



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:02 PM UTC

PDB ID : 7KYF / pdb_00007kyf
Title : Botulism Neurotoxin 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

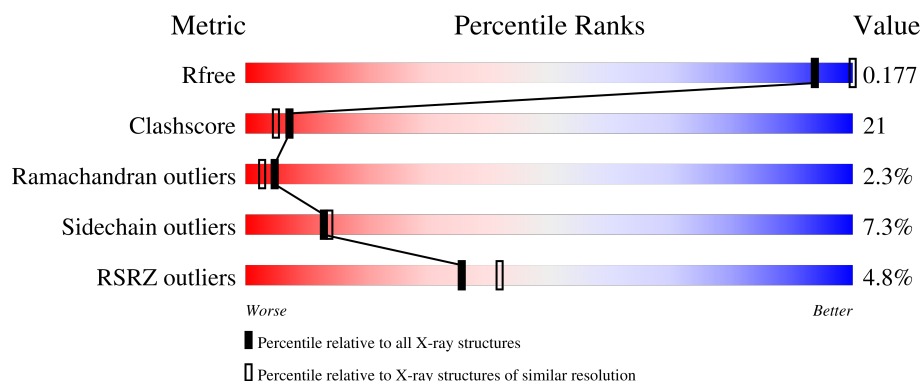
1 Overall quality at a glance

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (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 $\leq 5\%$. 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	

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			

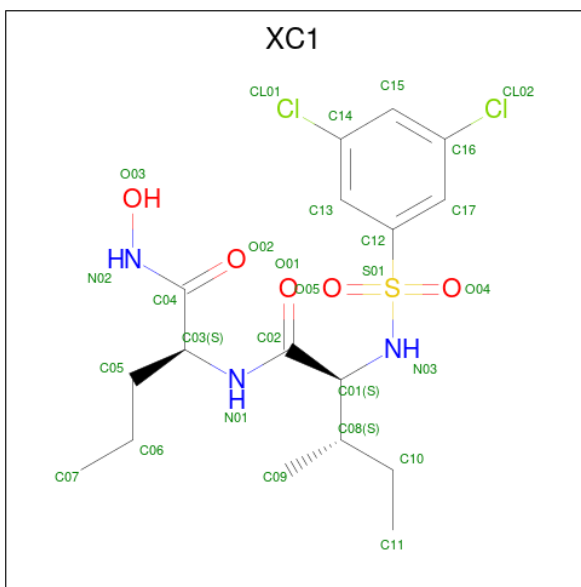
There are 2 discrepancies between the modelled and reference sequences:

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 (CCD ID: 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 (CCD ID: XC1) (formula: C₁₇H₂₅Cl₂N₃O₅S) (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		

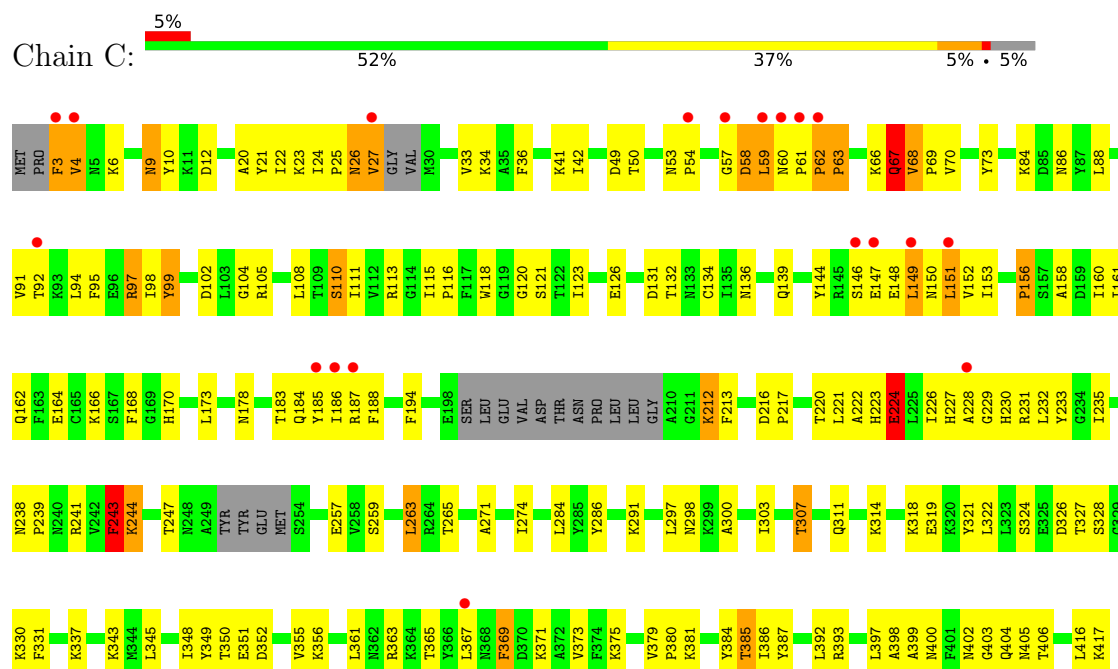
- Molecule 4 is water.

