Full wwPDB X-ray Structure Validation Report (i)

Oct 22, 2023 – 03:38 PM EDT

PDB ID	:	2Z93
Title	:	Crystal structure of Fab fragment of anti-ciguatoxin antibody 10C9 in complex with CTX3C-ABCD
Authors	:	Ui, M.; Tanaka, Y.; Tsumoto, K.
Deposited on	:	2007-09-14
Resolution	:	2.40 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
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
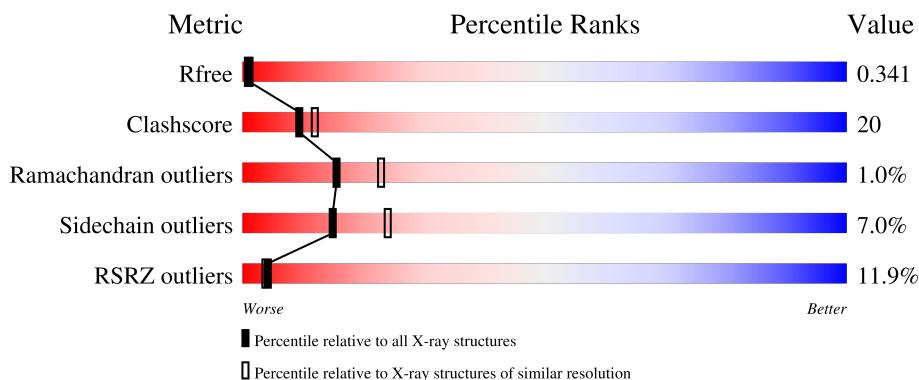
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
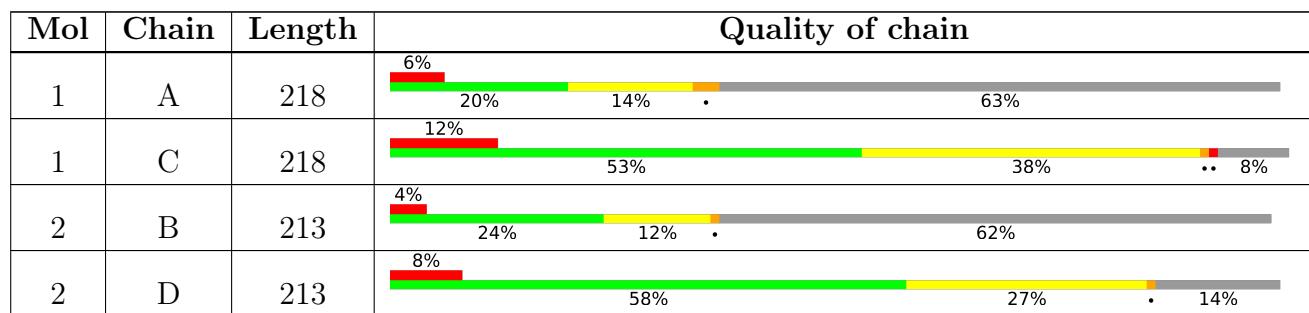
The reported resolution of this entry is 2.40 Å.

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		0.341
Clashscore		20
Ramachandran outliers		1.0%
Sidechain outliers		7.0%
RSRZ outliers		11.9%

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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	218	6% 20% 14% · 63%
1	C	218	12% 53% 38% ·· 8%
2	B	213	4% 24% 12% · 62%
2	D	213	8% 58% 27% · 14%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 4307 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.
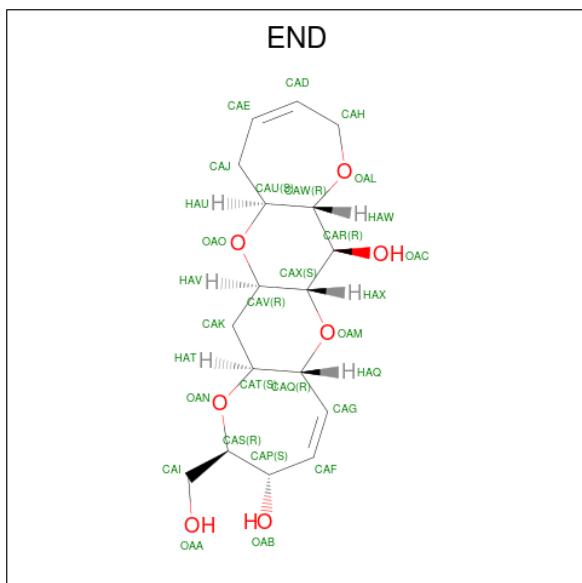
- Molecule 1 is a protein called Anti-ciguatoxin antibody 10C9 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	81	Total	C	N	O	S	0	0	0
			594	383	93	116	2			
1	C	201	Total	C	N	O	S	0	0	0
			1565	998	254	307	6			

- Molecule 2 is a protein called Anti-ciguatoxin antibody 10C9 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	80	Total	C	N	O	S	0	0	0
			623	389	106	125	3			
2	D	184	Total	C	N	O	S	0	0	0
			1380	859	226	286	9			

