WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Jun 11, 2024 – 02:52 PM EDT

PDB ID	:	6MIT
Title	:	LptBFGC from Enterobacter cloacae
Authors	:	Owens, T.W.; Kahne, D.; Kruse, A.C.
Deposited on	:	2018-09-20
Resolution	:	3.20 Å(reported)

The following versions of software and data (see references (i)) 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	:	2.36.2
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)	:	2.36.2

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 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
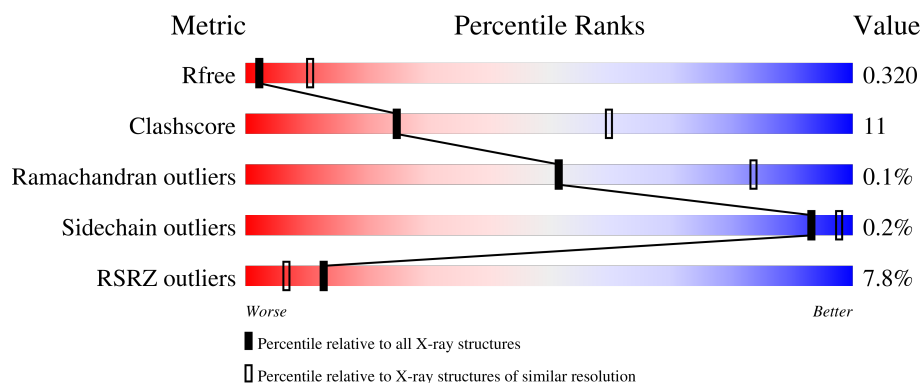
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	241	5% / 78% / 22%
1	B	241	8% / 76% / 24%
1	D	241	2% / 69% / 31%
1	E	241	12% / 77% / 22% / ·
2	C	195	8% / 67% / 23% / 10%

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Mol	Chain	Length	Quality of chain
2	H	195	14% / 64% / 26% / 10%
3	F	366	5% / 74% / 22% / ·
3	I	366	5% / 72% / 20% / 8%
4	G	360	6% / 77% / 22% / ·
4	J	360	11% / 65% / 21% / 14%

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
5	SO4	G	403	-	-	X	-
6	CL	A	303	-	-	-	X

2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 19733 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 Lipopolysaccharide export system ATP-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	240	Total	C	N	O	S	0	0	0
			1802	1134	323	341	4			
1	B	240	Total	C	N	O	S	0	0	0
			1792	1128	319	341	4			
1	D	240	Total	C	N	O	S	0	0	0
			1814	1144	326	340	4			
1	E	238	Total	C	N	O	S	0	0	0
			1736	1091	304	337	4			

- Molecule 2 is a protein called Lipopolysaccharide export system protein LptC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	175	Total	C	N	O	S	0	0	0
			1336	846	224	263	3			
2	H	175	Total	C	N	O	S	0	0	0
			1324	839	223	259	3			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	192	LEU	-	expression tag	UNP A0A0H3CU18
C	193	VAL	-	expression tag	UNP A0A0H3CU18
C	194	PRO	-	expression tag	UNP A0A0H3CU18
C	195	ARG	-	expression tag	UNP A0A0H3CU18
H	192	LEU	-	expression tag	UNP A0A0H3CU18
H	193	VAL	-	expression tag	UNP A0A0H3CU18
H	194	PRO	-	expression tag	UNP A0A0H3CU18
H	195	ARG	-	expression tag	UNP A0A0H3CU18

- Molecule 3 is a protein called LPS export ABC transporter permease LptF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	350	Total 2581	C 1679	N 425	O 460	S 17	0	0	0
3	I	335	Total 2435	C 1591	N 394	O 434	S 16	0	0	0

- Molecule 4 is a protein called Lipopolysaccharide export system permease protein LptG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	355	Total 2619	C 1708	N 426	O 468	S 17	0	0	0
4	J	309	Total 2186	C 1427	N 355	O 389	S 15	0	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
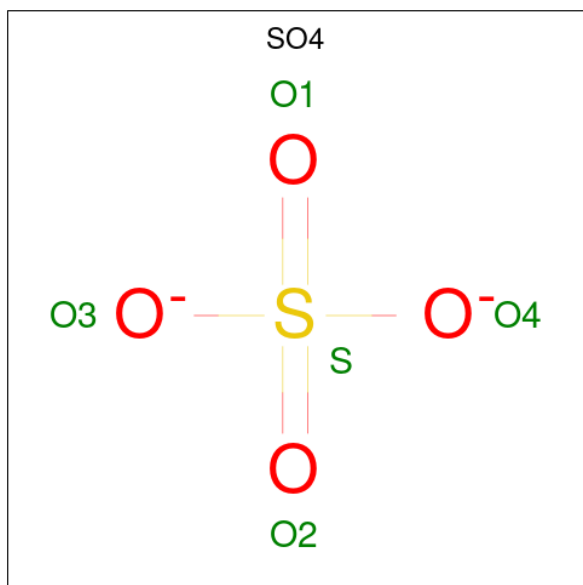
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 5	O 4	S 1	0	0
5	A	1	Total 5	O 4	S 1	0	0
5	B	1	Total 5	O 4	S 1	0	0
5	F	1	Total 5	O 4	S 1	0	0
5	G	1	Total 5	O 4	S 1	0	0
5	G	1	Total 5	O 4	S 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	G	1	Total 5	O 4	S 1	0	0
5	D	1	Total 5	O 4	S 1	0	0
5	E	1	Total 5	O 4	S 1	0	0
5	J	1	Total 5	O 4	S 1	0	0
5	J	1	Total 5	O 4	S 1	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total 1	Cl 1	0	0