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

3 Residue-property plots [i](#)

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

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 43.25 – 2.33	Depositor EDS
% Data completeness (in resolution range)	99.7 (43.25-2.33) 98.7 (43.25-2.33)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	50.60 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.160 , 0.179 0.171 , 0.177	Depositor DCC
R_{free} test set	2017 reflections (10.27%)	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)	0.40 , 290.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: 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	1.30	17/3300 (0.5%)	1.72	30/4461 (0.7%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	152	VAL	C-O	-9.29	1.14	1.24
1	C	221	LEU	C-O	-8.43	1.14	1.24
1	C	110	SER	C-O	7.19	1.32	1.24
1	C	111	ILE	C-O	-6.08	1.17	1.24
1	C	97	ARG	C-O	-5.92	1.17	1.24
1	C	311	GLN	C-O	-5.90	1.17	1.24
1	C	120	GLY	C-O	5.90	1.30	1.23
1	C	231	ARG	NE-CZ	-5.89	1.26	1.33
1	C	224	GLU	C-O	-5.83	1.17	1.24
1	C	350	THR	C-O	-5.70	1.16	1.23
1	C	314	LYS	C-O	-5.58	1.17	1.24
1	C	156	PRO	C-O	-5.44	1.17	1.23
1	C	42	ILE	C-O	-5.40	1.18	1.24
1	C	86	ASN	C-O	-5.19	1.18	1.24
1	C	178	ASN	N-CA	5.06	1.51	1.46
1	C	229	GLY	C-O	-5.06	1.17	1.23
1	C	20	ALA	C-O	-5.05	1.17	1.23

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	168	PHE	CA-C-N	7.96	130.50	122.30
1	C	168	PHE	C-N-CA	7.96	130.50	122.30
1	C	217	PRO	CA-C-N	7.71	130.94	120.38
1	C	217	PRO	C-N-CA	7.71	130.94	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	132	THR	CA-CB-OG1	6.79	119.79	109.60
1	C	99	TYR	CA-C-N	6.72	129.95	120.28
1	C	99	TYR	C-N-CA	6.72	129.95	120.28
1	C	115	ILE	N-CA-CB	6.23	117.08	110.17
1	C	220	THR	CA-CB-OG1	6.02	118.63	109.60
1	C	405	ASN	CA-C-N	5.99	129.41	120.31
1	C	405	ASN	C-N-CA	5.99	129.41	120.31
1	C	318	LYS	N-CA-C	-5.69	104.98	111.07
1	C	139	GLN	CB-CA-C	5.46	117.34	109.09
1	C	58	ASP	N-CA-C	-5.43	106.58	114.12
1	C	104	GLY	CA-C-N	5.41	127.79	120.38
1	C	104	GLY	C-N-CA	5.41	127.79	120.38
1	C	318	LYS	CA-C-N	5.40	128.06	120.28
1	C	318	LYS	C-N-CA	5.40	128.06	120.28
1	C	385	THR	CA-C-N	5.35	127.50	120.60
1	C	385	THR	C-N-CA	5.35	127.50	120.60
1	C	243	PHE	CA-C-N	5.32	131.71	121.54
1	C	243	PHE	C-N-CA	5.32	131.71	121.54
1	C	88	LEU	CA-C-N	5.24	127.62	120.54
1	C	88	LEU	C-N-CA	5.24	127.62	120.54
1	C	121	SER	CA-C-N	5.24	128.27	120.31
1	C	121	SER	C-N-CA	5.24	128.27	120.31
1	C	104	GLY	CA-C-O	-5.12	115.48	120.75
1	C	102	ASP	N-CA-C	-5.07	105.88	111.71
1	C	387	TYR	CA-C-O	-5.02	115.10	120.42
1	C	188	PHE	CA-CB-CG	5.00	118.80	113.80

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	C	3227	0	3186	132	0
2	C	1	0	0	0	0
3	C	28	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	19	0	0	22	0
All	All	3275	0	3186	133	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 21.