- Molecule 3 is 1,6:5,9:8,12:11,16-TETRAANHYDRO-2,3,4,10,13,14-HEXADEOXY-D-G LYCERO-D-ALLO-D-GULO-HEPTADECA-2,13-DIENITOL (three-letter code: END) (formula: $C_{17}H_{24}O_7$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total 24	C 17	O 7	0	0
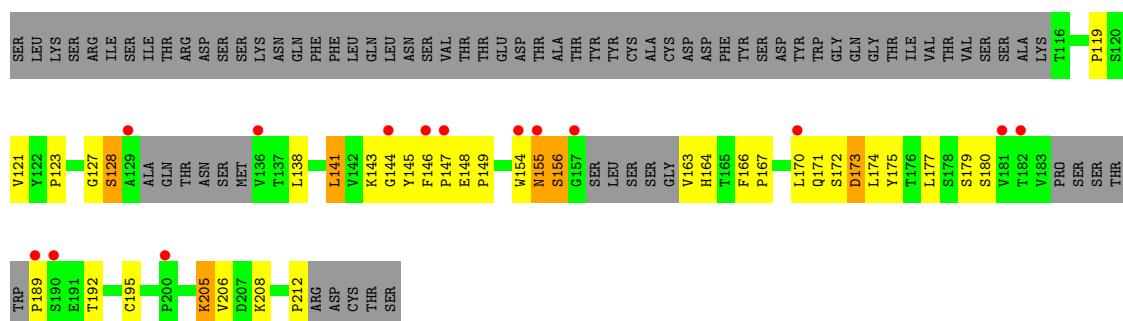
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	8	Total 8	O 8	0	0
4	B	18	Total 18	O 18	0	0
4	C	61	Total 61	O 61	0	0
4	D	34	Total 34	O 34	0	0
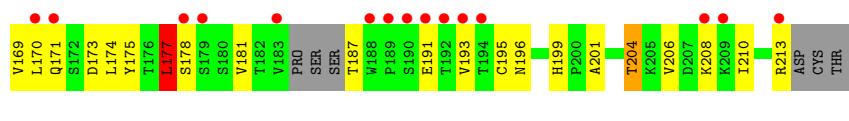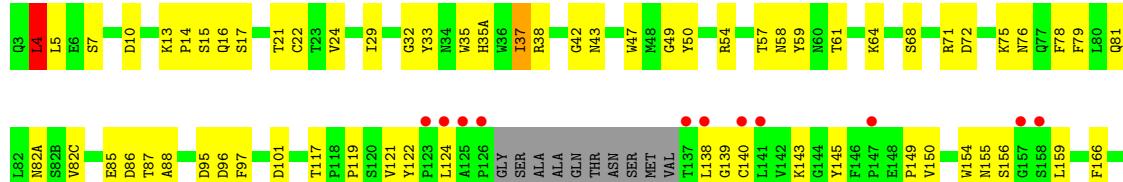
3 Residue-property plots ⓘ

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.
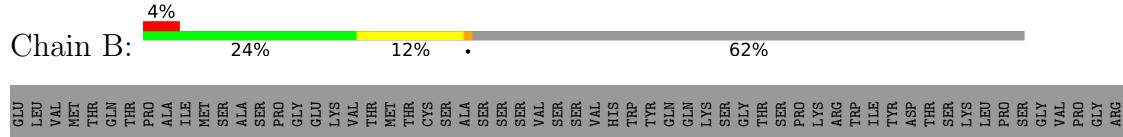
• Molecule 1: Anti-ciguatoxin antibody 10C9 Fab heavy chain
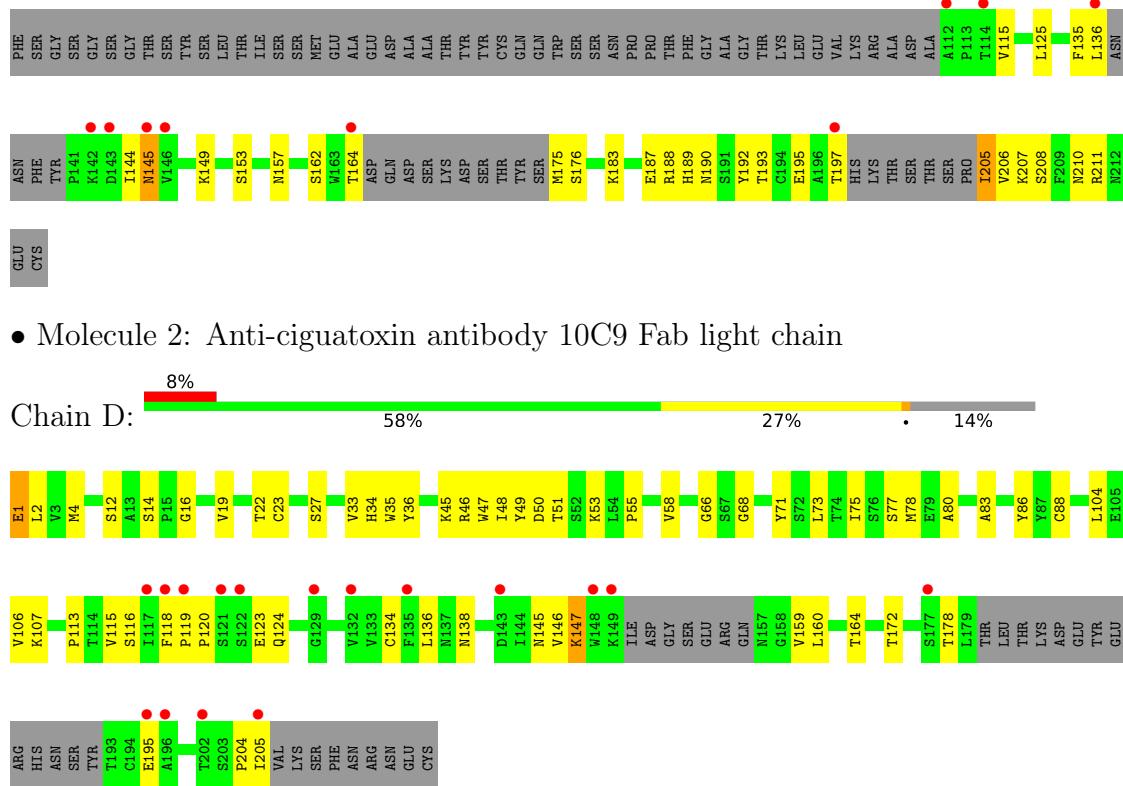
• Molecule 1: Anti-ciguatoxin antibody 10C9 Fab heavy chain

