Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 10:24 AM EDT

PDB ID : 7KYF
Title : Botulism Neurooxin Light Chain A app form
Authors : Ortega, M.E.; Salzameda, N.T.
Deposited on : 2020-12-07
Resolution : 2.33 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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:

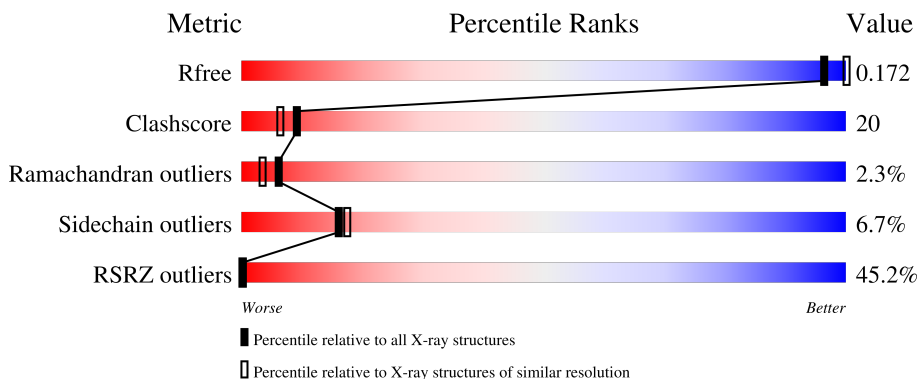|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.33 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		0.172
Clashscore		20
Ramachandran outliers		2.3%
Sidechain outliers		6.7%
RSRZ outliers		45.2%

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	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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	C	417	43% (upper bar); 59% / 32% / · 5%

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	XC1	C	502	-	X	-	-

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 3275 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 Bont/A1.

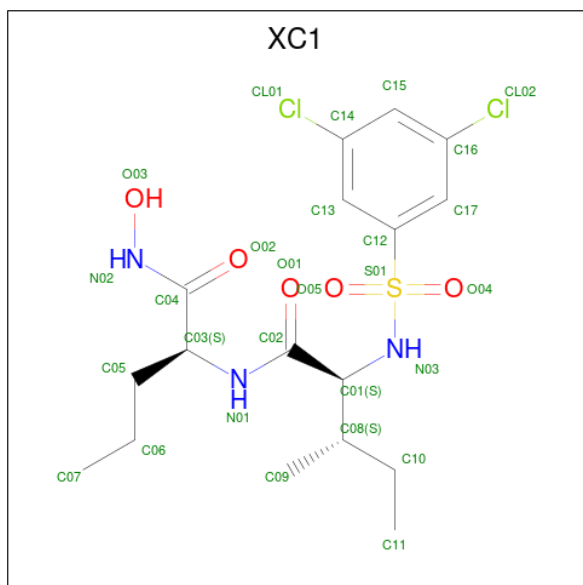| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	398	Total	C	N	O	S	0	0	0
			3227	2082	531	607	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	27	VAL	ALA	conflict	UNP C6K838
C	29	VAL	GLN	conflict	UNP C6K838

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total	Zn	0	0
			1	1		

- Molecule 3 is N-[(3,5-dichlorophenyl)sulfonyl]-L-isoleucyl-N-hydroxy-L-norvalinamide (three-letter code: XC1) (formula: $C_{17}H_{25}Cl_2N_3O_5S$) (labeled as "Ligand of Interest" by depositor).

| Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	C	1	Total	C	Cl	N	O	S	0	0
			28	17	2	3	5	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	19	Total	O	0	0
			19	19		

