wwPDB X-ray Structure Validation Summary Report (i)

Sep 6, 2023 – 07:52 PM EDT

PDB ID	:	4F21
Title	:	Crystal structure of carboxylesterase/phospholipase family protein from Francisella tularensis
Authors	:	Filippova, E.V.; Minasov, G.; Kuhn, M.; Wawrzak, Z.; Shuvalova, L.; Dubrovska, I.; Winsor, J.R.; Kiryukhina, O.; Becker, D.P.; Armoush, N.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on	:	2012-05-07
Resolution	:	2.50 Å(reported)

The following versions of software and data (see references ①) were used in the production of this report:

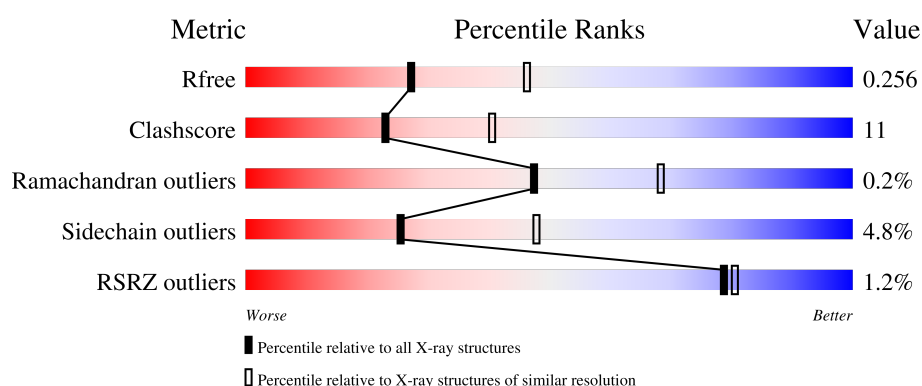|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.50 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		0.256
Clashscore		11
Ramachandran outliers		0.2%
Sidechain outliers		4.8%
RSRZ outliers		1.2%

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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	246	65% 22% • 12%
1	B	246	67% 22% • 11%
1	C	246	63% 24% • 11%
1	D	246	64% 24% • 11%
1	E	246	58% 25% 16%

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Mol	Chain	Length	Quality of chain
1	F	246	% 63% 18% • 17%
1	G	246	2% 60% 22% • 17%
1	H	246	3% 59% 22% • 17%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 13732 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 Carboxylesterase/phospholipase family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total 1701	C 1091	N 283	O 317	S 10	0	0	0
1	B	220	Total 1718	C 1101	N 285	O 321	S 11	0	0	0
1	C	220	Total 1718	C 1100	N 285	O 322	S 11	0	0	0
1	D	220	Total 1720	C 1101	N 286	O 322	S 11	0	0	0
1	E	206	Total 1607	C 1033	N 265	O 300	S 9	0	0	0
1	F	205	Total 1605	C 1030	N 267	O 298	S 10	0	1	0
1	G	204	Total 1598	C 1028	N 264	O 297	S 9	0	0	0
1	H	204	Total 1601	C 1032	N 264	O 296	S 9	0	0	0

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	expression tag	UNP Q5NI32
A	-22	HIS	-	expression tag	UNP Q5NI32
A	-21	HIS	-	expression tag	UNP Q5NI32
A	-20	HIS	-	expression tag	UNP Q5NI32
A	-19	HIS	-	expression tag	UNP Q5NI32
A	-18	HIS	-	expression tag	UNP Q5NI32
A	-17	HIS	-	expression tag	UNP Q5NI32
A	-16	SER	-	expression tag	UNP Q5NI32
A	-15	SER	-	expression tag	UNP Q5NI32
A	-14	GLY	-	expression tag	UNP Q5NI32
A	-13	VAL	-	expression tag	UNP Q5NI32
A	-12	ASP	-	expression tag	UNP Q5NI32
A	-11	LEU	-	expression tag	UNP Q5NI32

