wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 27, 2023 – 10:19 PM EDT

PDB ID	:	3L7M
Title	:	Structure of the Wall Teichoic Acid Polymerase TagF, H548A
Authors	:	Lovering, A.L.; Strynadka, N.C.J.
Deposited on	:	2009-12-28
Resolution	:	2.85 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:

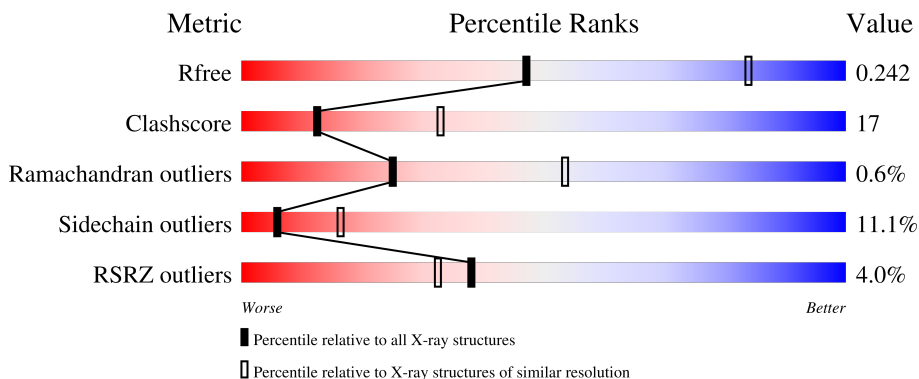|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.85 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Rfree		0.242
Clashscore		17
Ramachandran outliers		0.6%
Sidechain outliers		11.1%
RSRZ outliers		4.0%

Worse — *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	729	2% / 35% 18% • 44%
1	B	729	2% / 37% 16% • 44%
1	C	729	3% / 36% 18% • 44%
1	D	729	3% / 35% 19% • 43%

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	A	735	-	-	-	X
3	CL	A	736	-	-	-	X
3	CL	B	733	-	-	-	X
3	CL	B	734	-	-	-	X
3	CL	B	735	-	-	X	-
3	CL	B	736	-	-	X	-
4	EDT	A	738	-	-	X	-
4	EDT	D	735	-	-	X	-

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 13942 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	407	Total	C	N	O	S	0	0	0
			3434	2206	572	645	11			
1	B	411	Total	C	N	O	S	0	0	0
			3464	2226	577	650	11			
1	C	411	Total	C	N	O	S	0	0	0
			3464	2226	577	650	11			
1	D	412	Total	C	N	O	S	0	0	0
			3474	2232	580	651	11			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	584	ALA	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	584	ALA	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	584	ALA	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	584	ALA	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 PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).
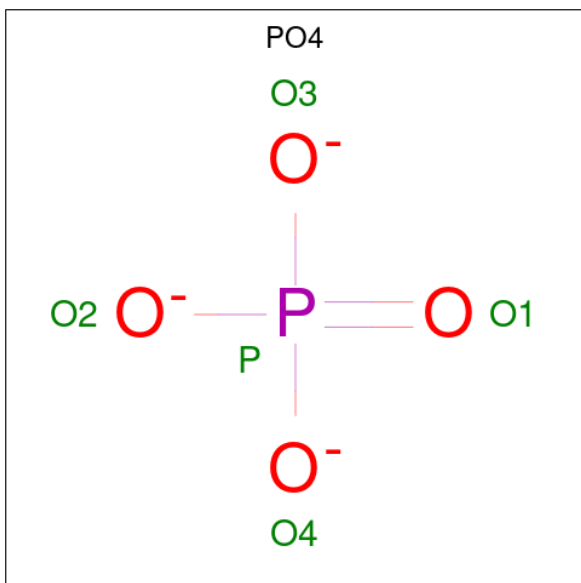
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	O 4	P 1	0	0
2	A	1	Total 5	O 4	P 1	0	0
2	B	1	Total 5	O 4	P 1	0	0
2	B	1	Total 5	O 4	P 1	0	0

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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total 6	Cl 6	0	0
3	B	6	Total 6	Cl 6	0	0
3	C	2	Total 2	Cl 2	0	0
3	D	4	Total 4	Cl 4	0	0