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: Bont/A1
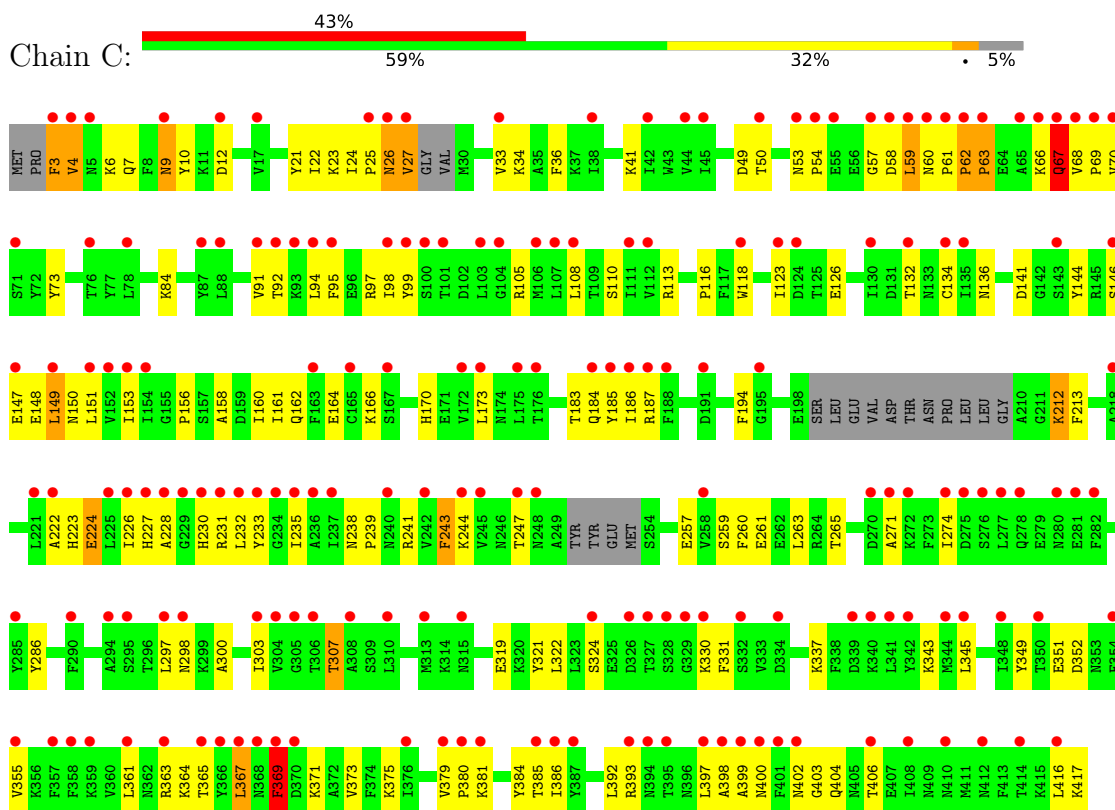
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	57.53Å 196.40Å 38.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.25 – 2.33 43.21 – 2.33	Depositor EDS
% Data completeness (in resolution range)	99.7 (43.25-2.33) 99.7 (43.21-2.33)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	50.60 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.160 , 0.179 0.167 , 0.172	Depositor DCC
R_{free} test set	1959 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å^2)	57.2	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.49 , 999.0	EDS
L-test for twinning[2]	$< |L| > = 0.51, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	3275	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.49% 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: XC1, ZN

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	C	0.91	1/3300 (0.0%)	1.08	3/4461 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	261	GLU	CD-OE2	5.18	1.31	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	231	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	C	132	THR	CA-CB-OG1	5.14	119.79	109.00
1	C	231	ARG	NE-CZ-NH1	5.03	122.82	120.30