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	GLY	-	expression tag	UNP Q5NI32
A	-9	THR	-	expression tag	UNP Q5NI32
A	-8	GLU	-	expression tag	UNP Q5NI32
A	-7	ASN	-	expression tag	UNP Q5NI32
A	-6	LEU	-	expression tag	UNP Q5NI32
A	-5	TYR	-	expression tag	UNP Q5NI32
A	-4	PHE	-	expression tag	UNP Q5NI32
A	-3	GLN	-	expression tag	UNP Q5NI32
A	-2	SER	-	expression tag	UNP Q5NI32
A	-1	ASN	-	expression tag	UNP Q5NI32
A	0	ALA	-	expression tag	UNP Q5NI32
B	-23	MET	-	expression tag	UNP Q5NI32
B	-22	HIS	-	expression tag	UNP Q5NI32
B	-21	HIS	-	expression tag	UNP Q5NI32
B	-20	HIS	-	expression tag	UNP Q5NI32
B	-19	HIS	-	expression tag	UNP Q5NI32
B	-18	HIS	-	expression tag	UNP Q5NI32
B	-17	HIS	-	expression tag	UNP Q5NI32
B	-16	SER	-	expression tag	UNP Q5NI32
B	-15	SER	-	expression tag	UNP Q5NI32
B	-14	GLY	-	expression tag	UNP Q5NI32
B	-13	VAL	-	expression tag	UNP Q5NI32
B	-12	ASP	-	expression tag	UNP Q5NI32
B	-11	LEU	-	expression tag	UNP Q5NI32
B	-10	GLY	-	expression tag	UNP Q5NI32
B	-9	THR	-	expression tag	UNP Q5NI32
B	-8	GLU	-	expression tag	UNP Q5NI32
B	-7	ASN	-	expression tag	UNP Q5NI32
B	-6	LEU	-	expression tag	UNP Q5NI32
B	-5	TYR	-	expression tag	UNP Q5NI32
B	-4	PHE	-	expression tag	UNP Q5NI32
B	-3	GLN	-	expression tag	UNP Q5NI32
B	-2	SER	-	expression tag	UNP Q5NI32
B	-1	ASN	-	expression tag	UNP Q5NI32
B	0	ALA	-	expression tag	UNP Q5NI32
C	-23	MET	-	expression tag	UNP Q5NI32
C	-22	HIS	-	expression tag	UNP Q5NI32
C	-21	HIS	-	expression tag	UNP Q5NI32
C	-20	HIS	-	expression tag	UNP Q5NI32
C	-19	HIS	-	expression tag	UNP Q5NI32
C	-18	HIS	-	expression tag	UNP Q5NI32
C	-17	HIS	-	expression tag	UNP Q5NI32

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-16	SER	-	expression tag	UNP Q5NI32
C	-15	SER	-	expression tag	UNP Q5NI32
C	-14	GLY	-	expression tag	UNP Q5NI32
C	-13	VAL	-	expression tag	UNP Q5NI32
C	-12	ASP	-	expression tag	UNP Q5NI32
C	-11	LEU	-	expression tag	UNP Q5NI32
C	-10	GLY	-	expression tag	UNP Q5NI32
C	-9	THR	-	expression tag	UNP Q5NI32
C	-8	GLU	-	expression tag	UNP Q5NI32
C	-7	ASN	-	expression tag	UNP Q5NI32
C	-6	LEU	-	expression tag	UNP Q5NI32
C	-5	TYR	-	expression tag	UNP Q5NI32
C	-4	PHE	-	expression tag	UNP Q5NI32
C	-3	GLN	-	expression tag	UNP Q5NI32
C	-2	SER	-	expression tag	UNP Q5NI32
C	-1	ASN	-	expression tag	UNP Q5NI32
C	0	ALA	-	expression tag	UNP Q5NI32
D	-23	MET	-	expression tag	UNP Q5NI32
D	-22	HIS	-	expression tag	UNP Q5NI32
D	-21	HIS	-	expression tag	UNP Q5NI32
D	-20	HIS	-	expression tag	UNP Q5NI32
D	-19	HIS	-	expression tag	UNP Q5NI32
D	-18	HIS	-	expression tag	UNP Q5NI32
D	-17	HIS	-	expression tag	UNP Q5NI32
D	-16	SER	-	expression tag	UNP Q5NI32
D	-15	SER	-	expression tag	UNP Q5NI32
D	-14	GLY	-	expression tag	UNP Q5NI32
D	-13	VAL	-	expression tag	UNP Q5NI32
D	-12	ASP	-	expression tag	UNP Q5NI32
D	-11	LEU	-	expression tag	UNP Q5NI32
D	-10	GLY	-	expression tag	UNP Q5NI32
D	-9	THR	-	expression tag	UNP Q5NI32
D	-8	GLU	-	expression tag	UNP Q5NI32
D	-7	ASN	-	expression tag	UNP Q5NI32
D	-6	LEU	-	expression tag	UNP Q5NI32
D	-5	TYR	-	expression tag	UNP Q5NI32
D	-4	PHE	-	expression tag	UNP Q5NI32
D	-3	GLN	-	expression tag	UNP Q5NI32
D	-2	SER	-	expression tag	UNP Q5NI32
D	-1	ASN	-	expression tag	UNP Q5NI32
D	0	ALA	-	expression tag	UNP Q5NI32
E	-23	MET	-	expression tag	UNP Q5NI32