- Molecule 4 is {[-(BIS-CARBOXYMETHYL-AMINO)-ETHYL]-CARBOXYMETHYL-AMINO}-ACETIC ACID (three-letter code: EDT) (formula: $C_{10}H_{16}N_2O_8$).
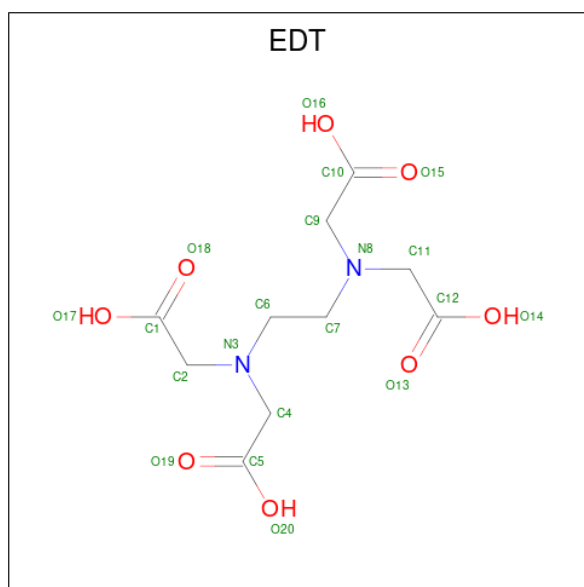
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 20	C 10	N 2	O 8	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total 20	C 10	N 2	O 8	0	0

- Molecule 5 is water.

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

MET ASN LYS LEU THR ILE ILE VAL THR TYR TYR ASN ALA GLU GLU TYR ILE THR GLY CYS LEU GLU SER ILE LYS GLN GLN ARG THR GLN ASP PHE ASN LEU ILE ILE VAL ASN ASP GLY SER THR ASP GLN SER LYS LYS LEU MET ASP ALA ILE LYS ASP TYR ASP LYS ASN ILE

ARG PHE ILE ASP LEU ASP GLU ASN SER GLY HIS ALA HIS ALA ARG ASN ILE ALA LEU GLU GLU VAL GLU THR PRO TYR PHE MET PHE LEU ASP ALA ASP ASP GLU LEU ALA SER TYR ALA ILE THR PHE TYR LEU GLU LYS PHE ASN ASN THR ASP GLY LEU ILE ALA PRO ILE HIS SER

PHE THR THR GLN ARG PRO GLN PHE VAL ASP LEU ASP ARG VAL ARG VAL GLU TYR PHE ASN ALA LYS GLU ASN ILE ASN SER PHE LEU ARG GLN SER ALA CYS ASN ILE ILE PHE ARG ARG THR ALA ILE VAL ARG ALA HIS HIS ILE ARG PHE ASN GLU LEU ASN THR TYR VAL ASP

TRP SER PHE VAL LEU GLU TYR MET LYS VAL ASN TYR VAL THR ALA LYS PHE VAL ARG ILE PHE ASN ASN PRO PHE TYR PHE ARG GLY GLU VAL TYR ASP PRO PHE GLU THR LEU LEU SER GLU ASN ASP ILE PHE LYS ASP TYR VAL ASN SER PHE ASP ALA ILE LYS ARG ALA

THR ASN PRO LYS VAL ARG GLU PHE ILE VAL THR LYS MET GLY ASN LYS ILE ALA ASN GLU PHE GLU PRO ARG TYR ASP ILE ASN GLU ARG TYR GLN THR HIS LYS ASP THR LEU VAL GLU LEU SER LYS PHE LEU HIS VAL HIS LEU VAL LYS ASN GLN LYS LEU ILE ASN LYS ILE

• Molecule 1: Teichoic acid biosynthesis protein F

Chain C:

MET ASN LYS LEU THR ILE ILE VAL THR TYR TYR ASN ALA GLU GLU TYR ILE THR GLY CYS LEU GLU SER ILE LYS GLN GLN ARG THR GLN ASP PHE ASN LEU ILE ILE VAL ASN ASP GLY SER THR ASP GLN SER LYS LYS LEU MET ASP ALA ILE LYS ASP TYR ASP LYS ASN ILE

