLY	GLY	ILE
M460	K370	GLN	GLN	TYP	ASN	LEU	LYS
	Y371	LYS	LYS	ASP	ASN	ILE	ASP
	T372	LEU	LEU	ALA	LEU	TYP	THR
T463	L371	ILE	ILE	ILE	THR	PRO	LYS
T464		ASN	ASN	LYS	THR	ILE	LYS
T465	Q377	THR	THR	TYP	THR	ASP	ASP
P466		LYS	LYS	ARG	HIS	HIS	ASN
P467	Y380	ILE	ILE	ALA	ASN	SER	THR

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	222.88Å 222.88Å 100.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.01 – 2.95 20.01 – 2.95	Depositor EDS
% Data completeness (in resolution range)	98.7 (20.01-2.95) 98.3 (20.01-2.95)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.93Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.193 , 0.254 0.186 , 0.250	Depositor DCC
R_{free} test set	2650 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	88.4	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 44.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13868	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.04% 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: C2G, CL, SO4, EDO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.63	0/3551	0.99	16/4798 (0.3%)
1	B	0.64	1/3556 (0.0%)	0.99	9/4805 (0.2%)
1	C	0.56	0/3556	0.96	4/4805 (0.1%)
1	D	0.61	0/3469	0.95	8/4688 (0.2%)
All	All	0.61	1/14132 (0.0%)	0.97	37/19096 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	425	ALA	CA-CB	-5.12	1.47	1.53

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	484	SER	CA-C-N	9.17	128.91	119.64
1	B	484	SER	C-N-CA	9.17	128.91	119.64
1	B	460	MET	CA-C-N	8.14	130.01	119.84
1	B	460	MET	C-N-CA	8.14	130.01	119.84
1	C	448	LEU	N-CA-C	-7.01	104.60	113.43

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	3462	0	3369	136	0
1	B	3467	0	3374	140	0
1	C	3467	0	3374	157	0
1	D	3383	0	3289	160	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	0	0
3	A	8	0	0	2	0
3	B	5	0	0	5	0
3	C	5	0	0	2	0
3	D	3	0	0	5	0
4	D	30	0	19	3	0
5	D	4	0	6	0	0
6	A	2	0	0	0	0
6	D	2	0	0	0	0
All	All	13868	0	13431	591	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 22.

The worst 5 of 591 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:333:ARG:HG2	1:A:333:ARG:HH11	1.13	1.13
1:D:333:ARG:HH11	1:D:333:ARG:HG2	1.16	1.08
1:D:470:ARG:HG2	1:D:470:ARG:HH11	1.07	1.08
1:B:470:ARG:HG2	1:B:470:ARG:HH11	1.24	1.01
1:B:333:ARG:HH11	1:B:333:ARG:HG2	1.24	1.00

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	408/729 (56%)	376 (92%)	28 (7%)	4 (1%)	12	32
1	B	409/729 (56%)	362 (88%)	38 (9%)	9 (2%)	5	15
1	C	409/729 (56%)	356 (87%)	46 (11%)	7 (2%)	7	20
1	D	397/729 (54%)	346 (87%)	42 (11%)	9 (2%)	5	14
All	All	1623/2916 (56%)	1440 (89%)	154 (10%)	29 (2%)	6	19

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	651	LEU
1	C	367	ASP
1	D	367	ASP
1	A	647	TYR
1	B	462	GLY

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	379/675 (56%)	333 (88%)	46 (12%)	5	14
1	B	379/675 (56%)	326 (86%)	53 (14%)	3	10
1	C	379/675 (56%)	334 (88%)	45 (12%)	5	15
1	D	370/675 (55%)	325 (88%)	45 (12%)	5	14
All	All	1507/2700 (56%)	1318 (88%)	189 (12%)	4	13