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-22	HIS	-	expression tag	UNP Q5NI32
E	-21	HIS	-	expression tag	UNP Q5NI32
E	-20	HIS	-	expression tag	UNP Q5NI32
E	-19	HIS	-	expression tag	UNP Q5NI32
E	-18	HIS	-	expression tag	UNP Q5NI32
E	-17	HIS	-	expression tag	UNP Q5NI32
E	-16	SER	-	expression tag	UNP Q5NI32
E	-15	SER	-	expression tag	UNP Q5NI32
E	-14	GLY	-	expression tag	UNP Q5NI32
E	-13	VAL	-	expression tag	UNP Q5NI32
E	-12	ASP	-	expression tag	UNP Q5NI32
E	-11	LEU	-	expression tag	UNP Q5NI32
E	-10	GLY	-	expression tag	UNP Q5NI32
E	-9	THR	-	expression tag	UNP Q5NI32
E	-8	GLU	-	expression tag	UNP Q5NI32
E	-7	ASN	-	expression tag	UNP Q5NI32
E	-6	LEU	-	expression tag	UNP Q5NI32
E	-5	TYR	-	expression tag	UNP Q5NI32
E	-4	PHE	-	expression tag	UNP Q5NI32
E	-3	GLN	-	expression tag	UNP Q5NI32
E	-2	SER	-	expression tag	UNP Q5NI32
E	-1	ASN	-	expression tag	UNP Q5NI32
E	0	ALA	-	expression tag	UNP Q5NI32
F	-23	MET	-	expression tag	UNP Q5NI32
F	-22	HIS	-	expression tag	UNP Q5NI32
F	-21	HIS	-	expression tag	UNP Q5NI32
F	-20	HIS	-	expression tag	UNP Q5NI32
F	-19	HIS	-	expression tag	UNP Q5NI32
F	-18	HIS	-	expression tag	UNP Q5NI32
F	-17	HIS	-	expression tag	UNP Q5NI32
F	-16	SER	-	expression tag	UNP Q5NI32
F	-15	SER	-	expression tag	UNP Q5NI32
F	-14	GLY	-	expression tag	UNP Q5NI32
F	-13	VAL	-	expression tag	UNP Q5NI32
F	-12	ASP	-	expression tag	UNP Q5NI32
F	-11	LEU	-	expression tag	UNP Q5NI32
F	-10	GLY	-	expression tag	UNP Q5NI32
F	-9	THR	-	expression tag	UNP Q5NI32
F	-8	GLU	-	expression tag	UNP Q5NI32
F	-7	ASN	-	expression tag	UNP Q5NI32
F	-6	LEU	-	expression tag	UNP Q5NI32
F	-5	TYR	-	expression tag	UNP Q5NI32

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-4	PHE	-	expression tag	UNP Q5NI32
F	-3	GLN	-	expression tag	UNP Q5NI32
F	-2	SER	-	expression tag	UNP Q5NI32
F	-1	ASN	-	expression tag	UNP Q5NI32
F	0	ALA	-	expression tag	UNP Q5NI32
G	-23	MET	-	expression tag	UNP Q5NI32
G	-22	HIS	-	expression tag	UNP Q5NI32
G	-21	HIS	-	expression tag	UNP Q5NI32
G	-20	HIS	-	expression tag	UNP Q5NI32
G	-19	HIS	-	expression tag	UNP Q5NI32
G	-18	HIS	-	expression tag	UNP Q5NI32
G	-17	HIS	-	expression tag	UNP Q5NI32
G	-16	SER	-	expression tag	UNP Q5NI32
G	-15	SER	-	expression tag	UNP Q5NI32
G	-14	GLY	-	expression tag	UNP Q5NI32
G	-13	VAL	-	expression tag	UNP Q5NI32
G	-12	ASP	-	expression tag	UNP Q5NI32
G	-11	LEU	-	expression tag	UNP Q5NI32
G	-10	GLY	-	expression tag	UNP Q5NI32
G	-9	THR	-	expression tag	UNP Q5NI32
G	-8	GLU	-	expression tag	UNP Q5NI32
G	-7	ASN	-	expression tag	UNP Q5NI32
G	-6	LEU	-	expression tag	UNP Q5NI32
G	-5	TYR	-	expression tag	UNP Q5NI32
G	-4	PHE	-	expression tag	UNP Q5NI32
G	-3	GLN	-	expression tag	UNP Q5NI32
G	-2	SER	-	expression tag	UNP Q5NI32
G	-1	ASN	-	expression tag	UNP Q5NI32
G	0	ALA	-	expression tag	UNP Q5NI32
H	-23	MET	-	expression tag	UNP Q5NI32
H	-22	HIS	-	expression tag	UNP Q5NI32
H	-21	HIS	-	expression tag	UNP Q5NI32
H	-20	HIS	-	expression tag	UNP Q5NI32
H	-19	HIS	-	expression tag	UNP Q5NI32
H	-18	HIS	-	expression tag	UNP Q5NI32
H	-17	HIS	-	expression tag	UNP Q5NI32
H	-16	SER	-	expression tag	UNP Q5NI32
H	-15	SER	-	expression tag	UNP Q5NI32
H	-14	GLY	-	expression tag	UNP Q5NI32
H	-13	VAL	-	expression tag	UNP Q5NI32
H	-12	ASP	-	expression tag	UNP Q5NI32
H	-11	LEU	-	expression tag	UNP Q5NI32