ARG PHE ILE ASP LEU ASP GLU ASN SER GLY HIS ALA HIS ALA ARG ASN ILE ALA LEU GLU GLU VAL GLU THR PRO TYR PHE MET PHE LEU ASP ALA ASP ASP GLU LEU ALA SER TYR ALA ILE THR PHE TYR LEU GLU LYS PHE ASN ASN THR ASP GLY LEU ILE ALA PRO ILE HIS SER

PHE THR THR GLN ARG PRO GLN PHE VAL ASP LEU ASP ARG VAL ARG VAL GLU TYR PHE ASN ALA LYS GLU ASN ILE ASN SER PHE LEU ARG GLN SER ALA CYS ASN ILE ILE PHE ARG ARG THR ALA ILE VAL ARG ALA HIS HIS ILE ARG PHE ASN GLU LEU ASN THR TYR VAL ASP

TRP SER PHE VAL LEU GLU TYR MET LYS VAL ASN TYR VAL THR ALA LYS PHE VAL ARG ILE PHE ASN ASN PRO PHE TYR PHE ARG GLY GLU VAL TYR ASP PRO PHE GLU THR LEU LEU SER GLU ASN ASP ILE PHE LYS ASP TYR VAL ASN SER PHE ASP ALA ILE LYS ARG ALA

THR ASN PRO LYS VAL ARG GLU PHE ILE VAL THR LYS MET GLY ASN LYS ILE ALA ASN GLU PHE GLU PRO ARG TYR ASP ILE ASN GLU ARG TYR GLN THR HIS LYS ASP THR LEU VAL GLU LEU SER LYS PHE LEU HIS VAL HIS LEU VAL LYS ASN GLN LYS LEU ILE ASN LYS ILE

• Molecule 1: Teichoic acid biosynthesis protein F

Chain D:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	223.51Å 223.51Å 101.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.94 – 2.85 19.94 – 2.85	Depositor EDS
% Data completeness (in resolution range)	90.0 (19.94-2.85) 89.9 (19.94-2.85)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.70 (at 2.83Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.191 , 0.251 0.185 , 0.242	Depositor DCC
R_{free} test set	2715 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	86.4	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 44.4	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13942	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 6.66% 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.

wwPDB X-ray Structure Validation Summary Report

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: EDT, CL, PO4

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	0.41	0/3521	0.59	0/4757
1	B	0.43	0/3553	0.60	1/4801 (0.0%)
1	C	0.40	0/3553	0.58	0/4801
1	D	0.39	0/3564	0.59	0/4816
All	All	0.41	0/14191	0.59	1/19175 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	619	LEU	CA-CB-CG	5.64	128.28	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	364	ASN	Peptide

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	3434	0	3342	121	0
1	B	3464	0	3373	103	0
1	C	3464	0	3373	118	0
1	D	3474	0	3380	123	0
2	A	10	0	0	1	0
2	B	10	0	0	1	0
2	C	10	0	0	0	0
2	D	10	0	0	1	0
3	A	6	0	0	2	0
3	B	6	0	0	5	0
3	C	2	0	0	1	0
3	D	4	0	0	2	0
4	A	20	0	16	10	0
4	D	20	0	16	7	0
5	A	1	0	0	0	0
5	B	4	0	0	2	0
5	C	1	0	0	0	0
5	D	2	0	0	0	0
All	All	13942	0	13500	462	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 17.

The worst 5 of 462 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:470:ARG:HH11	1:C:470:ARG:HG2	1.10	1.10
1:A:333:ARG:HG2	1:A:333:ARG:HH11	1.20	1.04
1:B:470:ARG:HG2	1:B:470:ARG:HH11	1.19	1.00
1:D:470:ARG:HG2	1:D:470:ARG:HH11	1.21	1.00
1:B:333:ARG:HH11	1:B:333:ARG:HG2	1.21	0.99

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	403/729 (55%)	369 (92%)	33 (8%)	1 (0%)	47	75
1	B	409/729 (56%)	366 (90%)	40 (10%)	3 (1%)	22	50
1	C	409/729 (56%)	363 (89%)	41 (10%)	5 (1%)	13	35
1	D	410/729 (56%)	372 (91%)	37 (9%)	1 (0%)	47	75
All	All	1631/2916 (56%)	1470 (90%)	151 (9%)	10 (1%)	25	53