- Molecule 7 is NOVOBIOCIN (three-letter code: NOV) (formula: $C_{31}H_{36}N_2O_{11}$).
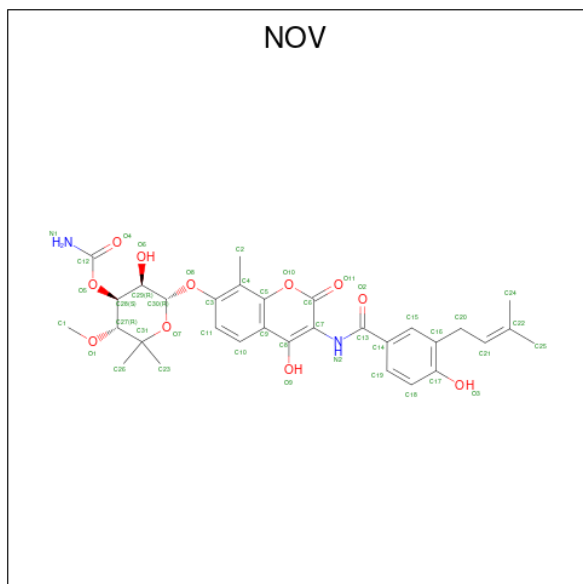
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	E	1	Total 44	C 31	N 2	O 11	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	3	Total 3	O 3	0	0
8	B	2	Total 2	O 2	0	0
8	D	2	Total 2	O 2	0	0
8	E	1	Total 1	O 1	0	0

3 Residue-property plots ⓘ

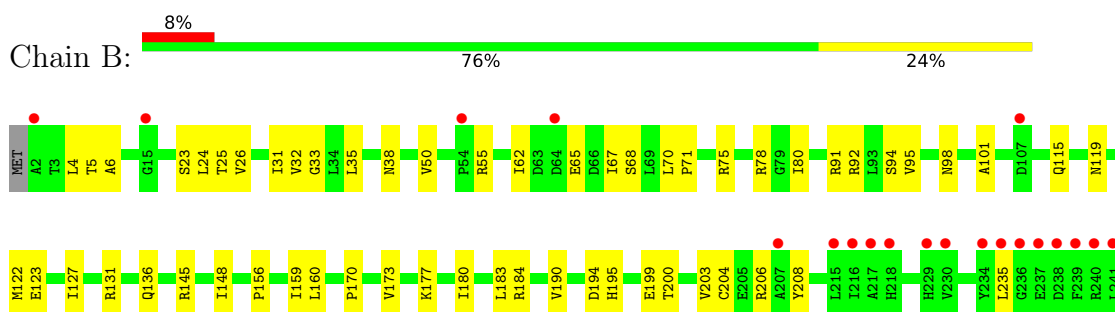These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Lipopolysaccharide export system ATP-binding protein