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	C	3227	0	3186	128	0
2	C	1	0	0	0	0
3	C	28	0	0	6	0
4	C	19	0	0	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3275	0	3186	129	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 (129) 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:62:PRO:HB2	1:C:63:PRO:CD	1.57	1.34
1:C:53:ASN:OD1	1:C:54:PRO:HD2	1.15	1.30
1:C:53:ASN:OD1	1:C:54:PRO:CD	1.92	1.18
1:C:244:LYS:HG2	4:C:609:HOH:O	1.43	1.18
1:C:66:LYS:HB3	1:C:70:VAL:CG1	1.87	1.04
1:C:66:LYS:CB	1:C:70:VAL:HG13	1.88	1.03
1:C:62:PRO:CB	1:C:63:PRO:HD3	1.90	1.01
1:C:194:PHE:CD1	4:C:606:HOH:O	2.18	0.96
1:C:62:PRO:HB2	1:C:63:PRO:HD3	0.98	0.96
1:C:62:PRO:CB	1:C:63:PRO:CD	2.41	0.96
1:C:4:VAL:HG21	1:C:92:THR:HG23	1.47	0.96
1:C:66:LYS:HB3	1:C:70:VAL:HG13	1.50	0.86
1:C:66:LYS:HB3	1:C:70:VAL:HG11	1.56	0.85
1:C:105:ARG:NH1	4:C:601:HOH:O	2.09	0.84
1:C:151:LEU:HD11	1:C:186:ILE:HD12	1.61	0.83
1:C:24:ILE:HG22	1:C:25:PRO:HD2	1.61	0.83
1:C:68:VAL:HG13	1:C:373:VAL:HG12	1.62	0.81
1:C:194:PHE:CE1	4:C:606:HOH:O	2.31	0.81
1:C:66:LYS:HB2	1:C:70:VAL:HG13	1.62	0.79
1:C:41:LYS:HE2	4:C:612:HOH:O	1.80	0.79
1:C:184:GLN:HG3	1:C:228:ALA:HA	1.65	0.79
1:C:194:PHE:CG	4:C:606:HOH:O	2.35	0.78
1:C:151:LEU:HD11	1:C:186:ILE:CD1	2.18	0.73
1:C:243:PHE:CD1	4:C:609:HOH:O	2.43	0.71
1:C:149:LEU:HD23	1:C:149:LEU:N	2.06	0.70
1:C:322:LEU:HB3	1:C:337:LYS:HE3	1.73	0.70
1:C:24:ILE:CG2	1:C:25:PRO:HD2	2.21	0.70
1:C:151:LEU:HD21	1:C:153:ILE:HD11	1.75	0.69
1:C:69:PRO:HG3	1:C:371:LYS:HA	1.74	0.69
1:C:352:ASP:O	1:C:355:VAL:HG22	1.94	0.68
1:C:230:HIS:NE2	1:C:345:LEU:O	2.28	0.67
1:C:3:PHE:CZ	1:C:108:LEU:HD22	2.29	0.67
1:C:243:PHE:CE1	4:C:609:HOH:O	2.47	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:363:ARG:NH1	3:C:502:XC1:O05	2.29	0.66
1:C:136:ASN:HB3	1:C:144:TYR:HB3	1.77	0.65
1:C:41:LYS:CE	4:C:612:HOH:O	2.40	0.65
1:C:224:GLU:O	1:C:227:HIS:HB2	1.98	0.64
1:C:23:LYS:HG3	1:C:144:TYR:CE1	2.33	0.64
1:C:222:ALA:O	1:C:226:ILE:HG12	1.98	0.62
1:C:113:ARG:NH2	1:C:319:GLU:O	2.33	0.62
1:C:149:LEU:HD23	1:C:149:LEU:H	1.64	0.61
1:C:62:PRO:HB2	1:C:63:PRO:HD2	1.72	0.61
1:C:212:LYS:HB3	1:C:213:PHE:CD2	2.36	0.61
1:C:50:THR:HG22	1:C:57:GLY:CA	2.31	0.61
1:C:321:TYR:HA	4:C:602:HOH:O	2.01	0.61
3:C:502:XC1:C11	4:C:605:HOH:O	2.50	0.59
1:C:365:THR:HG23	1:C:367:LEU:H	1.69	0.58
1:C:379:VAL:HB	1:C:380:PRO:HD3	1.87	0.57
1:C:375:LYS:HB2	1:C:416:LEU:HD11	1.87	0.57
1:C:232:LEU:HB2	4:C:617:HOH:O	2.04	0.56
1:C:298:ASN:HB3	1:C:330:LYS:HE2	1.89	0.55
1:C:393:ARG:CZ	4:C:608:HOH:O	2.55	0.55
1:C:162:GLN:HE22	3:C:502:XC1:C11	2.20	0.55
1:C:194:PHE:CD2	4:C:606:HOH:O	2.59	0.54
1:C:259:SER:CB	4:C:611:HOH:O	2.55	0.54
1:C:50:THR:HG22	1:C:57:GLY:HA3	1.89	0.54
1:C:94:LEU:O	1:C:98:ILE:HG13	2.08	0.54
1:C:164:GLU:HA	1:C:224:GLU:OE1	2.08	0.53
1:C:49:ASP:OD2	1:C:187:ARG:NE	2.34	0.53
1:C:369:PHE:HA	3:C:502:XC1:CL02	2.45	0.53
1:C:68:VAL:CG1	1:C:373:VAL:HG12	2.37	0.53
1:C:67:GLN:HE21	1:C:417:LYS:HG3	1.74	0.52