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	550	ASP
1	C	535	PRO
1	D	649	LYS
1	A	689	GLU
1	B	443	TRP

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	376/674 (56%)	332 (88%)	44 (12%)	5	14
1	B	378/674 (56%)	331 (88%)	47 (12%)	4	12
1	C	378/674 (56%)	341 (90%)	37 (10%)	8	21
1	D	379/674 (56%)	339 (89%)	40 (11%)	6	18
All	All	1511/2696 (56%)	1343 (89%)	168 (11%)	6	16

5 of 168 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	622	ASP
1	D	472	PHE
1	C	660	GLU
1	D	329	ILE
1	D	594	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	708	GLN
1	C	349	ASN
1	D	568	ASN
1	D	349	ASN
1	D	531	HIS

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 28 ligands modelled in this entry, 18 are monoatomic - leaving 10 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	PO4	A	730	-	4,4,4	0.82	0	6,6,6	0.65	0
2	PO4	C	731	-	4,4,4	0.85	0	6,6,6	0.47	0
4	EDT	A	738	-	19,19,19	1.59	4 (21%)	24,24,24	1.01	1 (4%)
2	PO4	A	731	-	4,4,4	0.82	0	6,6,6	0.47	0
2	PO4	B	731	-	4,4,4	0.89	0	6,6,6	0.58	0
4	EDT	D	735	-	19,19,19	1.62	4 (21%)	24,24,24	1.31	3 (12%)
2	PO4	D	730	-	4,4,4	0.96	0	6,6,6	0.33	0
2	PO4	D	731	-	4,4,4	0.72	0	6,6,6	0.75	0
2	PO4	C	730	-	4,4,4	0.83	0	6,6,6	0.49	0
2	PO4	B	730	-	4,4,4	0.88	0	6,6,6	0.41	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	EDT	A	738	-	-	14/21/21/21	-
4	EDT	D	735	-	-	13/21/21/21	-

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	735	EDT	O16-C10	3.32	1.41	1.30
4	A	738	EDT	O16-C10	3.10	1.41	1.30
4	D	735	EDT	O17-C1	3.09	1.41	1.30
4	D	735	EDT	O14-C12	2.99	1.40	1.30
4	A	738	EDT	O14-C12	2.98	1.40	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	735	EDT	C2-N3-C4	3.19	118.75	111.54
4	D	735	EDT	O20-C5-O19	-2.37	117.39	123.30
4	A	738	EDT	O14-C12-O13	-2.02	118.28	123.30
4	D	735	EDT	C4-N3-C6	2.01	116.84	111.94

There are no chirality outliers.