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-10	GLY	-	expression tag	UNP Q5NI32
H	-9	THR	-	expression tag	UNP Q5NI32
H	-8	GLU	-	expression tag	UNP Q5NI32
H	-7	ASN	-	expression tag	UNP Q5NI32
H	-6	LEU	-	expression tag	UNP Q5NI32
H	-5	TYR	-	expression tag	UNP Q5NI32
H	-4	PHE	-	expression tag	UNP Q5NI32
H	-3	GLN	-	expression tag	UNP Q5NI32
H	-2	SER	-	expression tag	UNP Q5NI32
H	-1	ASN	-	expression tag	UNP Q5NI32
H	0	ALA	-	expression tag	UNP Q5NI32

- Molecule 2 is N-((1R,2S)-2-allyl-4-oxocyclobutyl)-4-methylbenzenesulfonamide, bound form (three-letter code: 0S1) (formula: $C_{14}H_{19}NO_3S$).
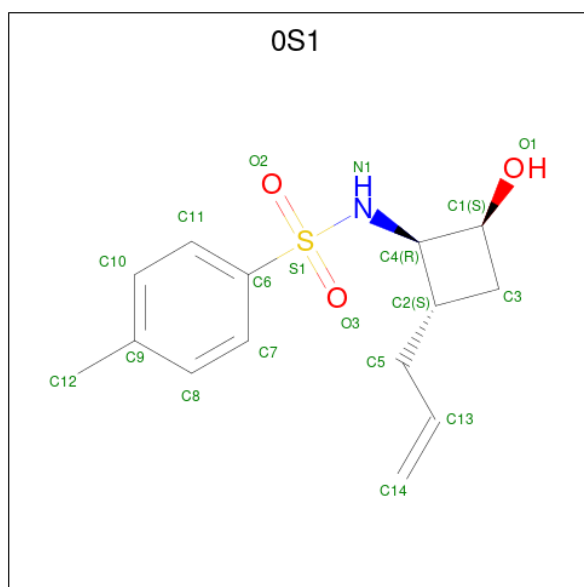
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total 5	C 4	O 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	66	Total 66	O 66	0	0
3	B	59	Total 59	O 59	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	87	Total 87	O 87	0	0
3	D	87	Total 87	O 87	0	0
3	E	47	Total 47	O 47	0	0
3	F	42	Total 42	O 42	0	0
3	G	37	Total 37	O 37	0	0
3	H	33	Total 34	O 34	1	1

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 proportio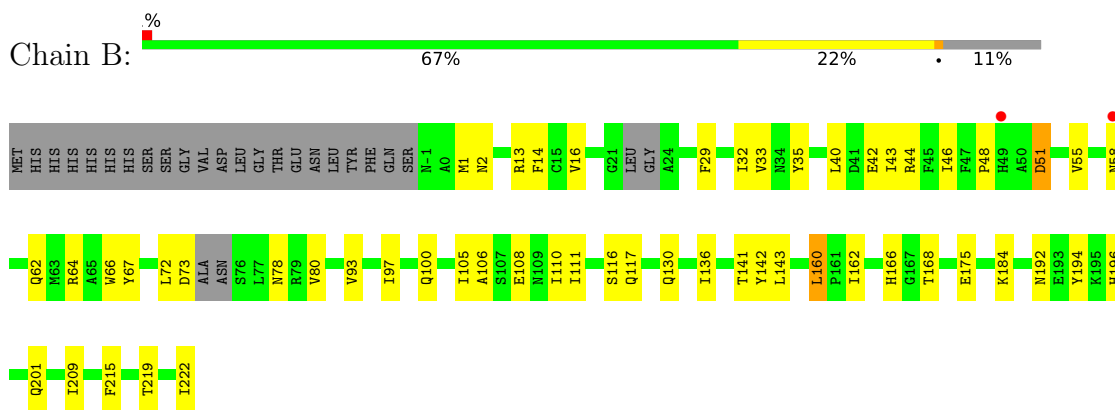ns of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 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: Carboxylesterase/phospholipase family protein

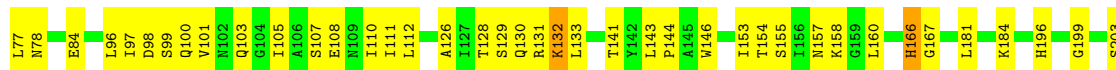- Molecule 1: Carboxylesterase/phospholipase family protein