1:C:10:TYR:O	1:C:34:LYS:NZ	2.32	0.52
1:C:118:TRP:HZ2	1:C:148:GLU:OE2	1.93	0.52
1:C:149:LEU:HG	1:C:183:THR:HG21	1.92	0.52
1:C:24:ILE:HG22	1:C:25:PRO:CD	2.36	0.52
1:C:223:HIS:NE2	3:C:502:XC1:O02	2.44	0.51
1:C:161:ILE:HB	1:C:194:PHE:HE1	1.75	0.51
1:C:66:LYS:CB	1:C:70:VAL:CG1	2.58	0.51
1:C:351:GLU:O	1:C:355:VAL:HG13	2.11	0.51
1:C:226:ILE:CG2	1:C:265:THR:HG23	2.42	0.50
1:C:24:ILE:HD12	1:C:185:TYR:HE2	1.75	0.50
1:C:194:PHE:CZ	4:C:606:HOH:O	2.60	0.50
1:C:10:TYR:CZ	1:C:84:LYS:HD2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:GLU:OE2	1:C:224:GLU:HA	2.13	0.49
1:C:3:PHE:CG	4:C:610:HOH:O	2.55	0.49
1:C:134:CYS:HA	1:C:147:GLU:O	2.12	0.49
1:C:53:ASN:CG	1:C:54:PRO:CD	2.77	0.48
1:C:68:VAL:HG13	1:C:373:VAL:CG1	2.37	0.48
1:C:399:ALA:O	1:C:402:ASN:ND2	2.43	0.48
1:C:381:LYS:HG2	1:C:385:THR:HG22	1.96	0.48
1:C:99:TYR:OH	1:C:105:ARG:CZ	2.62	0.48
1:C:26:ASN:HD22	1:C:26:ASN:HA	1.58	0.47
1:C:397:LEU:HD22	1:C:403:GLY:HA2	1.97	0.47
1:C:371:LYS:O	1:C:371:LYS:NZ	2.33	0.47
1:C:50:THR:HG22	1:C:57:GLY:HA2	1.97	0.46
1:C:69:PRO:HB3	1:C:371:LYS:C	2.36	0.46
1:C:149:LEU:N	1:C:149:LEU:CD2	2.76	0.46
1:C:4:VAL:HG12	1:C:6:LYS:O	2.16	0.46
1:C:97:ARG:HA	1:C:386:ILE:HG23	1.98	0.46
1:C:118:TRP:CZ3	1:C:303:ILE:HD11	2.50	0.46
1:C:324:SER:O	1:C:331:PHE:HA	2.16	0.45
1:C:58:ASP:C	1:C:60:ASN:H	2.20	0.45
1:C:110:SER:O	1:C:233:TYR:HE1	2.00	0.44
1:C:91:VAL:O	1:C:95:PHE:HD2	2.00	0.44
1:C:400:ASN:HB3	1:C:402:ASN:ND2	2.32	0.44
1:C:61:PRO:HG3	1:C:73:TYR:HB3	1.99	0.44
1:C:27:VAL:N	4:C:604:HOH:O	2.51	0.44
1:C:194:PHE:CE2	4:C:606:HOH:O	2.71	0.44
1:C:134:CYS:HA	1:C:149:LEU:CD2	2.48	0.44
1:C:212:LYS:O	1:C:406:THR:OG1	2.33	0.44
1:C:226:ILE:HD12	1:C:349:TYR:C	2.38	0.44
1:C:123:ILE:HG13	1:C:126:GLU:HB2	2.00	0.43
1:C:10:TYR:HA	1:C:36:PHE:CZ	2.52	0.43
1:C:68:VAL:HG21	1:C:417:LYS:C	2.39	0.43
1:C:3:PHE:CE1	1:C:108:LEU:HB3	2.54	0.43
1:C:9:ASN:HD22	1:C:12:ASP:CG	2.22	0.43
1:C:110:SER:O	1:C:233:TYR:CE1	2.72	0.43
1:C:392:LEU:O	1:C:398:ALA:HB2	2.19	0.43
1:C:243:PHE:HD1	4:C:609:HOH:O	1.89	0.43
1:C:166:LYS:HD2	1:C:187:ARG:HD2	2.01	0.42
1:C:156:PRO:HB2	1:C:160:ILE:HA	2.00	0.42
1:C:92:THR:O	1:C:92:THR:HG22	2.19	0.42
1:C:162:GLN:NE2	3:C:502:XC1:C11	2.82	0.42
1:C:244:LYS:CG	4:C:609:HOH:O	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:238:ASN:HA	1:C:239:PRO:HD3	1.92	0.42
1:C:367:LEU:HD23	1:C:367:LEU:O	2.20	0.41
1:C:66:LYS:O	1:C:70:VAL:CG1	2.68	0.41
1:C:21:TYR:HA	1:C:33:VAL:O	2.21	0.41
1:C:24:ILE:CG2	1:C:25:PRO:CD	2.94	0.41
1:C:50:THR:CG2	1:C:57:GLY:HA3	2.50	0.41
1:C:116:PRO:HD3	1:C:150:ASN:OD1	2.21	0.41
1:C:235:ILE:HG22	1:C:286:TYR:HB3	2.02	0.41
1:C:297:LEU:O	1:C:300:ALA:HB3	2.20	0.41
1:C:361:LEU:O	1:C:404:GLN:NE2	2.53	0.41
1:C:263:LEU:HD23	1:C:274:ILE:CG1	2.51	0.41
1:C:134:CYS:C	1:C:149:LEU:HD21	2.42	0.40
1:C:170:HIS:CG	1:C:173:LEU:HB2	2.56	0.40
1:C:4:VAL:CG2	1:C:92:THR:HG23	2.35	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	C	390/417 (94%)	344 (88%)	37 (10%)	9 (2%)	6	3