• Molecule 2: Anti-ciguatoxin antibody 10C9 Fab light chain

PHE SER GLY SER GLY SER GLY THR SER TYR SER SER LEU THR ILE SER SER MET GLU ALA ALA GLU ASP ALA ALA THR TYR TYR CYS GLN GLN TRP SER SER ASN PRO PRO THR PHE GLY ALA GLY THR LYS LEU GLU VAL LYS ARG ALA ASP ALA A112 P113 T114 V115 L125 F135 L136 ASN

ASN PHE TYR P141 K142 D143 I144 N145 V146 K149 S153 N157 S162 W163 T164 ASP GLN ASP SER LYS ASP SER THR TYR SER M175 S176 K183 E187 R188 H189 N190 S191 Y192 T193 C194 E195 A196 T197 HIS LYS THR SER THR SER PRO I205 V206 K207 S208 F209 N210 R211 N212

GLU CYS

• Molecule 2: Anti-ciguatoxin antibody 10C9 Fab light chain

Chain D:

E1 L2 V3 M4 S12 A13 S14 P15 G16 V19 T22 C23 S27 V33 H34 W35 Y36 K45 R46 W47 I48 Y49 D50 T51 S52 K53 L54 P55 V58 G66 S67 G68 Y71 S72 L73 T74 I75 S76 S77 M78 E79 A80 A83 Y86 Y87 C88 L104 E105

V106 K107 P113 T114 V115 S116 I117 F118 P119 P120 S121 S122 E123 Q124 G129 V132 V133 C134 F135 L136 N137 N138 D143 I144 N145 V146 K147 W148 K149 ILE ASP GLY SER GLU ARG GLN N157 G158 V159 L160 T164 T172 S177 T178 L179 THR LEU THR LYS ASP GLU TYR GLU

ARG HIS ASN SER TYR T193 C194 E195 A196 T202 S203 P204 I205 VAL LYS SER PHE ASN ARG ASN GLU CYS

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	80.72Å　45.41Å　122.37Å 90.00°　98.90°　90.00°	Depositor
Resolution (Å)	9.99 – 2.40 42.51 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.4 (9.99-2.40) 99.5 (42.51-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	4.17 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.297 , 0.340 0.302 , 0.341	Depositor DCC
R_{free} test set	3444 reflections (9.92%)	wwPDB-VP
Wilson B-factor (Å^2)	34.5	Xtriage
Anisotropy	0.932	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 49.9	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	4307	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.48% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: END

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	0.37	0/609	0.72	0/838
1	C	0.37	0/1609	0.72	2/2204 (0.1%)
2	B	0.35	0/633	0.63	0/854
2	D	0.41	0/1413	0.67	0/1922
All	All	0.38	0/4264	0.69	2/5818 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	4	LEU	CA-CB-CG	5.52	127.99	115.30
1	C	177	LEU	CA-CB-CG	5.28	127.44	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	594	0	594	31	0
1	C	1565	0	1510	67	0
2	B	623	0	603	27	0
2	D	1380	0	1320	46	0
3	C	24	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	8	0	0	2	0
4	B	18	0	0	2	0
4	C	61	0	0	2	0
4	D	34	0	0	3	0
All	All	4307	0	4051	162	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 20.