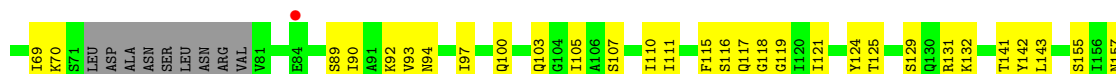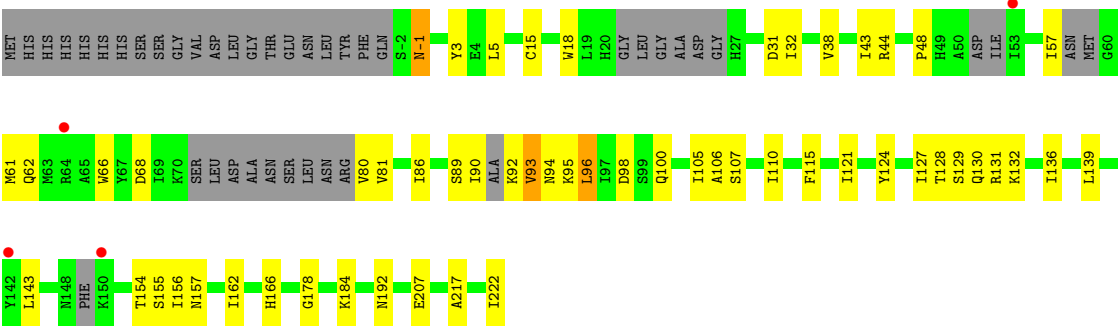- Molecule 1: Carboxylesterase/phospholipase family protein

G178 H179 G189 F190 A191 H196 Q201 H202 S203 K210 D211 I212 S213 N214 A217 K221 I222

• Molecule 1: Carboxylesterase/phospholipase family protein

Chain D: 64%   24%   •   11%

MET HIS HIS HIS HIS HIS SER SER GLY VAL ASP LEU GLY THR GLU ASN LEU TYR PHE GLN SER N-1 Y3 E4 W18 L19 H20 G21 LEU GLY A24 D31 L40 I43 P48 I53 M59 G60 M61 R64 A65 W66 Y67 D68 I69 D73 ALA ASN S76

L77 N78 E84 L96 I97 D98 S99 Q100 V101 N102 Q103 G104 I105 A106 S107 E108 N109 I110 I111 L112 A126 I127 T128 S129 Q130 R131 K132 L133 T141 Y142 L143 P144 A145 W146 I153 T154 S155 I156 N157 K158 G159 L160 H166 G167 L181 K184 H196 G199 S203

V204 K218 T219 F220 K221 I222

• Molecule 1: Carboxylesterase/phospholipase family protein

Chain E: 58%   25%   16%

MET HIS HIS HIS HIS HIS SER SER GLY VAL ASP LEU GLY THR GLU ASN LEU TYR PHE GLN S-2 Y3 E4 L5 M6 C15 V16 G21 L22 GLY ALA ASP G26 V38 S39 L40 I43 R44 F45 I46 F47 P48 I52 ILE PRO VAL THR ILE ASN MET G60 W66

I69 K70 S71 LEU ASP ALA ASN SER LEU ASN ARG VAL V81 E84 S89 I90 A91 K92 V93 N94 I97 Q100 Q103 G104 I105 A106 S107 I110 I111 F115 S116 Q117 G118 G119 I120 I121 Y124 T125 S129 Q130 R131 K132 T141 Y142 L143 S155 I156 N157

K158 G159 L160 P161 I162 L163 H166 D169 L173 K184 K195 H196 G199 C205 I209 S213 N214 F215 I216 T219 I222

• Molecule 1: Carboxylesterase/phospholipase family protein

Chain F: %   63%   18%   •   17%

MET HIS HIS HIS HIS HIS SER SER GLY VAL ASP LEU GLY THR GLU ASN LEU TYR PHE GLN S-2 Y3 E4 L5 M6 K10 R13 W18 L22 GLY ALA ASP G26 V38 F45 P48 I52 ILE PRO VAL THR ILE ASN M59 S71 LEU ASP ALA ASN

SER LEU ASN ARG VAL VAL ASP V83 N87 S88 S89 K92 V93 N94 K95 L96 I97 D98 I110 I111 L112 I121 A122 T125 Q130 R131 K132 M137 A138 L139 S140 T141 Y142 L143 P144 S155 I156 N157 K158 G159 L160 L163 H166 G167 L181 S182 D183 K184 L185

S188 G189 F190 E207 K210 D211 I212 F215 I216 A217 K218 T219 I222

• Molecule 1: Carboxylesterase/phospholipase family protein

Chain G: 2%   60%   22%   •   17%

MET HIS HIS HIS HIS HIS SER SER GLY VAL ASP LEU GLY THR GLU ASN LEU TYR PHE GLN S-2 N-1 Y3 E4 L5 C15 W18 L19 H20 GLY LEU GLY ALA ASP GLY H27 D31 I32 V38 I43 R44 P48 H49 A50 ASP ILE I53 I57 ASN MET G60

M61 Q62 M63 R64 A65 W66 Y67 D68 I69 K70 SER LEU ASP ALA ASN SER LEU ASN ARG V80 V81 I86 S89 I90 ALA K92 V93 N94 K95 L96 I97 D98 S99 Q100 I105 A106 S107 I110 F115 I121 Y124 I127 T128 S129 Q130 R131 K132 I136 L139

Y142 L143 N148 PHE K150 T154 S155 I156 N157 I162 H166 G178 K184 N192 E207 A217 I222

• Molecule 1: Carboxylesterase/phospholipase family protein

Chain H:

3%

59% 22% • 17%

MET HIS HIS HIS HIS HIS SER SER GLY VAL ASP LEU GLY THR GLU ASN LEU TYR PHE GLN S-2 N-1 Y3 E4 L5 M6 E7 P8 F14 C15 W18 G21 LEU GLY ALA ASP GLY H27 D31 I32 V33 V38 S39 L40 D41 R44 F45 P48 H49 A50 ASP

ILE I53 I57 ASN MET GLY MET GLN M63 D68 I69 K70 SER LEU ASP ALA ASN SER LEU ASN ARG V80 V81 S89 I90 V93 N94 K95 Q100 I105 N109 S116 Q117 I121 T125 S129 L133 L139 L143 P144 A145 W146 D147 N148 F149 K150

G151 I156 N157 L160 L163 V164 C165 H166 G167 T168 D169 D170 Q171 V172 L173 L181 E193 M200 Q201 H202 E207 K210 S213 A217 K218 T219 I222

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	51.00Å 64.42Å 139.04Å 94.89° 90.12° 89.96°	Depositor
Resolution (Å)	29.46 – 2.50 29.46 – 2.49	Depositor EDS
% Data completeness (in resolution range)	94.3 (29.46-2.50) 93.6 (29.46-2.49)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.29 (at 2.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.199 , 0.259 0.212 , 0.256	Depositor DCC
R_{free} test set	2922 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	33.0	Xtriage
Anisotropy	0.686	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 31.1	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.418 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13732	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 50.84 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.1070e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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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: 0S1

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	0.24	0/1732	0.42	0/2338
1	B	0.31	1/1751 (0.1%)	0.45	2/2367 (0.1%)
1	C	0.25	0/1751	0.46	0/2366
1	D	0.28	0/1753	0.48	0/2368
1	E	0.30	1/1638 (0.1%)	0.51	3/2210 (0.1%)
1	F	0.27	0/1636	0.46	1/2205 (0.0%)
1	G	0.26	0/1626	0.44	1/2191 (0.0%)
1	H	0.23	0/1632	0.44	0/2203
All	All	0.27	2/13519 (0.0%)	0.46	7/18248 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	201	GLN	C-N	7.37	1.51	1.34
1	E	199	GLY	C-N	-5.59	1.21	1.34

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	119	GLY	O-C-N	6.91	133.76	122.70
1	E	115	PHE	O-C-N	-6.26	112.68	122.70
1	G	93	VAL	N-CA-C	-5.48	96.21	111.00
1	E	119	GLY	CA-C-N	-5.39	105.33	117.20
1	F	160	LEU	CA-CB-CG	5.38	127.69	115.30

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	1701	0	1685	35	0
1	B	1718	0	1705	30	0
1	C	1718	0	1703	42	0
1	D	1720	0	1710	36	0
1	E	1607	0	1578	46	0
1	F	1605	0	1579	35	0
1	G	1598	0	1583	53	0
1	H	1601	0	1596	37	0
2	E	5	0	3	2	0
3	A	66	0	0	6	0
3	B	59	0	0	0	0
3	C	87	0	0	6	0
3	D	87	0	0	3	0
3	E	47	0	0	5	0
3	F	42	0	0	2	0
3	G	37	0	0	0	0
3	H	34	0	0	0	0
All	All	13732	0	13142	301	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 11.

The worst 5 of 301 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:H:80:VAL:HG12	1:H:81:VAL:N	1.65	1.06
1:F:141:THR:HG22	1:F:142:TYR:H	1.08	1.05
1:C:141:THR:HG22	1:C:142:TYR:H	1.18	1.05
1:C:141:THR:HG22	1:C:142:TYR:N	1.71	1.04
1:G:80:VAL:HG12	1:G:81:VAL:H	1.21	1.02

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	207/246 (84%)	189 (91%)	18 (9%)	0	100	100
1	B	214/246 (87%)	202 (94%)	12 (6%)	0	100	100
1	C	214/246 (87%)	199 (93%)	14 (6%)	1 (0%)	29	48
1	D	214/246 (87%)	199 (93%)	13 (6%)	2 (1%)	17	31
1	E	198/246 (80%)	186 (94%)	11 (6%)	1 (0%)	29	48
1	F	198/246 (80%)	178 (90%)	20 (10%)	0	100	100
1	G	190/246 (77%)	177 (93%)	13 (7%)	0	100	100
1	H	194/246 (79%)	179 (92%)	15 (8%)	0	100	100
All	All	1629/1968 (83%)	1509 (93%)	116 (7%)	4 (0%)	47	68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	0	ALA
1	D	69	ILE
1	E	69	ILE
1	D	144	PRO

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	184/211 (87%)	174 (95%)	10 (5%)	22	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	187/211 (89%)	178 (95%)	9 (5%)	25	48
1	C	187/211 (89%)	174 (93%)	13 (7%)	15	29
1	D	188/211 (89%)	176 (94%)	12 (6%)	17	33
1	E	171/211 (81%)	167 (98%)	4 (2%)	50	76
1	F	171/211 (81%)	160 (94%)	11 (6%)	17	33
1	G	173/211 (82%)	169 (98%)	4 (2%)	50	76
1	H	175/211 (83%)	168 (96%)	7 (4%)	31	56
All	All	1436/1688 (85%)	1366 (95%)	70 (5%)	25	47