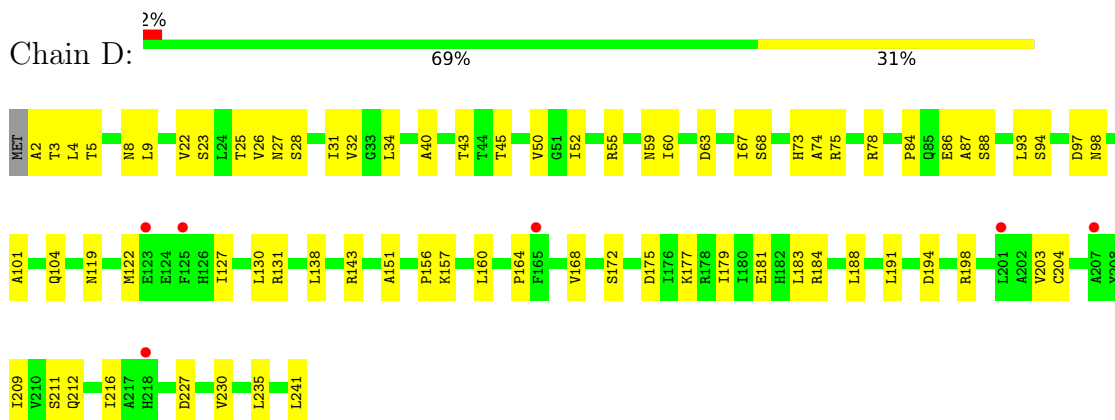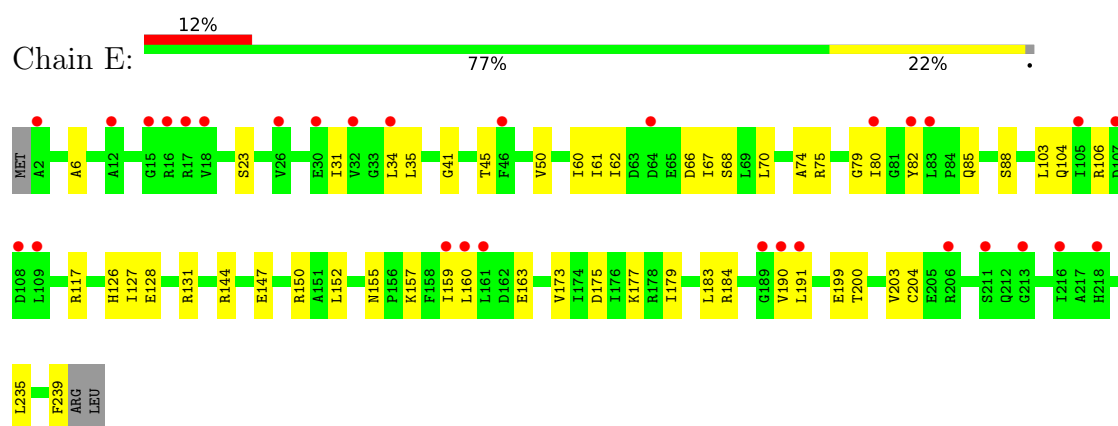- Molecule 1: Lipopolysaccharide export system ATP-binding protein

