Full wwPDB X-ray Structure Validation Report ⓘ

Jun 5, 2023 – 07:23 PM EDT

PDB ID	:	8D9Y
Title	:	Crystal structure of Taipan alpha-neurotoxin in complex with Centi-3FTX-D09 antibody
Authors	:	Pletnev, S.; Verardi, R.; Tully, E.S.; Glanville, J.; Kwong, P.D.
Deposited on	:	2022-06-12
Resolution	:	2.20 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:

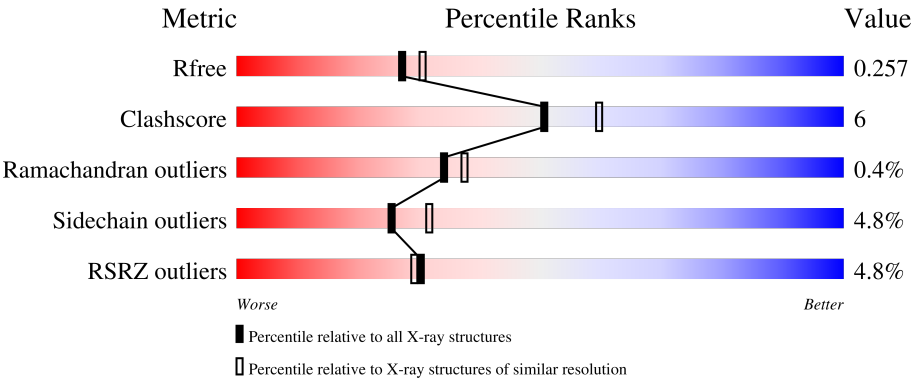
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.33
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	214	92% 7%
1	C	214	89% 9%
1	E	214	7% 82% 17%
1	G	214	13% 79% 18%
2	B	237	% 79% 12% 8%

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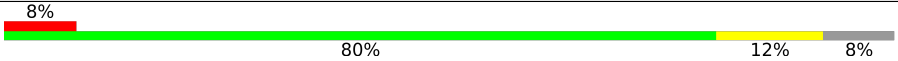
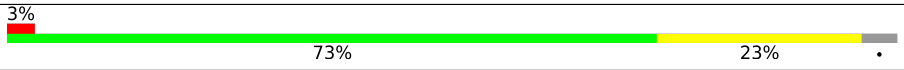
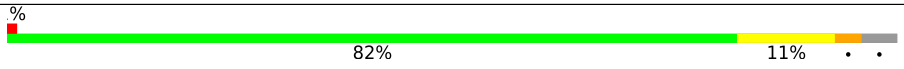
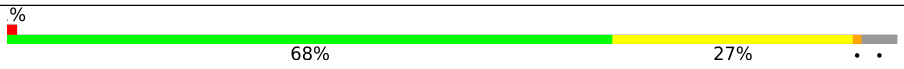
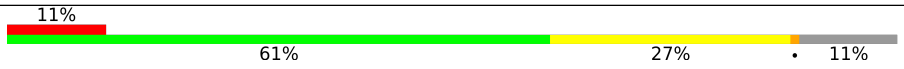
Mol	Chain	Length	Quality of chain
2	D	237	
2	F	237	
2	H	237	
3	I	71	
3	J	71	
3	K	71	
3	L	71	

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 16149 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 Centi-3FTX-D09 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	0	0
			1635	1023	271	337	4			
1	C	213	Total	C	N	O	S	0	0	0
			1635	1023	271	337	4			
1	E	213	Total	C	N	O	S	0	0	0
			1635	1023	271	337	4			
1	G	213	Total	C	N	O	S	0	0	0
			1635	1023	271	337	4			

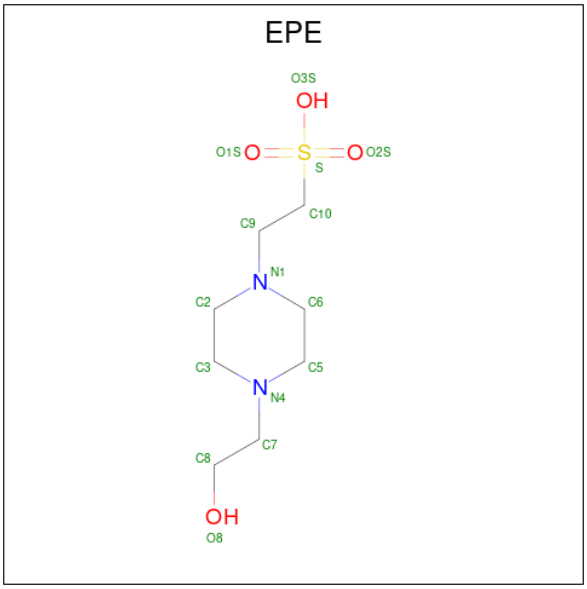
- Molecule 2 is a protein called Centi-3FTX-D09 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	219	Total	C	N	O	S	0	0	0
			1646	1042	278	320	6			
2	D	219	Total	C	N	O	S	0	0	0
			1646	1042	278	320	6			
2	F	219	Total	C	N	O	S	0	0	0
			1646	1042	278	320	6			
2	H	219	Total	C	N	O	S	0	0	0
			1646	1042	278	320	6			

- Molecule 3 is a protein called Long neurotoxin 1.