5 of 189 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	500	ASP
1	C	722	LEU
1	C	578	VAL
1	C	656	MET
1	D	337	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	703	ASN
1	D	436	ASN
1	C	382	ASN
1	D	317	ASN
1	C	349	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 29 ligands modelled in this entry, 21 are monoatomic - leaving 8 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	$\# Z > 2$
2	SO4	B	731	-	4,4,4	0.26	0	6,6,6	0.21	0
2	SO4	C	731	-	4,4,4	0.21	0	6,6,6	0.24	0
4	C2G	D	730	-	31,31,31	3.88	14 (45%)	42,46,46	1.10	4 (9%)
2	SO4	C	730	-	4,4,4	0.25	0	6,6,6	0.20	0
2	SO4	A	731	-	4,4,4	0.25	0	6,6,6	0.10	0
2	SO4	A	730	-	4,4,4	0.22	0	6,6,6	0.20	0
5	EDO	D	734	-	3,3,3	0.63	0	2,2,2	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	B	730	-	4,4,4	0.25	0	6,6,6	0.23	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
4	C2G	D	730	-	-	13/24/40/40	0/2/2/2
5	EDO	D	734	-	-	1/1/1/1	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	730	C2G	O2-C2	8.93	1.40	1.23
4	D	730	C2G	C4-N3	7.31	1.48	1.34
4	D	730	C2G	C6-C5	7.00	1.51	1.35
4	D	730	C2G	C2-N1	6.97	1.54	1.40
4	D	730	C2G	C2-N3	6.89	1.50	1.36

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	730	C2G	C1'-N1-C2	2.75	124.52	118.44
4	D	730	C2G	O2-C2-N3	-2.51	118.38	122.33
4	D	730	C2G	N4-C4-N3	2.29	122.00	117.91
4	D	730	C2G	C3'-C2'-C1'	2.27	105.76	101.46

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

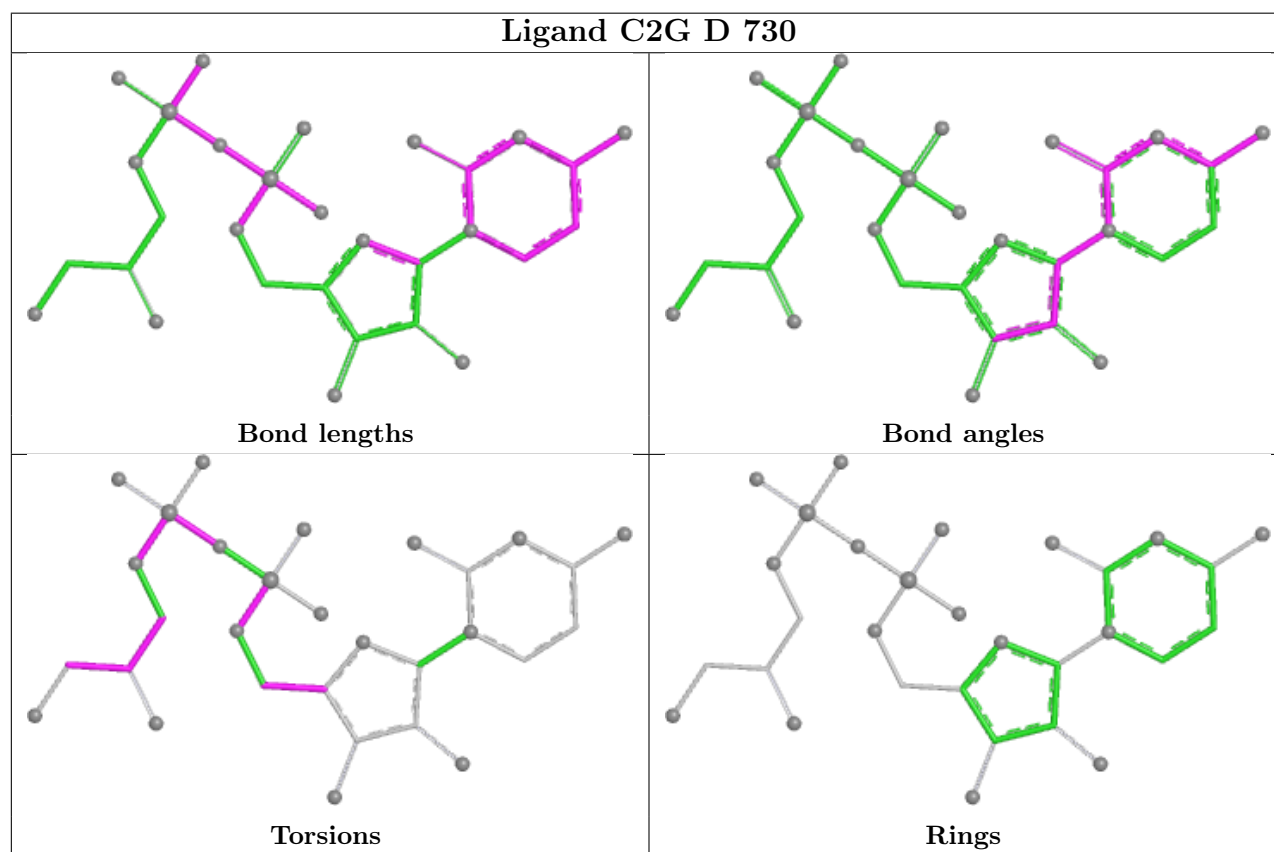
Mol	Chain	Res	Type	Atoms
4	D	730	C2G	C5'-O5'-PA-O1A
4	D	730	C2G	C5'-O5'-PA-O2A
4	D	730	C2G	C3G-O3B-PB-O3A
4	D	730	C2G	C3G-O3B-PB-O2B
4	D	730	C2G	O2G-C2G-C3G-O3B