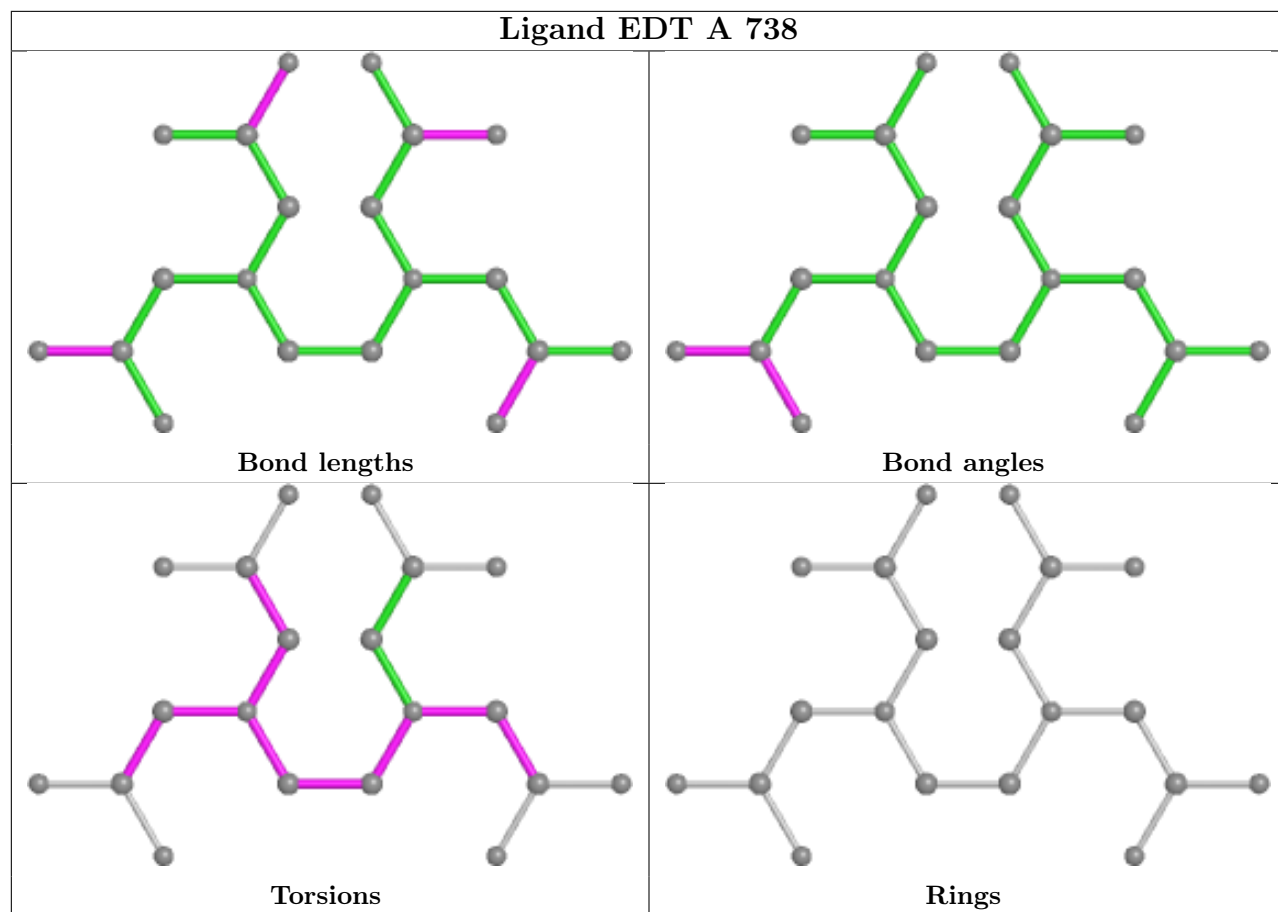5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	738	EDT	N3-C4-C5-O19
4	A	738	EDT	C5-C4-N3-C6
4	A	738	EDT	C7-C6-N3-C2
4	A	738	EDT	C10-C9-N8-C7
4	A	738	EDT	N8-C11-C12-O13

There are no ring outliers.

5 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	738	EDT	10	0
2	A	731	PO4	1	0
2	B	731	PO4	1	0
4	D	735	EDT	7	0
2	D	731	PO4	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 EDT A 738