All (162) 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:13:LYS:H	1:C:16:GLN:NE2	1.58	1.00
2:D:83:ALA:HB2	2:D:106:VAL:HG23	1.42	0.98
1:A:119:PRO:HB3	1:A:145:TYR:HB3	1.45	0.97
1:C:13:LYS:H	1:C:16:GLN:HE21	1.18	0.89
2:D:159:VAL:HA	2:D:178:THR:O	1.74	0.87
2:D:46:ARG:HD3	2:D:49:TYR:HB3	1.56	0.87
1:C:138:LEU:HD22	1:C:193:VAL:HG11	1.57	0.85
2:D:78:MET:HE1	2:D:104:LEU:HD21	1.59	0.84
1:C:124:LEU:HB2	1:C:139:GLY:HA3	1.58	0.83
2:D:46:ARG:HD2	4:D:216:HOH:O	1.82	0.80
1:C:187:THR:O	1:C:191:GLU:HB2	1.82	0.79
1:C:156:SER:H	1:C:196:ASN:HD21	1.31	0.76
1:C:177:LEU:HD23	1:C:178:SER:N	1.99	0.76
1:C:121:VAL:O	1:C:208:LYS:HE3	1.86	0.75
2:D:34:HIS:HD2	2:D:50:ASP:H	1.34	0.75
1:C:171:GLN:HG3	2:D:160:LEU:HD11	1.71	0.73
2:D:34:HIS:CD2	2:D:50:ASP:H	2.07	0.73
2:D:83:ALA:HB2	2:D:106:VAL:CG2	2.19	0.71
1:C:121:VAL:HG21	1:C:206:VAL:HB	1.73	0.70
1:C:154:TRP:CZ3	1:C:195:CYS:HB3	2.26	0.70
2:D:1:GLU:HG2	2:D:2:LEU:N	2.05	0.70
1:A:144:GLY:HA2	1:A:174:LEU:HB3	1.72	0.70
1:C:13:LYS:N	1:C:16:GLN:HE21	1.88	0.69
1:C:199:HIS:CE1	1:C:201:ALA:HB3	2.26	0.69
2:D:1:GLU:HA	4:D:231:HOH:O	1.93	0.69
1:C:169:VAL:HG11	2:D:160:LEU:HD22	1.75	0.68
2:D:55:PRO:HD2	2:D:58:VAL:HG21	1.76	0.68
1:C:61:THR:HA	1:C:64:LYS:HE2	1.77	0.67
1:C:119:PRO:HB3	1:C:145:TYR:HB3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:ARG:HH11	1:C:213:ARG:HG3	1.61	0.65
2:D:14:SER:OG	2:D:107:LYS:HD2	1.97	0.65
1:A:141:LEU:CD1	1:A:143:LYS:HG3	2.28	0.64
2:B:189:HIS:O	2:B:211:ARG:HD3	1.96	0.64
1:A:141:LEU:HD11	1:A:143:LYS:HG3	1.80	0.63
1:A:166:PHE:HB3	2:B:162:SER:OG	1.99	0.62
1:C:124:LEU:HB2	1:C:139:GLY:CA	2.30	0.61
1:A:170:LEU:HD12	1:A:175:TYR:CZ	2.36	0.60
1:C:71:ARG:HA	1:C:78:PHE:HA	1.83	0.60
2:D:1:GLU:CD	2:D:2:LEU:HD13	2.22	0.60
2:B:195:GLU:HG3	2:B:206:VAL:HG22	1.84	0.60
2:D:73:LEU:C	2:D:73:LEU:HD23	2.22	0.59
2:B:149:LYS:HB2	2:B:193:THR:HB	1.84	0.59
1:C:29:ILE:H	1:C:76:ASN:HD21	1.50	0.59
2:D:136:LEU:N	2:D:136:LEU:HD12	2.17	0.59
2:B:205:ILE:HD13	2:B:205:ILE:N	2.18	0.58
1:C:119:PRO:HD2	1:C:204:THR:HG21	1.84	0.58
2:D:1:GLU:CG	2:D:2:LEU:N	2.67	0.58
1:A:127:GLY:O	1:A:128:SER:C	2.41	0.57
1:C:170:LEU:HB2	1:C:175:TYR:CE2	2.39	0.57
1:C:37:ILE:HG13	1:C:38:ARG:N	2.18	0.57
1:A:170:LEU:HD12	1:A:175:TYR:OH	2.06	0.56
1:C:122:TYR:CE2	2:D:124:GLN:HG3	2.41	0.56
1:C:173:ASP:O	1:C:174:LEU:HD23	2.05	0.56
1:C:170:LEU:HD12	1:C:174:LEU:O	2.06	0.55
4:C:278:HOH:O	2:D:34:HIS:HE1	1.88	0.55
1:A:166:PHE:CD1	2:B:164:THR:HG23	2.42	0.55
1:A:119:PRO:CB	1:A:145:TYR:HB3	2.26	0.54
1:C:13:LYS:N	1:C:16:GLN:NE2	2.42	0.54
2:D:116:SER:O	2:D:134:CYS:HA	2.07	0.54
1:A:148:GLU:OE1	1:A:149:PRO:HA	2.08	0.54
1:A:170:LEU:C	1:A:170:LEU:HD23	2.29	0.54
2:B:205:ILE:HA	4:B:215:HOH:O	2.08	0.53
2:B:175:MET:HG2	2:B:176:SER:N	2.24	0.53
1:C:156:SER:N	1:C:196:ASN:HD21	2.04	0.53
1:C:14:PRO:O	1:C:15:SER:HB2	2.07	0.53
1:C:139:GLY:O	1:C:154:TRP:HH2	1.91	0.53
1:C:154:TRP:CH2	1:C:195:CYS:HB3	2.43	0.53
1:A:167:PRO:HD3	2:B:164:THR:HG22	1.91	0.52
2:B:136:LEU:HD12	2:B:136:LEU:N	2.24	0.52
1:A:121:VAL:HB	1:A:206:VAL:HG11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:CYS:HB2	1:C:154:TRP:CH2	2.45	0.52
1:C:138:LEU:HD12	1:C:138:LEU:N	2.25	0.51
1:C:199:HIS:HB3	1:C:204:THR:HG22	1.93	0.51
1:C:170:LEU:HD13	1:C:175:TYR:CZ	2.46	0.50
2:D:136:LEU:HD21	2:D:146:VAL:HG12	1.93	0.50
1:A:189:PRO:HG3	1:A:212:PRO:HG3	1.94	0.50
1:C:5:LEU:O	1:C:22:CYS:HA	2.12	0.50
1:C:150:VAL:HG23	1:C:199:HIS:HD2	1.77	0.49
1:C:101:ASP:O	2:D:45:LYS:NZ	2.40	0.49
2:D:80:ALA:HA	2:D:106:VAL:HG21	1.93	0.49