5 of 70 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	160	LEU
1	G	-1	ASN
1	H	68	ASP
1	C	83	VAL
1	C	62	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	B	201	GLN
1	D	157	ASN
1	E	196	HIS
1	G	94	ASN

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 (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	0S1	E	301	1	3,5,20	0.32	0	3,6,29	3.37	2 (66%)

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
2	0S1	E	301	1	-	-	0/1/1/2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

| Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	301	0S1	O1-C1-C4	-4.44	110.98	119.15
2	E	301	0S1	O1-C1-C3	-3.68	112.36	119.15

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	301	0S1	2	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 0S1 E 301
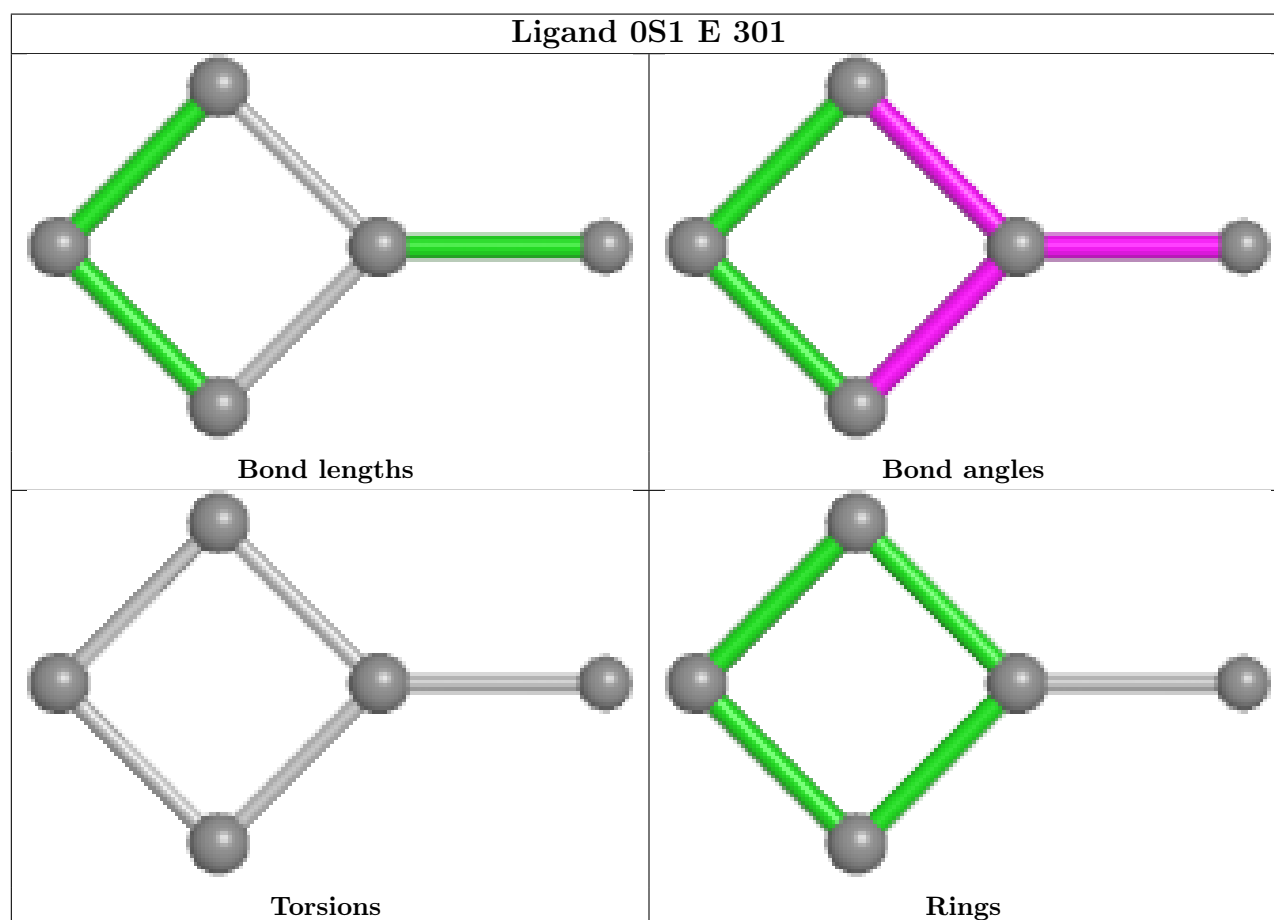
5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	217/246 (88%)	-0.46	3 (1%)	75	77	17, 45, 79, 131	0
1	B	220/246 (89%)	-0.55	2 (0%)	84	86	16, 43, 85, 162	0
1	C	220/246 (89%)	-0.65	1 (0%)	91	91	5, 37, 62, 103	0
1	D	220/246 (89%)	-0.70	0	100	100	7, 32, 59, 83	0
1	E	206/246 (83%)	-0.61	1 (0%)	91	91	15, 43, 75, 126	0
1	F	205/246 (83%)	-0.61	2 (0%)	82	84	12, 42, 73, 111	0
1	G	204/246 (82%)	-0.37	4 (1%)	65	68	24, 50, 88, 113	0
1	H	204/246 (82%)	-0.24	7 (3%)	45	48	20, 56, 103, 163	0
All	All	1696/1968 (86%)	-0.53	20 (1%)	79	80	5, 44, 83, 163	0