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	59	LEU
1	C	212	LYS
1	C	307	THR
1	C	62	PRO
1	C	63	PRO
1	C	158	ALA
1	C	369	PHE

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Mol	Chain	Res	Type
1	C	67	GLN
1	C	271	ALA

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	C	357/374 (96%)	333 (93%)	24 (7%)	16	17

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	3	PHE
1	C	4	VAL
1	C	7	GLN
1	C	9	ASN
1	C	22	ILE
1	C	26	ASN
1	C	27	VAL
1	C	59	LEU
1	C	67	GLN
1	C	141	ASP
1	C	146	SER
1	C	149	LEU
1	C	224	GLU
1	C	241	ARG
1	C	243	PHE
1	C	247	THR
1	C	257	GLU
1	C	260	PHE
1	C	307	THR
1	C	343	LYS
1	C	364	LYS
1	C	367	LEU
1	C	369	PHE
1	C	384	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	9	ASN
1	C	26	ASN
1	C	67	GLN
1	C	139	GLN
1	C	162	GLN
1	C	368	ASN
1	C	412	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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	#$|Z| > 2$
3	XC1	C	502	2	28,28,28	5.29	17 (60%)	37,39,39	3.44	18 (48%)

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	XC1	C	502	2	-	13/34/34/34	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	502	XC1	S01-N03	18.67	1.93	1.61
3	C	502	XC1	C05-C03	-10.40	1.29	1.53
3	C	502	XC1	C04-N02	7.90	1.44	1.33
3	C	502	XC1	C14-CL01	-6.14	1.61	1.74
3	C	502	XC1	C01-C02	5.93	1.68	1.52
3	C	502	XC1	C10-C08	-5.55	1.35	1.53
3	C	502	XC1	O05-S01	-5.01	1.37	1.43
3	C	502	XC1	O03-N02	4.80	1.52	1.40
3	C	502	XC1	C01-N03	-4.13	1.39	1.46
3	C	502	XC1	C03-N01	3.91	1.54	1.45
3	C	502	XC1	C09-C08	-3.73	1.44	1.53
3	C	502	XC1	C13-C12	-3.58	1.32	1.39
3	C	502	XC1	O04-S01	-3.34	1.39	1.43
3	C	502	XC1	C08-C01	-2.95	1.46	1.54
3	C	502	XC1	C16-CL02	2.79	1.80	1.74
3	C	502	XC1	C12-S01	2.43	1.80	1.76
3	C	502	XC1	O02-C04	-2.41	1.18	1.23

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	502	XC1	C13-C14-CL01	-7.99	109.17	119.15
3	C	502	XC1	C15-C14-CL01	7.87	128.98	119.15
3	C	502	XC1	C02-C01-N03	-7.66	96.66	110.46
3	C	502	XC1	O05-S01-C12	6.75	116.28	107.97
3	C	502	XC1	O04-S01-C12	-5.99	100.58	107.97
3	C	502	XC1	C01-N03-S01	-5.38	106.69	121.02
3	C	502	XC1	C17-C12-S01	-4.83	113.67	119.08
3	C	502	XC1	C13-C12-S01	4.38	123.98	119.08
3	C	502	XC1	C03-N01-C02	3.51	129.20	121.67
3	C	502	XC1	C05-C03-C04	3.28	117.86	110.20
3	C	502	XC1	C11-C10-C08	3.23	126.72	113.84
3	C	502	XC1	C17-C16-C15	-3.01	117.92	121.66
3	C	502	XC1	C16-C17-C12	2.52	120.49	118.23
3	C	502	XC1	C17-C16-CL02	2.48	122.25	119.15
3	C	502	XC1	C16-C15-C14	2.35	120.12	117.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	502	XC1	C10-C08-C01	2.29	116.86	111.17
3	C	502	XC1	C08-C01-C02	2.27	115.88	111.62
3	C	502	XC1	C12-S01-N03	-2.08	104.90	107.78

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	502	XC1	C04-C03-C05-C06
3	C	502	XC1	C03-C05-C06-C07
3	C	502	XC1	C13-C12-S01-N03
3	C	502	XC1	C09-C08-C10-C11
3	C	502	XC1	N01-C03-C05-C06
3	C	502	XC1	C17-C12-S01-N03
3	C	502	XC1	C08-C01-C02-O01
3	C	502	XC1	C17-C12-S01-O04
3	C	502	XC1	C08-C01-C02-N01
3	C	502	XC1	C13-C12-S01-O05
3	C	502	XC1	C13-C12-S01-O04
3	C	502	XC1	N01-C03-C04-O02
3	C	502	XC1	N03-C01-C02-N01