1:C:29:ILE:HA	1:C:35:TRP:CZ2	2.48	0.49
2:D:4:MET:HE2	2:D:88:CYS:SG	2.53	0.49
1:C:87:THR:O	1:C:88:ALA:HB2	2.12	0.49
2:D:19:VAL:HG21	2:D:78:MET:CE	2.42	0.49
2:D:78:MET:HE3	2:D:78:MET:HB2	1.58	0.49
2:D:147:LYS:HB3	2:D:195:GLU:HB3	1.95	0.49
1:C:42:GLY:O	1:C:43:ASN:HB2	2.13	0.49
1:A:180:SER:HB3	2:B:135:PHE:CE2	2.48	0.48
2:D:19:VAL:HG21	2:D:78:MET:HE3	1.93	0.48
2:B:190:ASN:O	2:B:210:ASN:HA	2.13	0.48
1:C:143:LYS:HG3	4:C:248:HOH:O	2.13	0.48
2:B:145:ASN:O	2:B:197:THR:N	2.32	0.48
1:A:163:VAL:HA	1:A:180:SER:O	2.14	0.48
1:C:138:LEU:HD23	1:C:210:ILE:HG21	1.96	0.48
1:A:147:PRO:HB2	4:A:221:HOH:O	2.14	0.47
1:C:17:SER:HA	1:C:82(A):ASN:HA	1.96	0.47
1:C:47:TRP:CZ2	1:C:49:GLY:HA2	2.49	0.47
2:D:27:SER:HB2	4:D:227:HOH:O	2.15	0.47
1:C:82(C):VAL:HA	1:C:86:ASP:OD2	2.13	0.47
2:B:190:ASN:HD21	2:B:210:ASN:HB3	1.80	0.47
2:B:193:THR:CG2	2:B:206:VAL:HG13	2.44	0.47
1:C:170:LEU:HD13	1:C:175:TYR:CE2	2.50	0.47
1:C:4:LEU:HD13	1:C:24:VAL:HG22	1.97	0.47
1:A:154:TRP:CZ3	1:A:195:CYS:HB3	2.50	0.46
2:D:75:ILE:HD12	2:D:78:MET:CE	2.46	0.46
1:C:121:VAL:HB	1:C:206:VAL:HG11	1.98	0.46
1:C:13:LYS:HB2	1:C:16:GLN:HE21	1.81	0.46
2:D:115:VAL:HG21	2:D:205:ILE:HG23	1.98	0.46
1:A:175:TYR:HE2	4:A:218:HOH:O	1.98	0.46
1:C:154:TRP:HB3	1:C:159:LEU:HD23	1.98	0.45
2:B:145:ASN:H	2:B:197:THR:CG2	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:22:THR:HG22	2:D:23:CYS:N	2.31	0.45
1:C:7:SER:OG	1:C:21:THR:HB	2.16	0.45
1:C:213:ARG:HH11	1:C:213:ARG:CG	2.26	0.45
2:D:46:ARG:HD3	2:D:49:TYR:CB	2.40	0.45
2:B:157:ASN:HA	4:B:225:HOH:O	2.17	0.45
2:D:66:GLY:HA3	2:D:71:TYR:HA	1.99	0.45
2:B:144:ILE:HD12	2:B:197:THR:HG23	1.98	0.45
2:D:35:TRP:HB2	2:D:48:ILE:HB	1.98	0.45
2:B:190:ASN:ND2	2:B:210:ASN:HB3	2.32	0.44
1:A:172:SER:O	1:A:173:ASP:CB	2.65	0.44
2:B:192:TYR:O	2:B:208:SER:HB2	2.18	0.44
2:B:125:LEU:O	2:B:183:LYS:HD2	2.18	0.44
2:B:115:VAL:HA	2:B:135:PHE:O	2.18	0.43
1:C:35(A):HIS:ND1	1:C:50:TYR:HB3	2.32	0.43
2:D:36:TYR:O	2:D:86:TYR:HA	2.18	0.43
1:A:164:HIS:O	1:A:179:SER:HA	2.18	0.43
2:B:145:ASN:H	2:B:197:THR:HG23	1.83	0.43
1:A:154:TRP:O	1:A:156:SER:N	2.51	0.43
1:C:138:LEU:HB2	1:C:181:VAL:CG1	2.48	0.43
2:D:50:ASP:HB3	2:D:53:LYS:CE	2.49	0.43
2:D:4:MET:HE3	2:D:23:CYS:SG	2.58	0.42
2:D:19:VAL:CG2	2:D:78:MET:HE3	2.49	0.42
1:C:13:LYS:CB	1:C:16:GLN:HE21	2.32	0.42
1:C:154:TRP:CE3	1:C:195:CYS:HB3	2.54	0.42
1:A:172:SER:O	1:A:173:ASP:HB2	2.20	0.42
2:B:144:ILE:HA	2:B:197:THR:CG2	2.49	0.42
2:D:113:PRO:O	2:D:205:ILE:HD13	2.19	0.42
1:A:123:PRO:HD3	1:A:208:LYS:HD2	2.02	0.42
1:A:146:PHE:CD1	1:A:147:PRO:HA	2.55	0.42
2:D:138:ASN:HA	2:D:172:THR:OG1	2.20	0.42
2:D:16:GLY:HA2	2:D:77:SER:OG	2.19	0.42
1:C:35:TRP:CD1	1:C:35:TRP:N	2.87	0.41
2:D:50:ASP:O	2:D:51:THR:HB	2.20	0.41
1:A:205:LYS:O	1:A:206:VAL:HG23	2.20	0.41
2:D:118:PHE:HA	2:D:119:PRO:HD3	1.92	0.41
1:C:29:ILE:H	1:C:76:ASN:ND2	2.16	0.41
1:C:117:THR:O	1:C:145:TYR:HA	2.20	0.41
1:A:154:TRP:CH2	1:A:195:CYS:HB3	2.56	0.41
1:C:59:TYR:HB2	1:C:64:LYS:HD3	2.01	0.41
1:C:213:ARG:CG	1:C:213:ARG:NH1	2.82	0.41
1:C:96:ASP:O	1:C:97:PHE:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:LEU:HD13	1:A:143:LYS:HG3	2.00	0.41
1:A:154:TRP:C	1:A:155:ASN:OD1	2.58	0.41
2:B:187:GLU:OE2	2:B:211:ARG:NH2	2.54	0.40
1:A:154:TRP:C	1:A:156:SER:N	2.74	0.40
2:B:144:ILE:HG13	2:B:145:ASN:N	2.37	0.40
1:C:32:GLY:O	1:C:33:TYR:HB2	2.21	0.40
2:B:136:LEU:O	2:B:175:MET:N	2.55	0.40
1:C:155:ASN:OD1	1:C:193:VAL:HA	2.21	0.40
1:C:166:PHE:CD1	2:D:164:THR:HG23	2.57	0.40
1:C:72:ASP:OD2	1:C:75:LYS:HE2	2.20	0.40