- Molecule 1: Lipopolysaccharide export system ATP-binding protein

- Molecule 1: Lipopolysaccharide export system ATP-binding protein

Chain E:
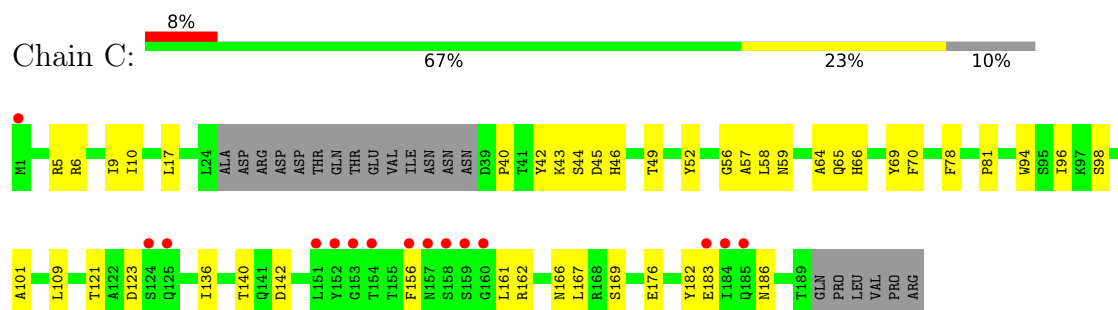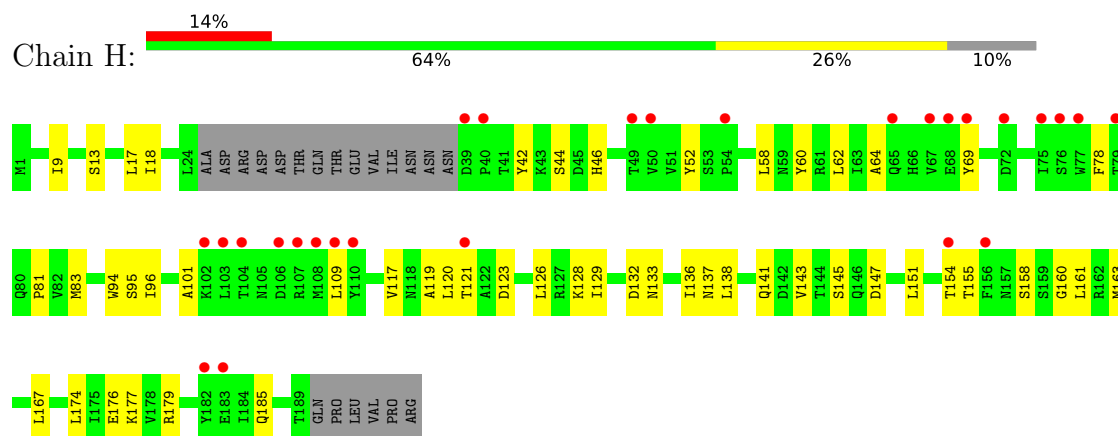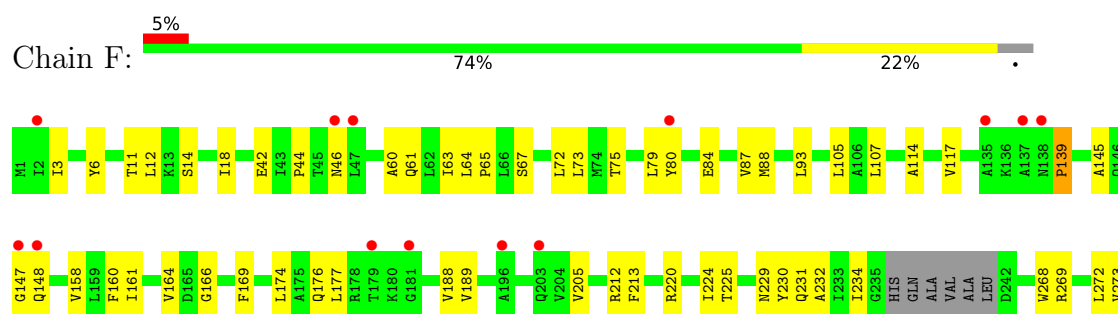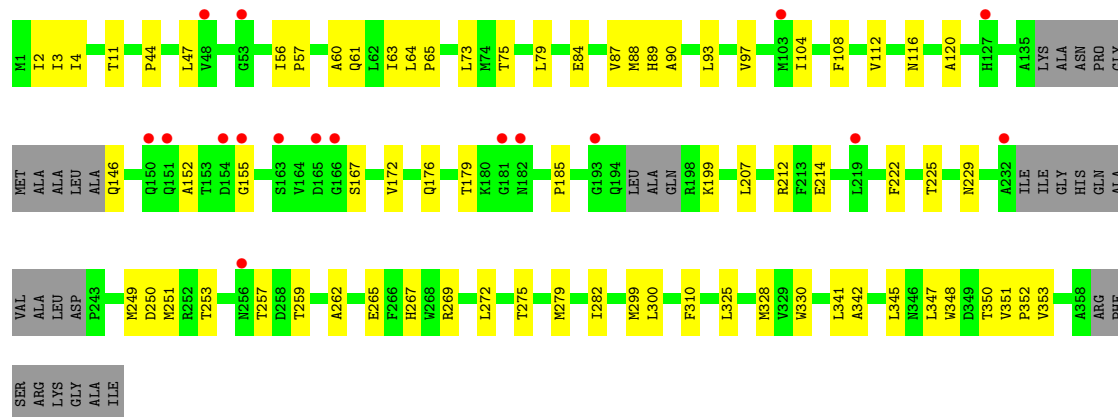

• Molecule 2: Lipopolysaccharide export system protein LptC

Chain C:

• Molecule 2: Lipopolysaccharide export system protein LptC

Chain H:
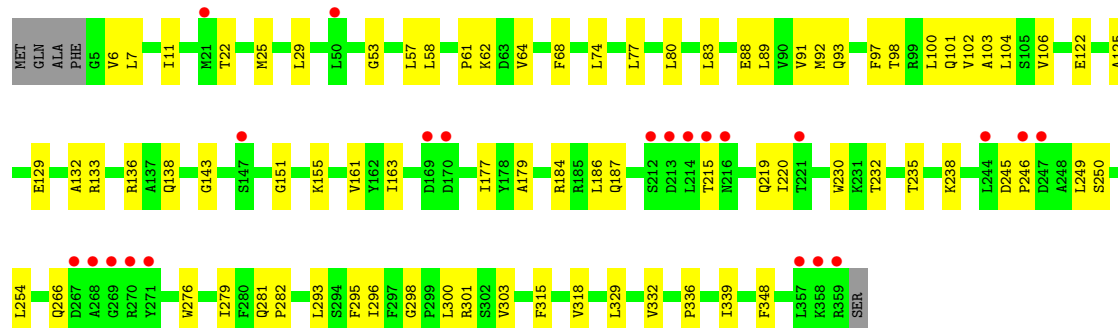

• Molecule 3: LPS export ABC transporter permease LptF

Chain F:

F274 T275 V276 F277 M278 M279 I282 P285 V288 M299 L300 P301 Y306 F310 N319 D326 V329 Y338 L341 L345 N346 L347 W348 D349 T350 V351 P352 V353 I356 ARG ALA ARG PHE SER ARG GLY ALA ILE

● Molecule 3: LPS export ABC transporter permease LptF

Chain I:

M1 I2 I3 I4 T11 P44 L47 V48 G53 I56 P57 A60 Q61 L62 I63 L64 P65 L73 M74 T75 L79 E84 V87 M88 H89 A90 L93 V97 M103 I104 F108 V112 N116 A120 H127 A135 LYS ALA ASN PRO GLY

MET ALA ALA LEU ALA Q146 Q150 Q151 A152 T153 D154 G155 S163 V164 D165 G166 S167 V172 Q176 T179 K180 G181 N182 P185 G193 Q194 LEU ALA GLN R198 K199 L207 R212 F213 E214 L219 F222 T225 N229 A232 ILE ILE GLY HIS GLN ALA

VAL ALA LEU ASP P243 M249 D250 M251 R252 T253 N256 T257 D258 T259 A262 E265 F266 H267 W268 R269 L272 T275 M279 I282 M299 L300 F310 L325 M328 V329 W330 L341 A342 L345 N346 L347 W348 D349 T350 V351 P352 V353 A358 ARG PHE

SER ARG LYS ALA ILE

● Molecule 4: Lipopolysaccharide export system permease protein LptG

Chain G:

MET GLN ALA PHE G5 V6 L7 I11 M21 T22 M25 L29 I50 G53 L57 L58 P61 K62 D63 V64 F68 L74 L77 L80 L83 E88 L89 V90 V91 M92 Q93 F97 T98 R99 L100 Q101 V102 A103 L104 S105 V106 E122 A125

E129 A132 R133 R136 A137 Q138 G143 S147 G151 K155 V161 Y162 I163 D169 D170 I177 Y178 A179 R184 R185 L186 Q187 S212 D213 L214 T215 N216 Q219 I220 I221 W230 K231 T232 T235 K238 L244 D245 P246 D247 A248 L249 S250

L254 Q266 D267 A268 C269 R270 Y271 W276 I279 F280 Q281 P282 L293 S294 F295 I296 F297 G298 P299 L300 R301 S302 V303 F315 V318 L329 V332 P336 I339 F348 L357 K358 R359 SER

● Molecule 4: Lipopolysaccharide export system permease protein LptG

Chain J:

MET Q2 V6 L7 I11 L23 F24 M25 L26 V27 S28 L29 K34 F35 V36 D37 Q38 G43 S46 G53 M54 Y55 T56 L57 L58 P61 V64 M70 L73 L74 L80 E88 L89 V90 V91 M92 Q93 F97 L100 Q101 V102 A103 L104 S105 V106

T109 V114 T117 E122 W123 P126 Q127 Q130 M131 A132 R133 N134 Y135 R136 A137 Q138 A139 M140 TYR GLY GLY SER LEU LEU SER THR GLN GLN G151 L152 W153 V161 E164 ARG VAL LYS GLY ASP ASP GLU LEU GLY GLY VAL S176 I177 N181 ASP GLU ARG ARG

L186 Q187 S188 A192 SER SER ALA LYS PHE ASP PRO GLU HIS LYS GLN TRP ARG LEU SER GLN V209 D210 E211 S212 D213 L214 T215 N216 P217 K218 Q219 I220 T221 V226 SER GLY THR TRP LYS T232 L239 V242 D247 A248 L249 S252 H255 N256 Y257 V258 K259 Y260 L261

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α, β, γ	116.43Å 156.98Å 295.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.33 – 3.20 49.33 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.33-3.20) 99.3 (49.33-3.20)	Depositor EDS
R_{merge}	0.48	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.08 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.279 , 0.320 0.279 , 0.320	Depositor DCC
R_{free} test set	1641 reflections (1.83%)	wwPDB-VP
Wilson B-factor (Å^2)	111.8	Xtriage
Anisotropy	0.322	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 85.1	EDS
L-test for twinning [2]	$< |L| > = 0.44, < L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	19733	wwPDB-VP
Average B, all atoms (Å^2)	136.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, SO4, NOV

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	0.39	0/1828	0.58	0/2483
1	B	0.38	0/1818	0.61	0/2470
1	D	0.42	0/1840	0.61	0/2496
1	E	0.33	0/1761	0.52	0/2400
2	C	0.45	0/1359	0.65	0/1857
2	H	0.39	0/1346	0.59	0/1841
3	F	0.42	0/2627	0.61	0/3586
3	I	0.36	0/2476	0.56	0/3381
4	G	0.36	0/2675	0.57	0/3642
4	J	0.37	0/2224	0.53	0/3026
All	All	0.38	0/19954	0.58	0/27182

There are no bond length outliers.