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	502	XC1	6	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 XC1 C 502

Bond lengths

Bond angles

Torsions

Rings
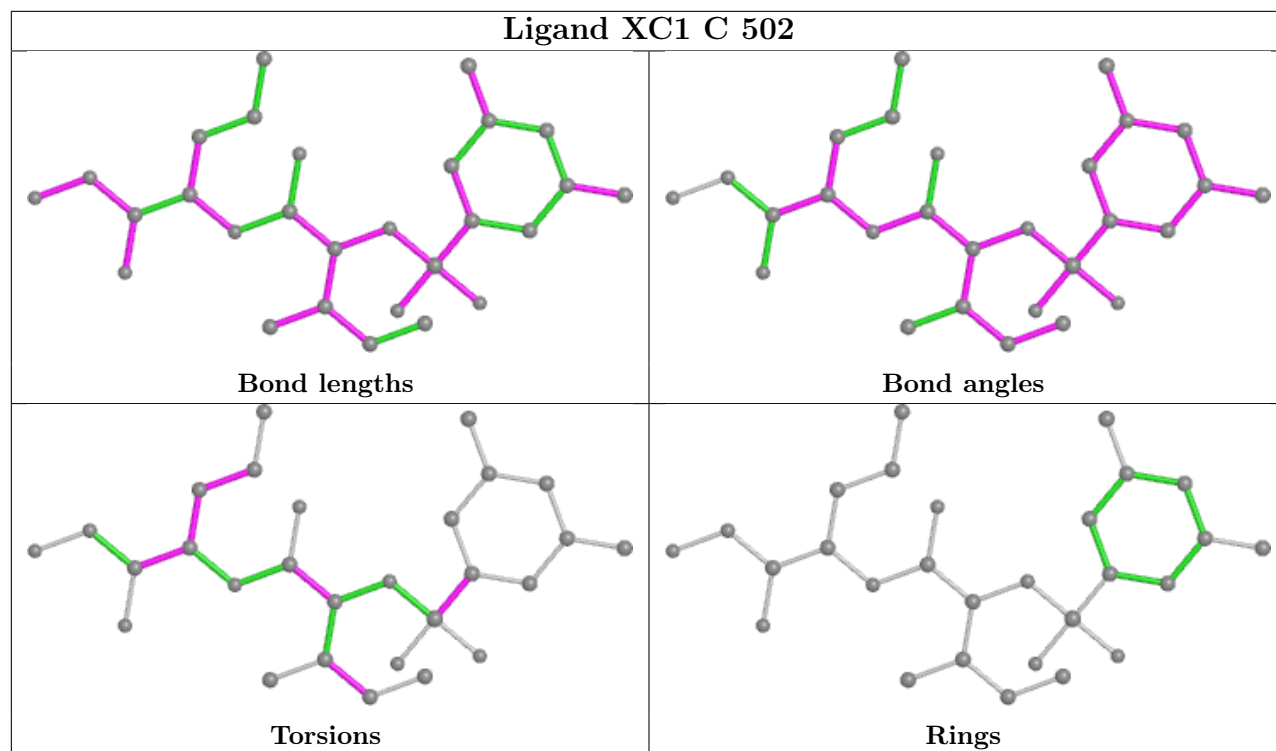
5.7 Other polymers (i)

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(Å^2)	Q<0.9
1	C	398/417 (95%)	2.07	180 (45%)	0	0	30, 56, 95, 115	0