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	73/218 (34%)	64 (88%)	7 (10%)	2 (3%)	5	5
1	C	195/218 (89%)	180 (92%)	15 (8%)	0	100	100
2	B	72/213 (34%)	71 (99%)	1 (1%)	0	100	100
2	D	178/213 (84%)	170 (96%)	5 (3%)	3 (2%)	9	11
All	All	518/862 (60%)	485 (94%)	28 (5%)	5 (1%)	15	23

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	128	SER
1	A	155	ASN
2	D	204	PRO
2	D	120	PRO
2	D	68	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	72/196 (37%)	64 (89%)	8 (11%)	6	8
1	C	182/196 (93%)	168 (92%)	14 (8%)	13	20
2	B	73/188 (39%)	68 (93%)	5 (7%)	16	25
2	D	160/188 (85%)	153 (96%)	7 (4%)	28	45
All	All	487/768 (63%)	453 (93%)	34 (7%)	15	24

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	LEU
1	A	141	LEU
1	A	156	SER
1	A	171	GLN
1	A	173	ASP
1	A	177	LEU
1	A	192	THR
1	A	205	LYS
2	B	145	ASN
2	B	153	SER
2	B	188	ARG
2	B	205	ILE
2	B	207	LYS
1	C	4	LEU
1	C	10	ASP
1	C	37	ILE
1	C	54	ARG
1	C	57	THR
1	C	58	ASN
1	C	68	SER
1	C	79	PHE
1	C	81	GLN
1	C	85	GLU
1	C	95	ASP

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Mol	Chain	Res	Type
1	C	149	PRO
1	C	177	LEU
1	C	204	THR
2	D	1	GLU
2	D	12	SER
2	D	33	VAL
2	D	47	TRP
2	D	123	GLU
2	D	145	ASN
2	D	147	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	171	GLN
1	A	196	ASN
2	B	145	ASN
2	B	156	GLN
2	B	212	ASN
1	C	16	GLN
1	C	76	ASN
1	C	77	GLN
1	C	81	GLN
1	C	196	ASN
2	D	34	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 (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	#$|Z| > 2$
3	END	C	1	-	26,27,27	1.87	5 (19%)	27,39,39	2.68	8 (29%)