There are no bond angle outliers.

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	1802	0	1771	40	0
1	B	1792	0	1743	42	0
1	D	1814	0	1809	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1736	0	1647	39	0
2	C	1336	0	1269	36	0
2	H	1324	0	1258	37	0
3	F	2581	0	2574	62	0
3	I	2435	0	2409	48	0
4	G	2619	0	2602	59	0
4	J	2186	0	2118	49	0
5	A	10	0	0	0	0
5	B	5	0	0	0	0
5	D	5	0	0	1	0
5	E	5	0	0	0	0
5	F	5	0	0	0	0
5	G	15	0	0	2	0
5	J	10	0	0	1	0
6	A	1	0	0	0	0
7	E	44	0	34	3	0
8	A	3	0	0	0	0
8	B	2	0	0	0	0
8	D	2	0	0	0	0
8	E	1	0	0	0	0
All	All	19733	0	19234	422	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 422 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)
4:G:136:ARG:NH1	5:G:403:SO4:O3	2.06	0.88
2:H:58:LEU:HD23	4:J:218:LYS:HB3	1.52	0.87
1:B:94:SER:O	1:B:98:ASN:ND2	2.13	0.81
2:H:9:ILE:HD13	3:I:300:LEU:HD23	1.63	0.79
1:D:181:GLU:OE1	1:D:184:ARG:NH2	2.19	0.75

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	238/241 (99%)	221 (93%)	16 (7%)	1 (0%)	34	69
1	B	238/241 (99%)	221 (93%)	17 (7%)	0	100	100
1	D	238/241 (99%)	219 (92%)	19 (8%)	0	100	100
1	E	236/241 (98%)	225 (95%)	11 (5%)	0	100	100
2	C	171/195 (88%)	160 (94%)	11 (6%)	0	100	100
2	H	171/195 (88%)	159 (93%)	12 (7%)	0	100	100
3	F	346/366 (94%)	328 (95%)	17 (5%)	1 (0%)	41	74
3	I	327/366 (89%)	313 (96%)	14 (4%)	0	100	100
4	G	353/360 (98%)	338 (96%)	15 (4%)	0	100	100
4	J	295/360 (82%)	284 (96%)	11 (4%)	0	100	100
All	All	2613/2806 (93%)	2468 (94%)	143 (6%)	2 (0%)	51	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F	139	PRO
1	A	71	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	183/202 (91%)	182 (100%)	1 (0%)	88	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	179/202 (89%)	179 (100%)	0	100	100
1	D	187/202 (93%)	186 (100%)	1 (0%)	88	95
1	E	170/202 (84%)	170 (100%)	0	100	100
2	C	141/179 (79%)	140 (99%)	1 (1%)	84	94
2	H	138/179 (77%)	138 (100%)	0	100	100
3	F	261/307 (85%)	261 (100%)	0	100	100
3	I	242/307 (79%)	242 (100%)	0	100	100
4	G	266/300 (89%)	265 (100%)	1 (0%)	91	95
4	J	209/300 (70%)	209 (100%)	0	100	100
All	All	1976/2380 (83%)	1972 (100%)	4 (0%)	93	98

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ILE
2	C	183	GLU
4	G	68	PHE
1	D	52	ILE

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

Mol	Chain	Res	Type
1	B	38	ASN
1	B	195	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 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 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	SO4	A	302	-	4,4,4	0.19	0	6,6,6	0.69	0
7	NOV	E	302	-	47,47,47	1.69	7 (14%)	66,70,70	1.52	11 (16%)
5	SO4	G	402	-	4,4,4	0.30	0	6,6,6	0.88	0
5	SO4	E	301	-	4,4,4	0.20	0	6,6,6	0.29	0
5	SO4	G	401	-	4,4,4	0.20	0	6,6,6	0.44	0
5	SO4	G	403	-	4,4,4	0.17	0	6,6,6	0.23	0
5	SO4	A	301	-	4,4,4	0.17	0	6,6,6	0.20	0
5	SO4	B	301	-	4,4,4	0.14	0	6,6,6	0.26	0
5	SO4	D	301	-	4,4,4	0.16	0	6,6,6	0.69	0
5	SO4	J	401	-	4,4,4	0.11	0	6,6,6	0.66	0
5	SO4	F	401	-	4,4,4	0.20	0	6,6,6	0.42	0
5	SO4	J	402	-	4,4,4	0.22	0	6,6,6	0.44	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
7	NOV	E	302	-	-	6/23/46/46	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	302	NOV	O7-C31	-6.70	1.38	1.45
7	E	302	NOV	C28-C27	3.48	1.59	1.52
7	E	302	NOV	C12-N1	3.39	1.40	1.33
7	E	302	NOV	O7-C30	-3.37	1.36	1.42
7	E	302	NOV	C9-C8	-3.21	1.40	1.45

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	E	302	NOV	C20-C21-C22	-3.68	123.11	127.59
7	E	302	NOV	C5-O10-C6	-3.09	119.14	122.68
7	E	302	NOV	C2-C4-C3	3.00	125.19	120.69
7	E	302	NOV	C6-C7-N2	2.99	118.50	112.39
7	E	302	NOV	O7-C30-C29	-2.92	104.55	110.42

There are no chirality outliers.