All (180) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	62	PRO	10.4
1	C	247	THR	8.3
1	C	60	ASN	7.9
1	C	57	GLY	7.5
1	C	54	PRO	7.3
1	C	397	LEU	7.2
1	C	398	ALA	6.1
1	C	59	LEU	6.0
1	C	367	LEU	5.7
1	C	186	ILE	5.4
1	C	3	PHE	5.4
1	C	92	THR	5.3
1	C	185	TYR	5.2
1	C	123	ILE	5.0
1	C	107	LEU	4.7
1	C	275	ASP	4.7
1	C	68	VAL	4.6
1	C	67	GLN	4.5
1	C	295	SER	4.5
1	C	369	PHE	4.4
1	C	329	GLY	4.3
1	C	221	LEU	4.3
1	C	354	PHE	4.3
1	C	98	ILE	4.2
1	C	326	ASP	4.1
1	C	341	LEU	4.0
1	C	222	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	328	SER	3.9
1	C	368	ASN	3.9
1	C	271	ALA	3.8
1	C	344	MET	3.8
1	C	276	SER	3.8
1	C	151	LEU	3.8
1	C	91	VAL	3.8
1	C	65	ALA	3.7
1	C	225	LEU	3.7
1	C	38	ILE	3.7
1	C	274	ILE	3.7
1	C	143	SER	3.7
1	C	108	LEU	3.6
1	C	226	ILE	3.6
1	C	227	HIS	3.5
1	C	95	PHE	3.5
1	C	184	GLN	3.5
1	C	358	PHE	3.5
1	C	153	ILE	3.5
1	C	101	THR	3.4
1	C	69	PRO	3.4
1	C	330	LYS	3.4
1	C	27	VAL	3.4
1	C	277	LEU	3.3
1	C	4	VAL	3.3
1	C	58	ASP	3.3
1	C	163	PHE	3.3
1	C	401	PHE	3.3
1	C	332	SER	3.3
1	C	366	TYR	3.3
1	C	42	ILE	3.3
1	C	111	ILE	3.3
1	C	165	CYS	3.2
1	C	94	LEU	3.2
1	C	187	ARG	3.2
1	C	280	ASN	3.2
1	C	135	ILE	3.1
1	C	387	TYR	3.1
1	C	149	LEU	3.1
1	C	305	GLY	3.1
1	C	12	ASP	3.1
1	C	298	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	245	VAL	3.1
1	C	244	LYS	3.1
1	C	350	THR	3.1
1	C	70	VAL	3.0
1	C	124	ASP	3.0
1	C	376	ILE	3.0
1	C	195	GLY	3.0
1	C	232	LEU	3.0
1	C	248	ASN	3.0
1	C	61	PRO	3.0
1	C	410	ASN	3.0
1	C	172	VAL	2.9
1	C	191	ASP	2.9
1	C	100	SER	2.9
1	C	282	PHE	2.9
1	C	112	VAL	2.9
1	C	380	PRO	2.9
1	C	104	GLY	2.8
1	C	44	VAL	2.8
1	C	25	PRO	2.8
1	C	50	THR	2.8
1	C	381	LYS	2.8
1	C	334	ASP	2.8
1	C	45	ILE	2.8
1	C	237	ILE	2.8
1	C	152	VAL	2.7
1	C	408	ILE	2.7
1	C	147	GLU	2.7
1	C	294	ALA	2.7
1	C	242	VAL	2.7
1	C	103	LEU	2.7
1	C	386	ILE	2.7
1	C	53	ASN	2.7
1	C	379	VAL	2.7
1	C	230	HIS	2.7
1	C	310	LEU	2.7
1	C	342	TYR	2.6
1	C	345	LEU	2.6
1	C	132	THR	2.6
1	C	228	ALA	2.6
1	C	146	SER	2.6
1	C	327	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	414	THR	2.6
1	C	313	MET	2.6
1	C	278	GLN	2.6
1	C	359	LYS	2.6
1	C	355	VAL	2.5
1	C	175	LEU	2.5
1	C	258	VAL	2.5
1	C	365	THR	2.5
1	C	134	CYS	2.5
1	C	118	TRP	2.5
1	C	71	SER	2.5
1	C	99	TYR	2.5
1	C	76	THR	2.5
1	C	33	VAL	2.5
1	C	173	LEU	2.5
1	C	281	GLU	2.4
1	C	78	LEU	2.4
1	C	357	PHE	2.4
1	C	306	THR	2.4
1	C	188	PHE	2.4
1	C	130	ILE	2.4
1	C	285	TYR	2.4
1	C	231	ARG	2.4
1	C	270	ASP	2.4
1	C	395	THR	2.4
1	C	394	ASN	2.4
1	C	235	ILE	2.3
1	C	402	ASN	2.3
1	C	88	LEU	2.3
1	C	324	SER	2.3
1	C	370	ASP	2.3
1	C	234	GLY	2.3
1	C	400	ASN	2.3
1	C	218	ALA	2.3
1	C	229	GLY	2.3
1	C	315	ASN	2.3
1	C	63	PRO	2.3
1	C	412	ASN	2.2
1	C	406	THR	2.2
1	C	361	LEU	2.2
1	C	87	TYR	2.2
1	C	17	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	303	ILE	2.2
1	C	348	ILE	2.2
1	C	399	ALA	2.2
1	C	304	VAL	2.2
1	C	416	LEU	2.2
1	C	290	PHE	2.2
1	C	106	MET	2.2
1	C	5	ASN	2.1
1	C	339	ASP	2.1
1	C	176	THR	2.1
1	C	93	LYS	2.1
1	C	26	ASN	2.1
1	C	240	ASN	2.1
1	C	55	GLU	2.1
1	C	363	ARG	2.1
1	C	308	ALA	2.1
1	C	385	THR	2.1
1	C	154	ILE	2.0
1	C	297	LEU	2.0
1	C	167	SER	2.0
1	C	340	LYS	2.0
1	C	9	ASN	2.0
1	C	393	ARG	2.0
1	C	66	LYS	2.0
1	C	233	TYR	2.0
1	C	236	ALA	2.0
1	C	272	LYS	2.0