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
3	END	C	1	-	-	0/2/55/55	0/3/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	END	CAQ-CAG	-6.29	1.40	1.49
3	C	1	END	CAJ-CAE	-4.04	1.40	1.50
3	C	1	END	CAH-CAD	-3.80	1.40	1.49
3	C	1	END	CAP-CAF	3.18	1.54	1.51
3	C	1	END	CAG-CAF	2.37	1.38	1.32

All (8) bond angle outliers are listed below:

| Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	END	OAL-CAH-CAD	7.47	127.88	113.69
3	C	1	END	CAH-OAL-CAW	6.84	122.06	114.89
3	C	1	END	OAM-CAQ-CAT	5.91	113.82	108.84
3	C	1	END	CAS-OAN-CAT	-4.01	107.29	114.64
3	C	1	END	CAI-CAS-CAP	-3.62	107.52	112.51
3	C	1	END	CAP-CAF-CAG	2.59	133.23	127.69
3	C	1	END	CAW-CAR-CAX	2.13	113.39	108.96
3	C	1	END	OAN-CAT-CAK	2.08	110.66	107.42
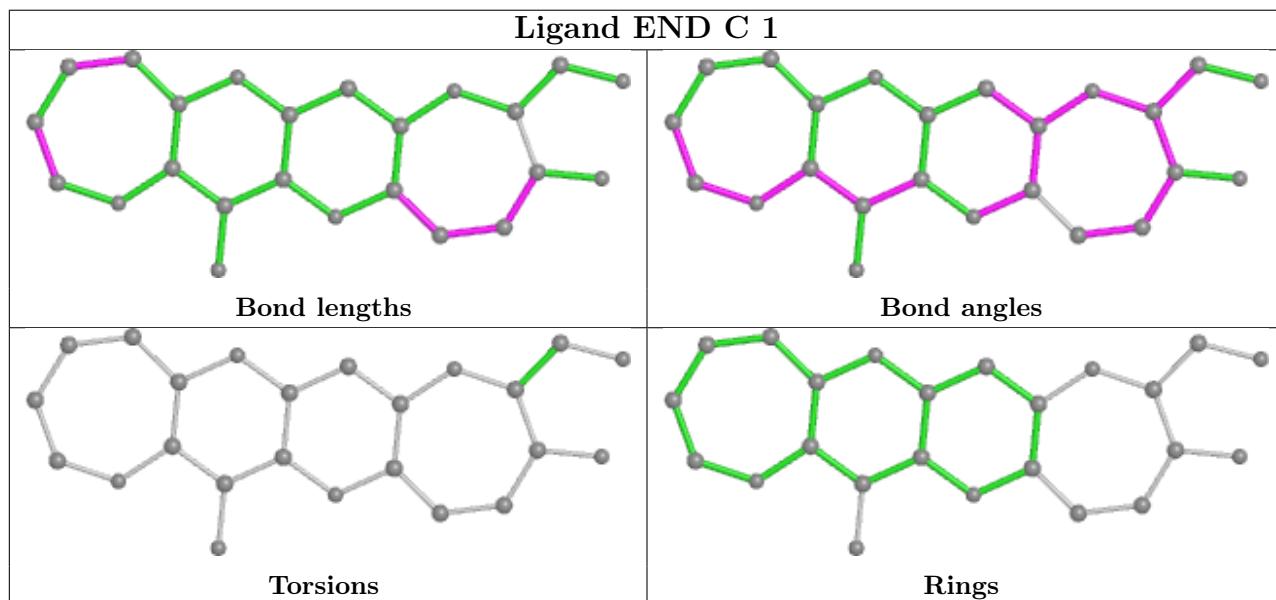
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 END C 1