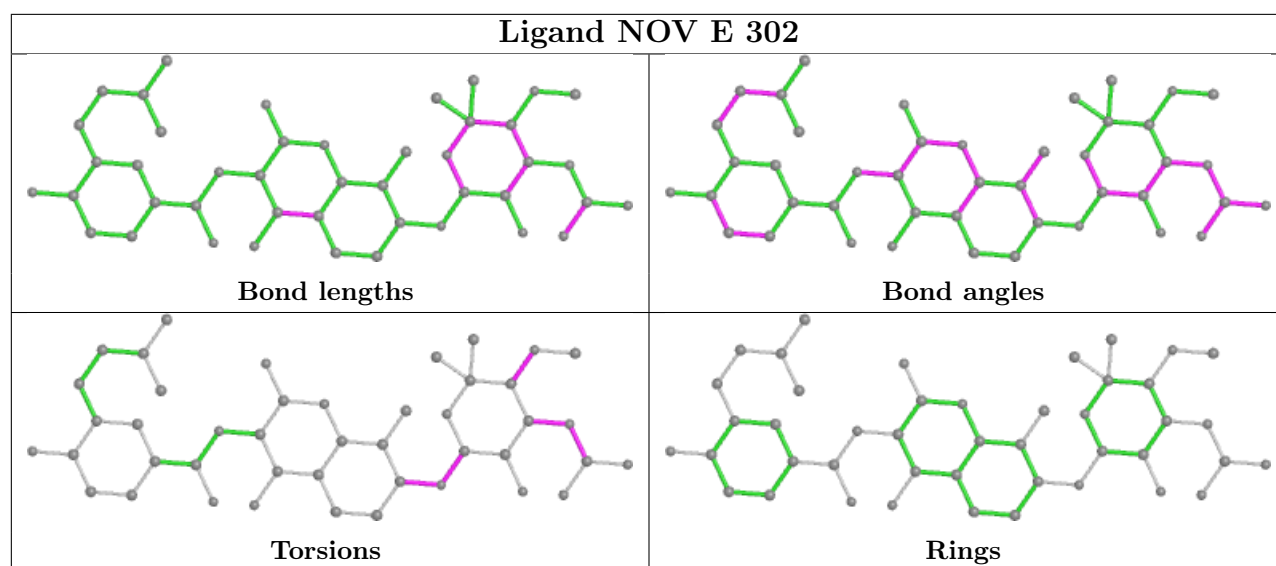5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	E	302	NOV	N1-C12-O5-C28
7	E	302	NOV	O4-C12-O5-C28
7	E	302	NOV	C27-C28-O5-C12
7	E	302	NOV	O7-C30-O8-C3
7	E	302	NOV	C4-C3-O8-C30

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	302	NOV	3	0
5	G	403	SO4	2	0
5	D	301	SO4	1	0
5	J	402	SO4	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 NOV E 302

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(Å²)	Q<0.9
1	A	240/241 (99%)	0.19	11 (4%)	32	20	99, 132, 164, 180	0
1	B	240/241 (99%)	0.40	20 (8%)	11	6	93, 139, 173, 202	0
1	D	240/241 (99%)	0.13	6 (2%)	57	43	86, 120, 148, 170	0
1	E	238/241 (98%)	0.52	30 (12%)	3	2	106, 144, 181, 195	0
2	C	175/195 (89%)	0.16	15 (8%)	10	5	88, 130, 159, 173	0
2	H	175/195 (89%)	0.55	27 (15%)	2	1	95, 142, 189, 203	0
3	F	350/366 (95%)	0.27	19 (5%)	25	14	78, 123, 177, 211	0
3	I	335/366 (91%)	0.15	17 (5%)	28	16	93, 134, 195, 229	0
4	G	355/360 (98%)	0.25	22 (6%)	20	11	89, 131, 175, 203	0
4	J	309/360 (85%)	0.57	39 (12%)	3	2	94, 154, 199, 225	0
All	All	2657/2806 (94%)	0.31	206 (7%)	13	7	78, 134, 186, 229	0

The worst 5 of 206 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	J	263	SER	15.1
4	J	264	SER	11.0
4	J	215	THR	9.7
4	J	212	SER	7.8
4	J	262	LYS	7.6