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

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

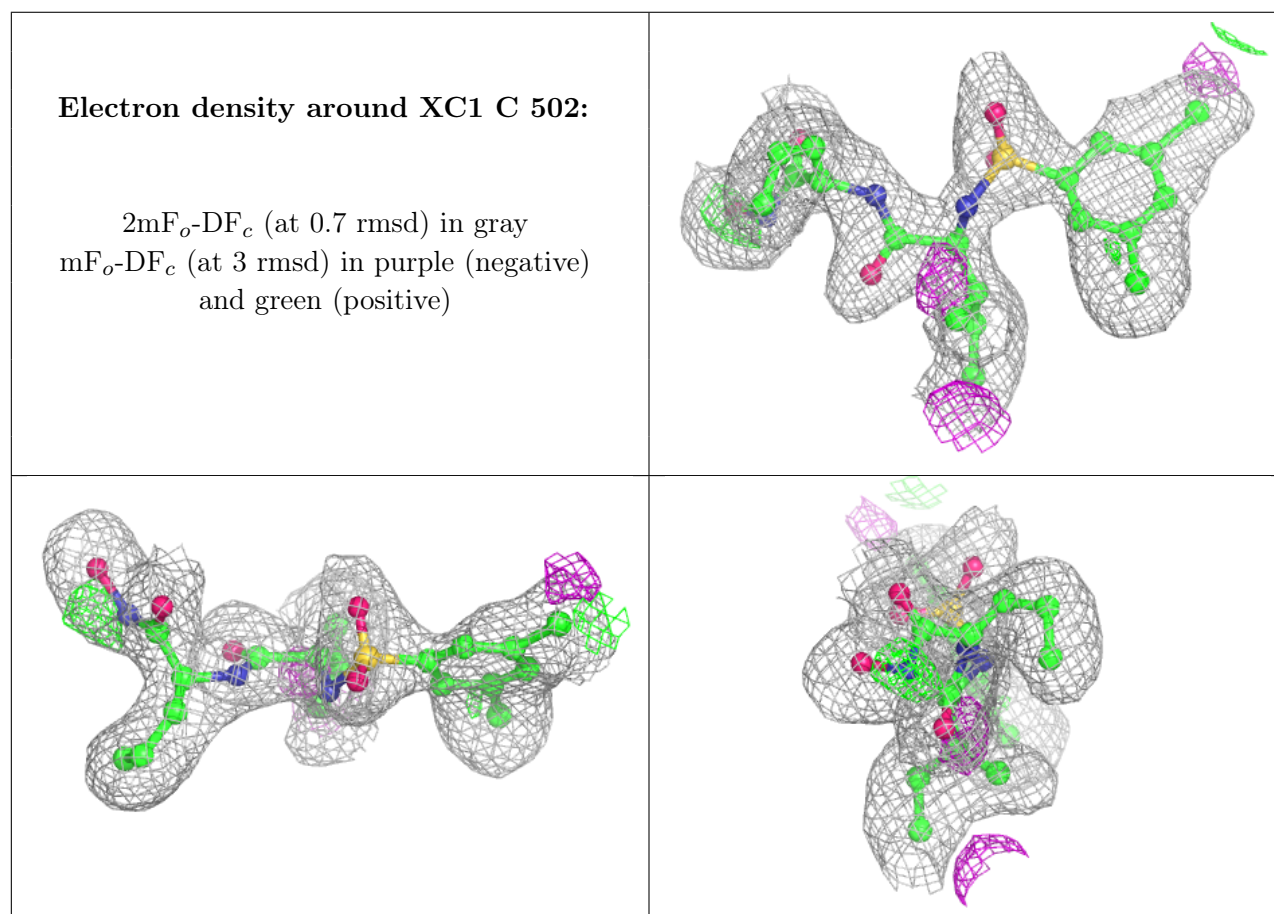## 6.3 Carbohydrates ⓘ

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	XC1	C	502	28/28	0.86	0.25	8,15,30,61	0
2	ZN	C	501	1/1	0.93	1.01	356,356,356,356	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 XC1 C 502:

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

6.5   Other polymers ⓘ

There are no such residues in this entry.