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	730	C2G	3	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 ⓘ

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	410/729 (56%)	-0.58	1 (0%) 91 90	61, 83, 149, 220	0
1	B	411/729 (56%)	-0.56	2 (0%) 87 83	64, 85, 159, 242	0
1	C	411/729 (56%)	-0.51	1 (0%) 91 90	69, 94, 166, 263	0
1	D	401/729 (55%)	-0.51	2 (0%) 87 83	66, 92, 151, 279	0
All	All	1633/2916 (56%)	-0.54	6 (0%) 88 86	61, 88, 156, 279	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	560	PHE	3.0
1	D	587	ILE	2.4
1	A	560	PHE	2.4
1	D	651	LEU	2.1
1	B	559	LEU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

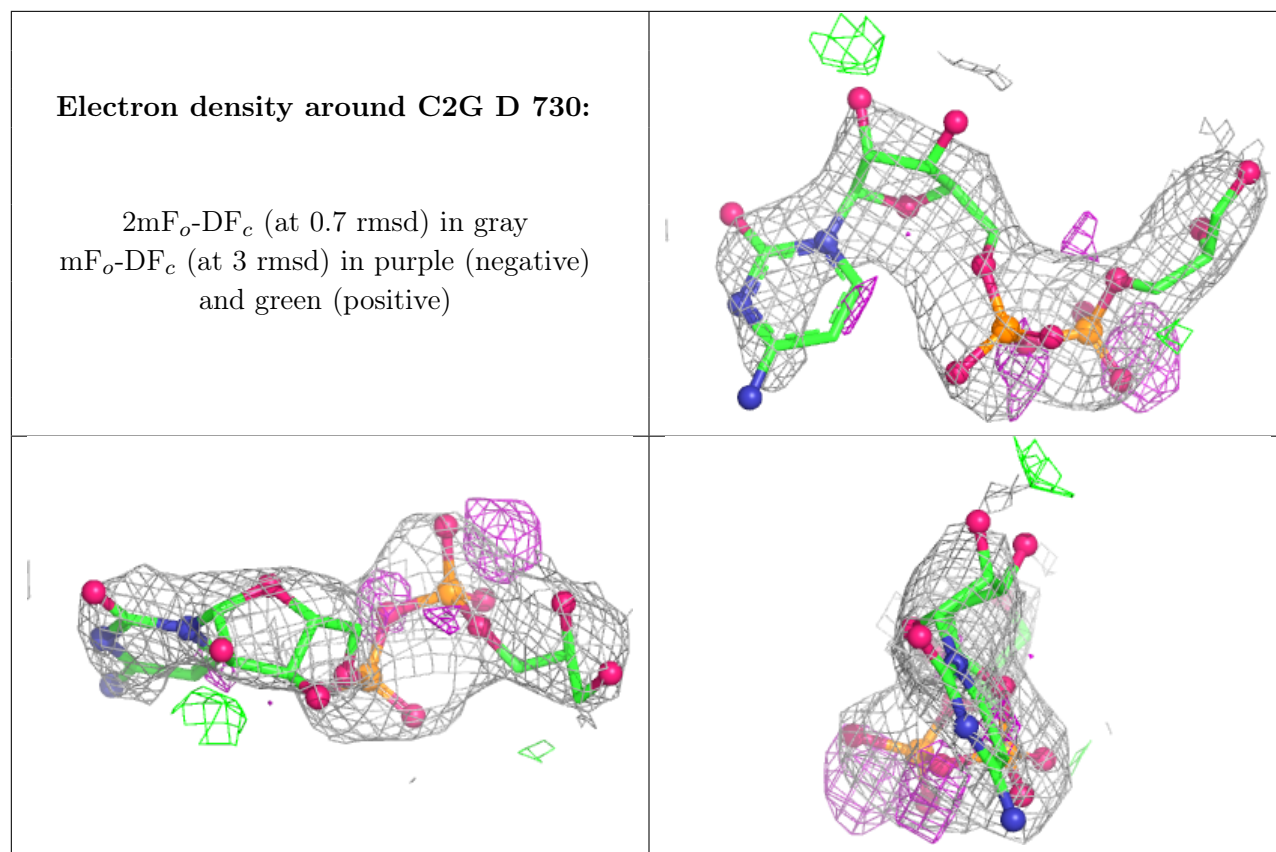
There are no oligosaccharides in this entry.