Bond lengths

Bond angles

Torsions

Rings

Ligand EDT D 735

Bond lengths

Bond angles

Torsions

Rings
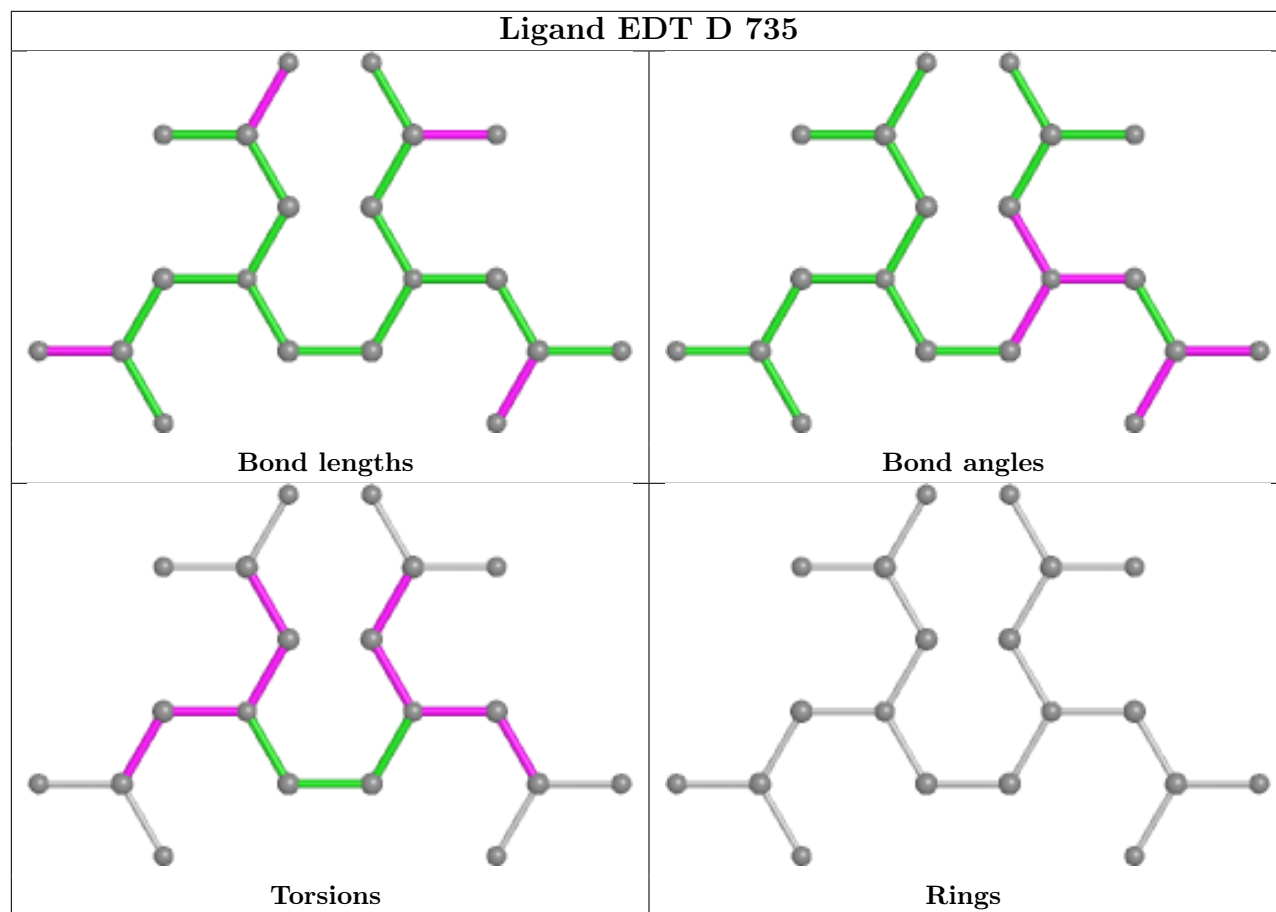
5.7 Other polymers ⓘ

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	407/729 (55%)	-0.19	11 (2%)	54	50	57, 87, 151, 221	0
1	B	411/729 (56%)	-0.20	16 (3%)	39	34	58, 84, 147, 265	0
1	C	411/729 (56%)	-0.06	19 (4%)	32	27	59, 96, 163, 264	0
1	D	412/729 (56%)	-0.11	19 (4%)	32	27	63, 89, 163, 306	0
All	All	1641/2916 (56%)	-0.14	65 (3%)	38	32	57, 89, 160, 306	0

The worst 5 of 65 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	724	HIS	7.9
1	C	558	TYR	7.3
1	D	652	ARG	5.9
1	B	555	LYS	5.6
1	D	558	TYR	5.1