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

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

WORLDWIDE
wwPDB
PROTEIN DATA BANK
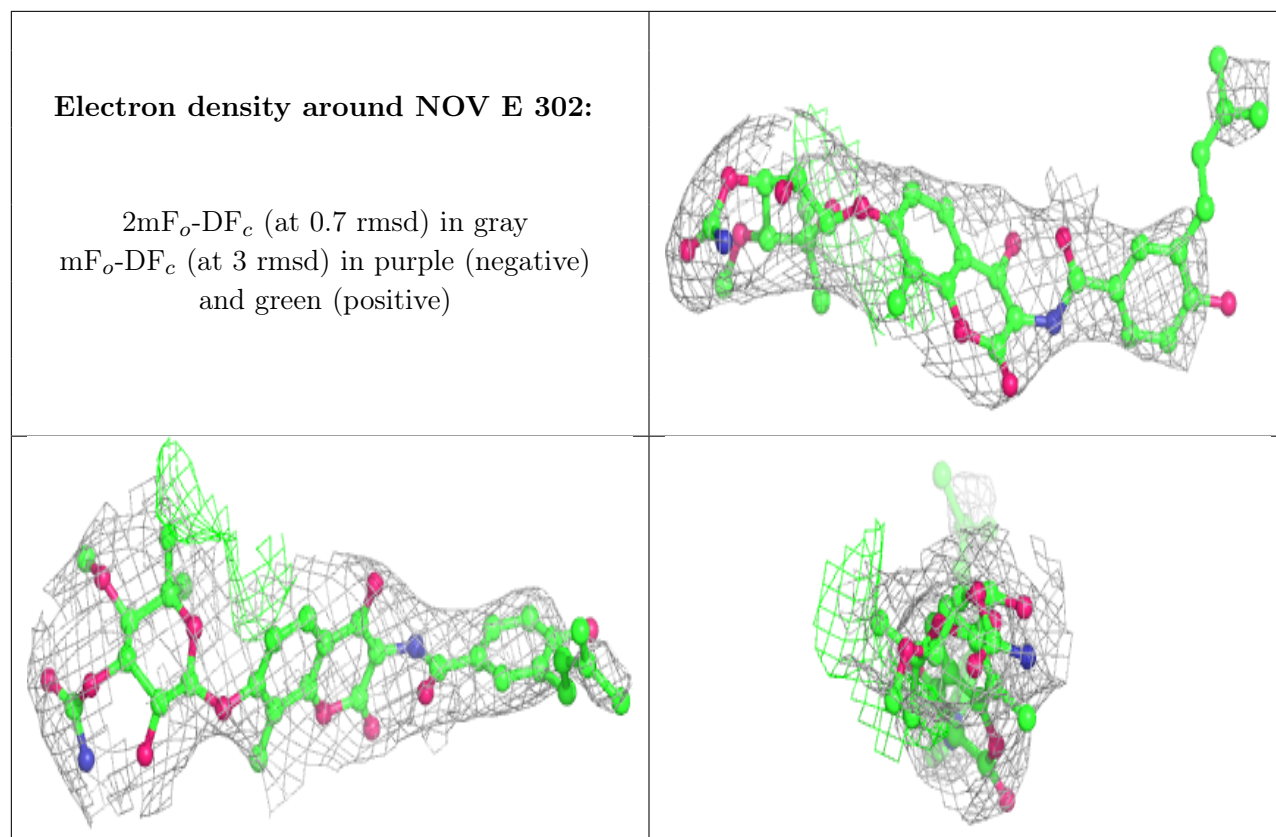
6.3 Carbohydrates ⓘ

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
6	CL	A	303	1/1	0.07	0.80	195,195,195,195	0
7	NOV	E	302	44/44	0.81	0.34	102,152,167,171	0
5	SO4	A	301	5/5	0.84	0.21	152,153,159,175	0
5	SO4	B	301	5/5	0.87	0.14	144,149,163,166	0
5	SO4	F	401	5/5	0.89	0.16	107,115,139,139	0
5	SO4	J	402	5/5	0.90	0.17	109,136,140,141	0
5	SO4	G	403	5/5	0.92	0.12	151,156,173,177	0
5	SO4	G	401	5/5	0.92	0.12	128,130,146,153	0
5	SO4	E	301	5/5	0.93	0.11	142,159,167,168	0
5	SO4	A	302	5/5	0.96	0.13	117,136,145,146	0
5	SO4	D	301	5/5	0.96	0.37	114,118,127,133	0
5	SO4	G	402	5/5	0.96	0.42	81,90,116,131	0
5	SO4	J	401	5/5	0.97	0.20	105,108,118,141	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 NOV E 302:

$2mF_o$-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.