All (133) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:243:PHE:CE1	4:C:609:HOH:O	2.47	0.67
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:53:ASN:CG	1:C:54:PRO:CD	2.77	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:69:PRO:HB3	1:C:371:LYS:C	2.36	0.50
1:C:226:ILE:CG2	1:C:265:THR:HG23	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:58:ASP:C	1:C:60:ASN:H	2.20	0.49
1:C:10:TYR:CZ	1:C:84:LYS:HD2	2.47	0.49
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:226:ILE:HD12	1:C:349:TYR:C	2.38	0.48
1:C:68:VAL:HG13	1:C:373:VAL:CG1	2.37	0.48
1:C:68:VAL:HG21	1:C:417:LYS:C	2.39	0.48
1:C:399:ALA:O	1:C:402:ASN:ND2	2.43	0.48
1:C:9:ASN:HD22	1:C:12:ASP:CG	2.22	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: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:134:CYS:C	1:C:149:LEU:HD21	2.42	0.45
1:C:324:SER:O	1:C:331:PHE:HA	2.16	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: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:3:PHE:CE1	1:C:108:LEU:HB3	2.54	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:216:ASP:OD1	1:C:384:TYR:OH	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:THR:O	1:C:92:THR:HG22	2.19	0.42
1:C:326:ASP:OD1	1:C:328:SER:OG	2.32	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
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:58:ASP:C	1:C:60:ASN:N	2.79	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:131:ASP:CG	4:C:603:HOH:O	2.64	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: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 [i](#)

5.3.1 Protein backbone [i](#)

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%)	5 3

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	59	LEU
1	C	212	LYS

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Mol	Chain	Res	Type
1	C	307	THR
1	C	62	PRO
1	C	63	PRO
1	C	158	ALA
1	C	369	PHE
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%)	331 (93%)	26 (7%)	13	14

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	3	PHE
1	C	4	VAL
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	68	VAL
1	C	146	SER
1	C	149	LEU
1	C	151	LEU
1	C	224	GLU
1	C	241	ARG
1	C	243	PHE
1	C	244	LYS
1	C	247	THR
1	C	257	GLU
1	C	263	LEU

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Mol	Chain	Res	Type
1	C	284	LEU
1	C	291	LYS
1	C	307	THR
1	C	327	THR
1	C	343	LYS
1	C	348	ILE
1	C	356	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	9	ASN
1	C	26	ASN
1	C	60	ASN
1	C	67	GLN
1	C	136	ASN
1	C	139	GLN
1	C	162	GLN
1	C	240	ASN
1	C	368	ASN
1	C	412	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	27,28,28	5.23	16 (59%)	36,39,39	3.51	20 (55%)

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	-	12/34/34/34	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	502	XC1	S01-N03	19.10	1.93	1.61
3	C	502	XC1	C05-C03	-10.46	1.29	1.53
3	C	502	XC1	C01-C02	6.14	1.68	1.52
3	C	502	XC1	C14-CL01	-5.68	1.61	1.74
3	C	502	XC1	C10-C08	-5.48	1.35	1.53
3	C	502	XC1	O03-N02	5.08	1.52	1.40
3	C	502	XC1	O05-S01	-4.95	1.37	1.43
3	C	502	XC1	C01-N03	-4.24	1.39	1.46
3	C	502	XC1	C03-N01	3.95	1.54	1.45
3	C	502	XC1	C13-C12	-3.68	1.32	1.39
3	C	502	XC1	C09-C08	-3.57	1.44	1.53
3	C	502	XC1	O04-S01	-3.31	1.39	1.43
3	C	502	XC1	C08-C01	-2.94	1.46	1.54
3	C	502	XC1	C16-CL02	2.64	1.80	1.74
3	C	502	XC1	O02-C04	-2.49	1.18	1.23
3	C	502	XC1	C12-S01	2.43	1.80	1.76