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 ⓘ

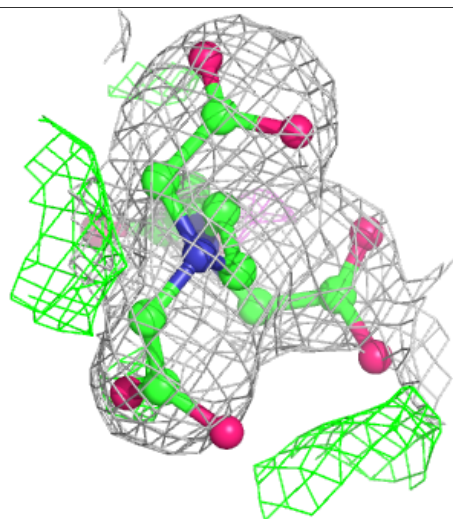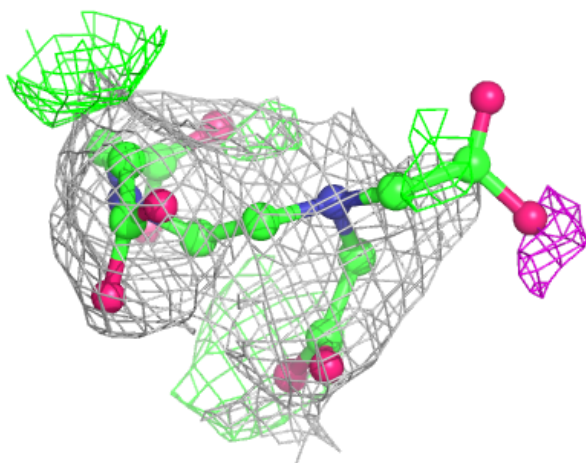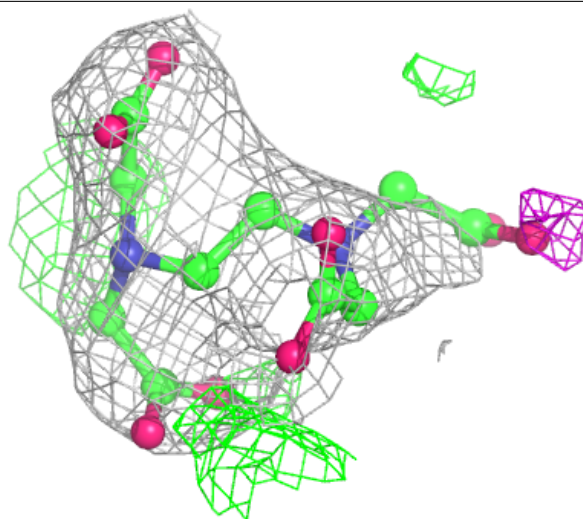There are no monosaccharides in this entry.