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	81/218 (37%)	1.12	14 (17%)	1	1	42, 54, 75, 83	0
1	C	201/218 (92%)	0.65	26 (12%)	3	3	18, 37, 69, 77	0
2	B	80/213 (37%)	0.74	9 (11%)	5	4	28, 43, 59, 63	0
2	D	184/213 (86%)	0.54	16 (8%)	10	9	13, 29, 71, 76	0
All	All	546/862 (63%)	0.70	65 (11%)	4	4	13, 41, 70, 83	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	140	CYS	5.7
1	C	189	PRO	4.6
1	C	193	VAL	4.6
2	D	205	ILE	4.3
1	A	190	SER	4.1
1	C	137	THR	4.0
1	C	125	ALA	4.0
2	B	164	THR	3.8
2	B	145	ASN	3.7
1	A	181	VAL	3.7
1	C	183	VAL	3.6
1	A	154	TRP	3.5
1	C	191	GLU	3.5
1	C	126	PRO	3.4
2	B	197	THR	3.4
1	C	171	GLN	3.3
2	D	121	SER	3.3
2	D	195	GLU	3.3
2	D	122	SER	3.3
2	B	136	LEU	3.2
1	A	170	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
2	D	132	VAL	3.2
1	C	190	SER	3.1
2	D	196	ALA	3.1
1	C	192	THR	3.0
1	A	136	VAL	3.0
1	C	194	THR	2.9
1	A	182	THR	2.9
1	A	155	ASN	2.8
2	D	117	ILE	2.8
2	B	143	ASP	2.8
1	C	124	LEU	2.7
1	A	189	PRO	2.7
1	A	129	ALA	2.7
1	C	141	LEU	2.6
2	D	119	PRO	2.6
2	D	202	THR	2.6
1	C	188	TRP	2.6
1	C	123	PRO	2.5
2	B	114	THR	2.5
1	A	146	PHE	2.4
1	A	144	GLY	2.4
2	B	112	ALA	2.4
1	C	157	GLY	2.4
1	A	200	PRO	2.4
2	D	177	SER	2.4
1	A	147	PRO	2.4
1	C	179	SER	2.4
2	D	143	ASP	2.3
1	C	213	ARG	2.3
1	C	138	LEU	2.3
1	C	178	SER	2.3
1	C	170	LEU	2.3
2	B	142	LYS	2.2
2	D	129	GLY	2.2
1	C	158	SER	2.2
2	D	135	PHE	2.2
2	B	146	VAL	2.1
2	D	148	TRP	2.1
2	D	149	LYS	2.1
1	C	208	LYS	2.1
1	C	147	PRO	2.1
1	C	209	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	118	PHE	2.1
1	A	157	GLY	2.0

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 ⓘ
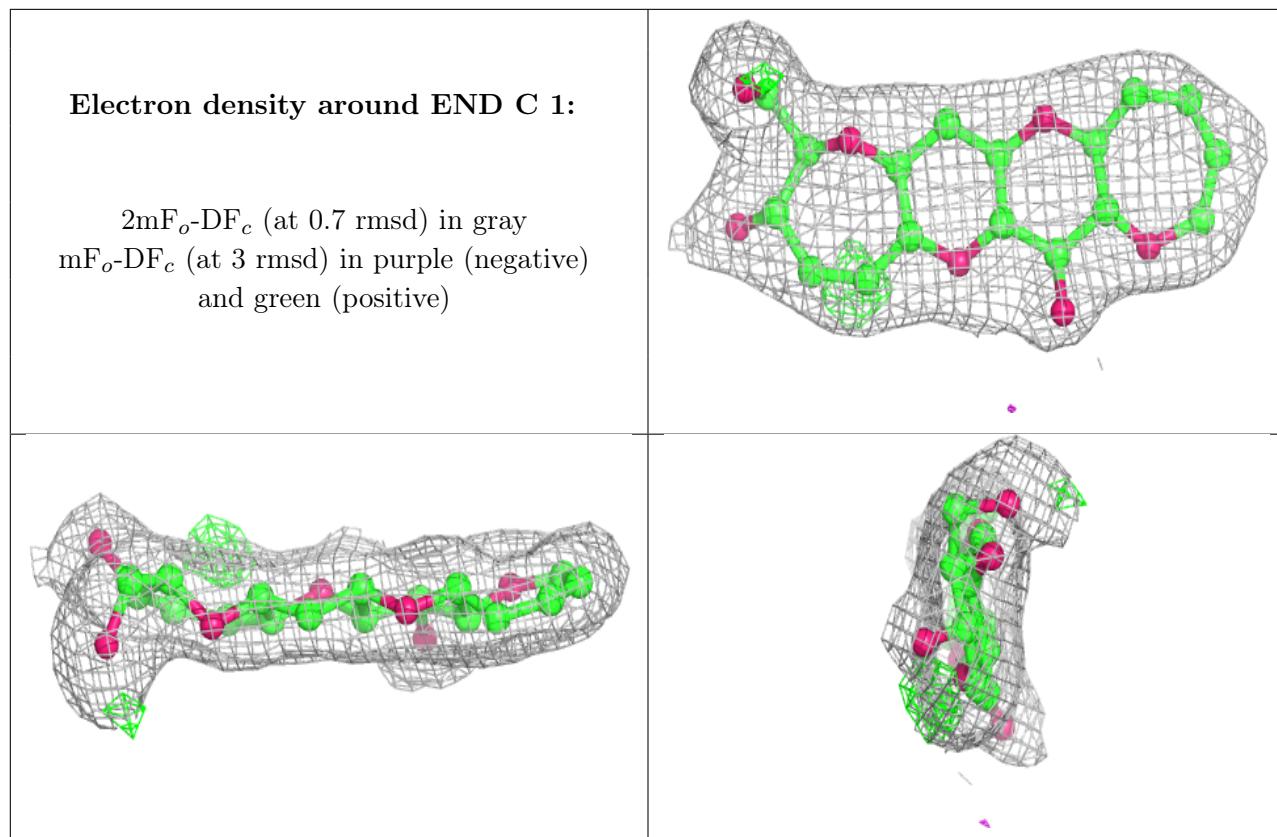
There are no monosaccharides in this entry.

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	END	C	1	24/24	0.94	0.17	16,19,24,26	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 END C 1:

$2mF_o$-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.