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
2	SO4	B	731	5/5	0.57	0.12	171,171,171,171	0
2	SO4	A	731	5/5	0.74	0.12	166,166,166,166	0
3	CL	B	734	1/1	0.81	0.09	111,111,111,111	0
3	CL	C	735	1/1	0.81	0.12	118,118,118,118	0
3	CL	C	734	1/1	0.85	0.10	106,106,106,106	0
3	CL	A	732	1/1	0.87	0.06	114,114,114,114	0
5	EDO	D	734	4/4	0.87	0.10	90,90,90,90	0
3	CL	D	733	1/1	0.88	0.06	92,92,92,92	0
4	C2G	D	730	30/30	0.89	0.11	122,122,123,123	0
3	CL	A	737	1/1	0.89	0.07	108,108,108,108	0
3	CL	A	733	1/1	0.90	0.09	130,130,130,130	0
2	SO4	C	731	5/5	0.90	0.08	124,125,127,128	0
3	CL	A	739	1/1	0.90	0.12	88,88,88,88	0
3	CL	D	732	1/1	0.91	0.06	101,101,101,101	0
3	CL	B	735	1/1	0.91	0.09	127,127,127,127	0
3	CL	A	736	1/1	0.91	0.08	106,106,106,106	0
2	SO4	C	730	5/5	0.91	0.07	129,129,131,132	0
3	CL	C	733	1/1	0.92	0.04	102,102,102,102	0
3	CL	B	733	1/1	0.93	0.08	121,121,121,121	0
2	SO4	A	730	5/5	0.93	0.09	103,104,105,107	0
2	SO4	B	730	5/5	0.93	0.07	90,90,91,94	0
3	CL	C	736	1/1	0.93	0.06	106,106,106,106	0
3	CL	B	732	1/1	0.94	0.12	100,100,100,100	0
3	CL	A	734	1/1	0.95	0.07	96,96,96,96	0
3	CL	B	736	1/1	0.95	0.06	83,83,83,83	0
3	CL	A	735	1/1	0.96	0.09	94,94,94,94	0
3	CL	C	732	1/1	0.96	0.04	107,107,107,107	0
3	CL	A	738	1/1	0.97	0.06	97,97,97,97	0
3	CL	D	731	1/1	0.99	0.12	68,68,68,68	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.