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.
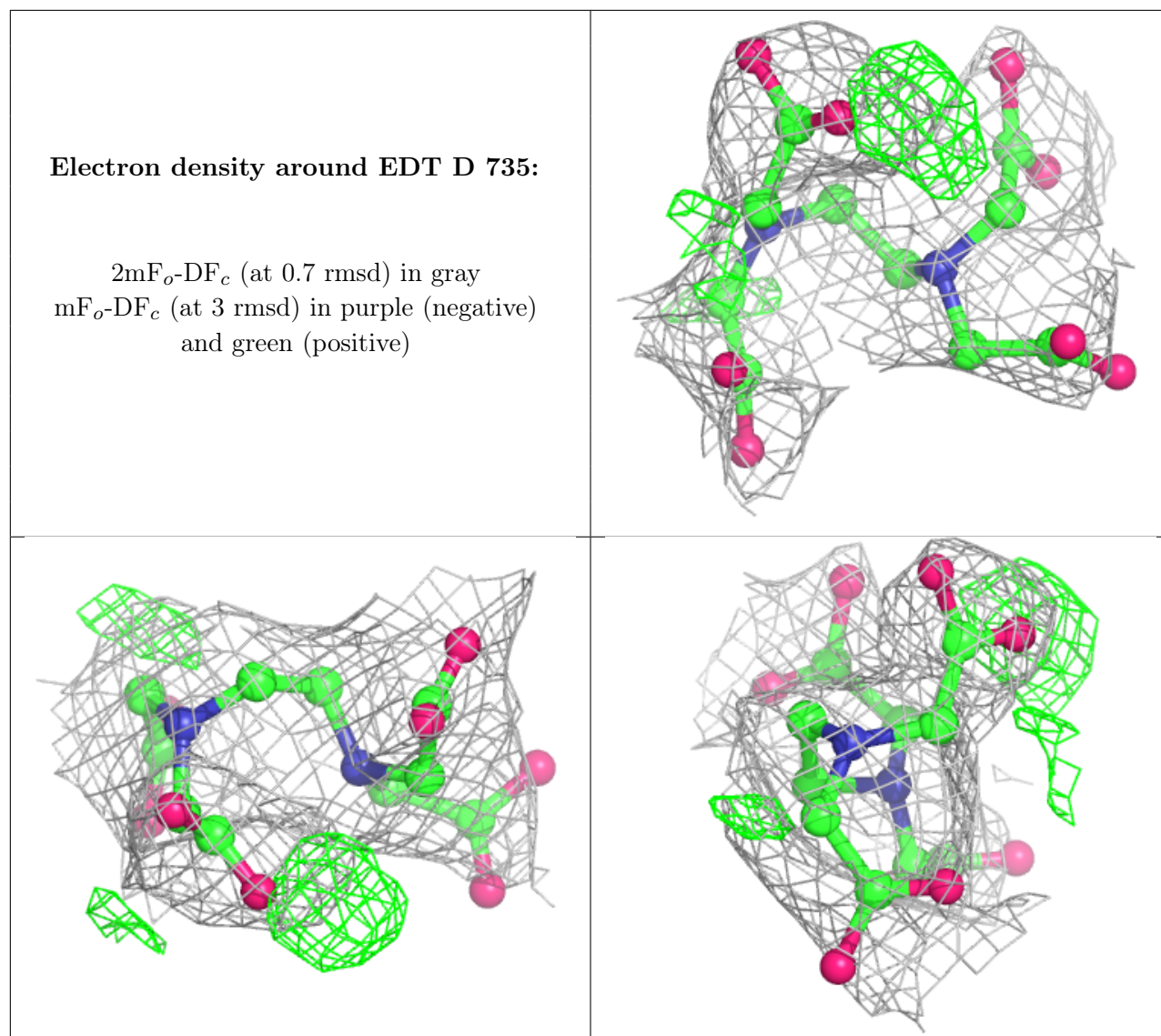
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CL	A	736	1/1	0.61	0.44	111,111,111,111	0
3	CL	B	734	1/1	0.68	0.51	141,141,141,141	0
3	CL	D	733	1/1	0.69	0.34	124,124,124,124	0
3	CL	A	735	1/1	0.71	0.66	104,104,104,104	0
3	CL	A	737	1/1	0.77	0.22	115,115,115,115	0
4	EDT	A	738	20/20	0.78	0.30	134,134,134,134	0
4	EDT	D	735	20/20	0.78	0.29	132,132,132,132	0
3	CL	B	733	1/1	0.80	0.48	109,109,109,109	0
3	CL	C	733	1/1	0.83	0.27	108,108,108,108	0
3	CL	D	732	1/1	0.85	0.11	107,107,107,107	0
3	CL	B	737	1/1	0.87	0.21	99,99,99,99	0
3	CL	C	732	1/1	0.88	0.20	119,119,119,119	0
3	CL	A	732	1/1	0.88	0.57	126,126,126,126	0
3	CL	B	735	1/1	0.89	0.18	107,107,107,107	0
3	CL	D	736	1/1	0.89	0.18	87,87,87,87	0
2	PO4	C	731	5/5	0.90	0.26	152,152,152,152	0
3	CL	D	734	1/1	0.92	0.43	113,113,113,113	0
2	PO4	D	731	5/5	0.93	0.15	133,133,133,133	0
3	CL	B	736	1/1	0.94	0.50	140,140,140,140	0
2	PO4	B	731	5/5	0.95	0.17	123,123,123,123	0
3	CL	A	734	1/1	0.95	0.16	102,102,102,102	0
2	PO4	C	730	5/5	0.95	0.10	125,125,125,125	0
2	PO4	A	731	5/5	0.96	0.12	124,124,124,124	0
2	PO4	B	730	5/5	0.97	0.10	112,112,112,112	0
3	CL	A	733	1/1	0.98	0.39	93,93,93,93	0
2	PO4	A	730	5/5	0.98	0.09	102,102,102,102	0
2	PO4	D	730	5/5	0.98	0.12	125,125,125,125	0
3	CL	B	732	1/1	0.99	0.07	69,69,69,69	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 EDT A 738:

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

Electron density around EDT D 735:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

6.5 Other polymers ⓘ

There are no such residues in this entry.