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	XC1	C13-C14-CL01	-7.97	109.17	119.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	XC1	C15-C14-CL01	7.82	128.98	119.17
3	C	502	XC1	C02-C01-N03	-7.77	96.66	110.46
3	C	502	XC1	O05-S01-C12	6.58	116.28	107.98
3	C	502	XC1	O04-S01-C12	-5.86	100.58	107.98
3	C	502	XC1	C01-N03-S01	-5.34	106.69	121.06
3	C	502	XC1	C17-C12-S01	-5.27	113.67	119.06
3	C	502	XC1	C13-C12-S01	4.81	123.98	119.06
3	C	502	XC1	C03-N01-C02	3.52	129.20	121.65
3	C	502	XC1	C05-C03-C04	3.17	117.86	110.11
3	C	502	XC1	C11-C10-C08	3.11	126.72	113.81
3	C	502	XC1	C17-C16-C15	-3.06	117.92	121.64
3	C	502	XC1	C16-C17-C12	2.83	120.49	118.12
3	C	502	XC1	C17-C16-CL02	2.46	122.25	119.17
3	C	502	XC1	C10-C08-C01	2.26	116.86	111.17
3	C	502	XC1	C08-C01-C02	2.24	115.88	111.64
3	C	502	XC1	C16-C15-C14	2.24	120.12	117.43
3	C	502	XC1	C12-S01-N03	-2.11	104.90	107.79
3	C	502	XC1	C09-C08-C01	2.07	115.92	110.98
3	C	502	XC1	C06-C05-C03	2.00	126.08	114.52

There are no chirality outliers.

All (12) torsion outliers are listed below:

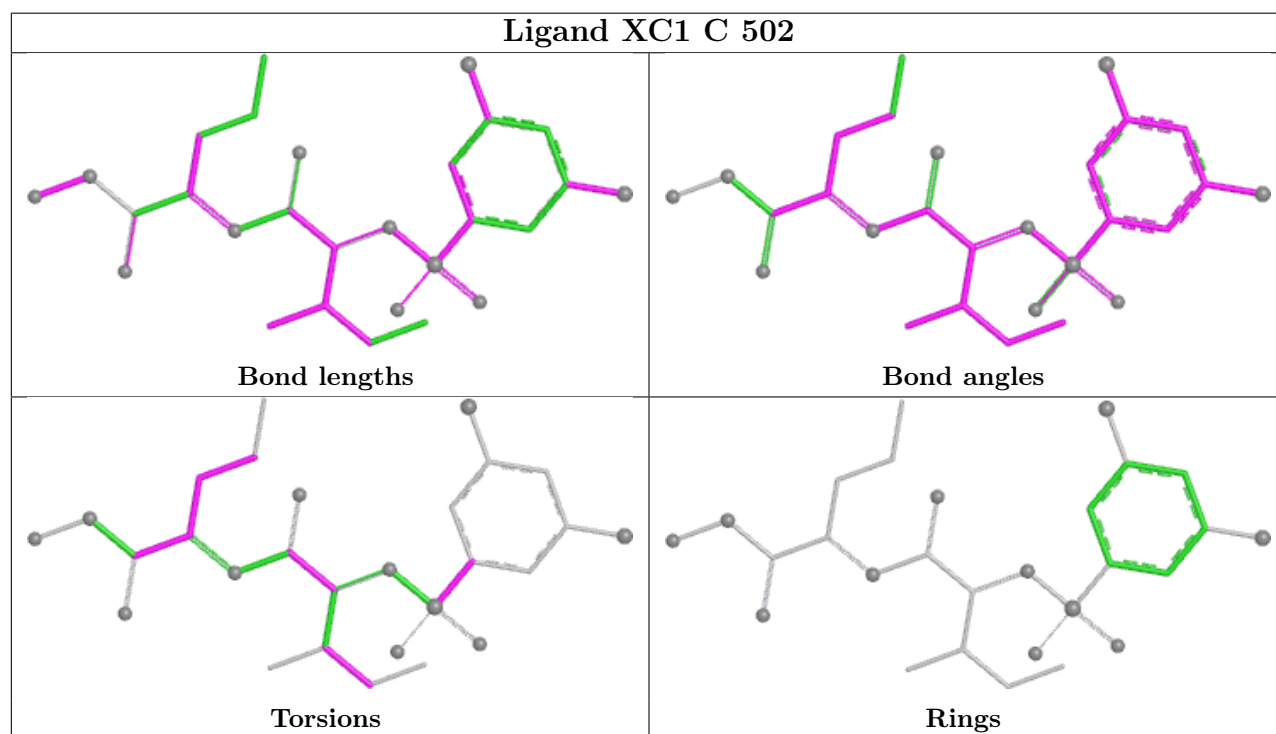
Mol	Chain	Res	Type	Atoms
3	C	502	XC1	C04-C03-C05-C06
3	C	502	XC1	C03-C05-C06-C07
3	C	502	XC1	C13-C12-S01-N03
3	C	502	XC1	C09-C08-C10-C11
3	C	502	XC1	N01-C03-C05-C06
3	C	502	XC1	C17-C12-S01-N03
3	C	502	XC1	C08-C01-C02-O01
3	C	502	XC1	C17-C12-S01-O04
3	C	502	XC1	C08-C01-C02-N01
3	C	502	XC1	C13-C12-S01-O05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