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	49	HIS	3.8
1	H	149	PHE	3.6
1	H	151	GLY	3.6
1	A	72	LEU	3.6
1	B	58	ASN	3.5

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

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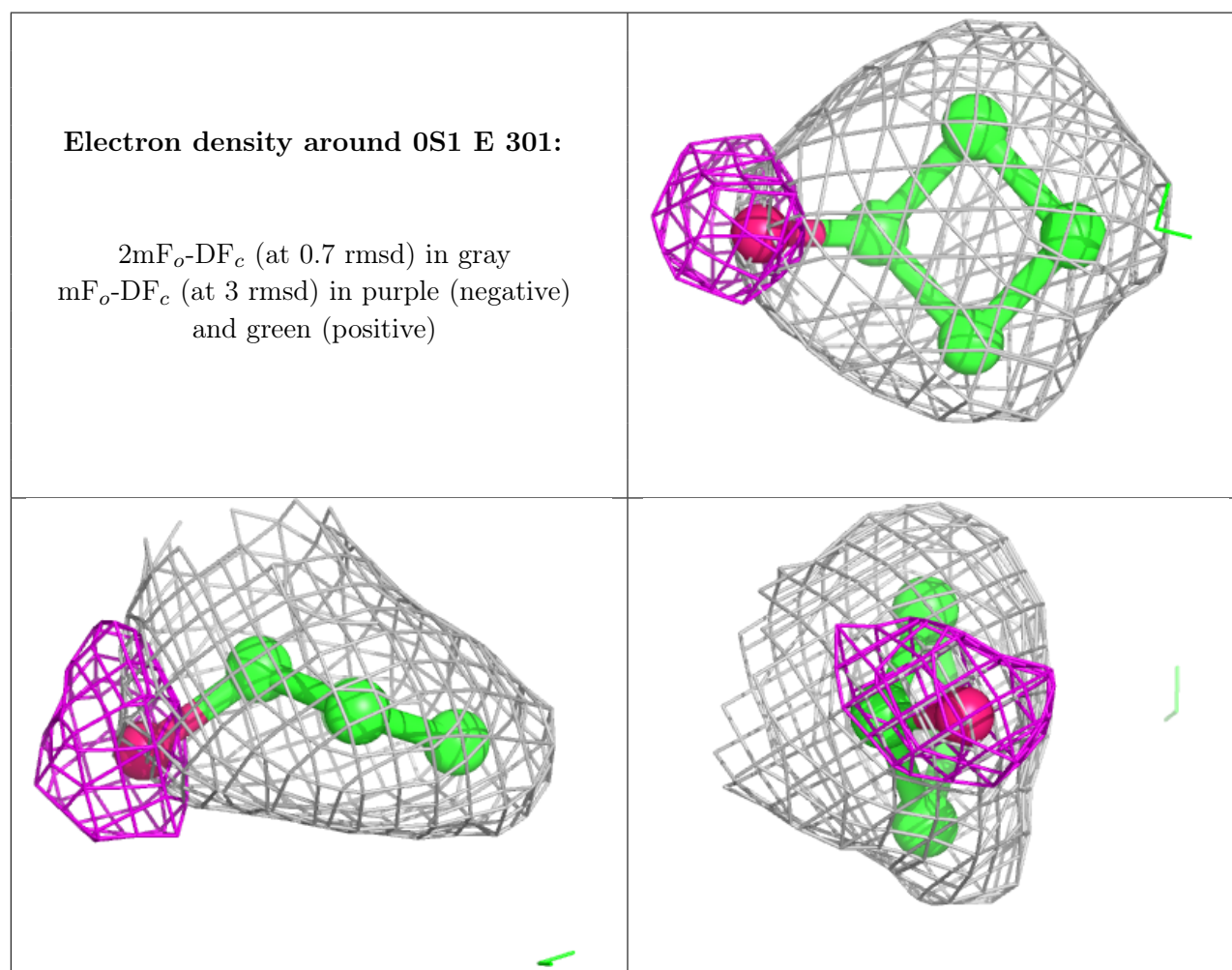
6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4   Ligands (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($Å^2$)	Q<0.9
2	0S1	E	301	5/19	0.91	0.16	17,28,38,46	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 0S1 E 301:

$2mF_o$-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.