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 than 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.



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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.11	19 (4%)	35 42	30, 56, 95, 115	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	62	PRO	6.5
1	C	27	VAL	4.5
1	C	3	PHE	4.5
1	C	147	GLU	4.3
1	C	54	PRO	4.2
1	C	186	ILE	4.0
1	C	187	ARG	3.3
1	C	59	LEU	3.3
1	C	57	GLY	3.3
1	C	185	TYR	3.3
1	C	92	THR	3.2
1	C	149	LEU	2.9
1	C	151	LEU	2.9
1	C	367	LEU	2.8
1	C	228	ALA	2.6
1	C	4	VAL	2.5
1	C	60	ASN	2.5
1	C	146	SER	2.3
1	C	61	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

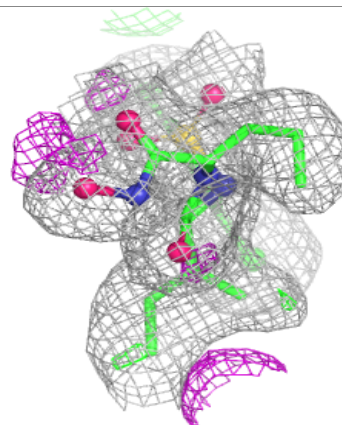
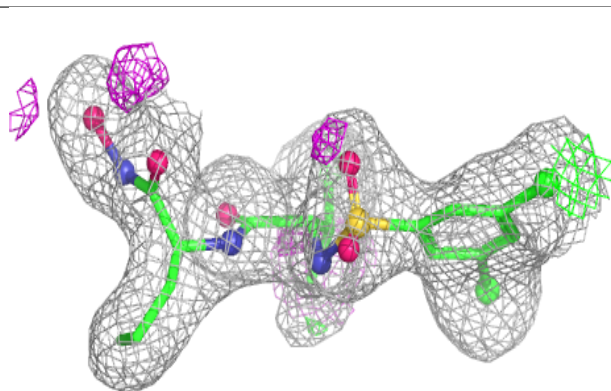
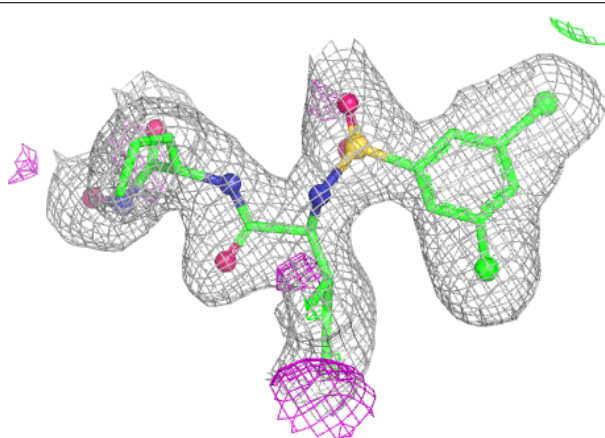
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	C	501	1/1	0.96	0.15	356,356,356,356	0
3	XC1	C	502	28/28	0.99	0.04	8,15,30,61	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:

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.