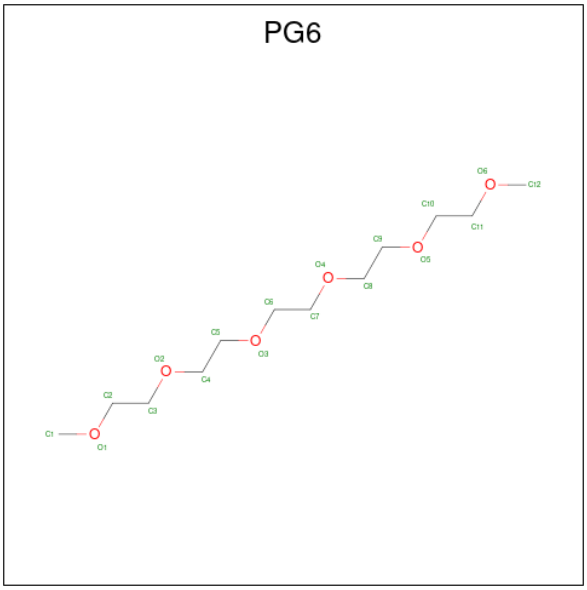
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	68	Total	C	N	O	S	0	0	0
			517	314	98	97	8			
3	J	68	Total	C	N	O	S	0	0	0
			517	314	98	97	8			
3	K	68	Total	C	N	O	S	0	0	0
			517	314	98	97	8			
3	L	63	Total	C	N	O	S	0	0	0
			470	284	87	91	8			

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



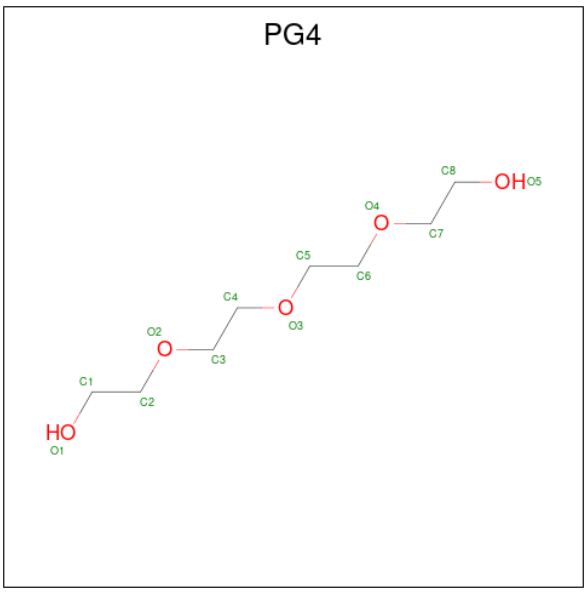
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 5 is 1-(2-METHOXY-ETHOXY)-2-{2-[2-(2-METHOXY-ETHOXY]-ETHOXY}-ETHANE (three-letter code: PG6) (formula: $C_{12}H_{26}O_6$).



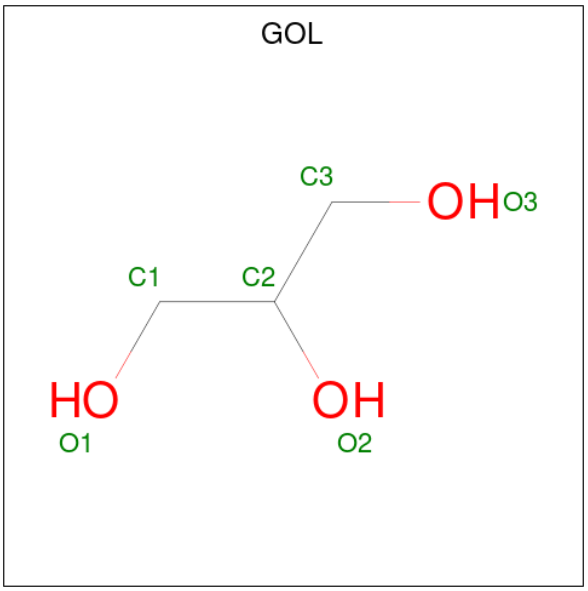
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			18	12	6		

- Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	J	1	Total C O 13 8 5	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	K	1	Total C O 6 3 3	0	0

- Molecule 8 is water.

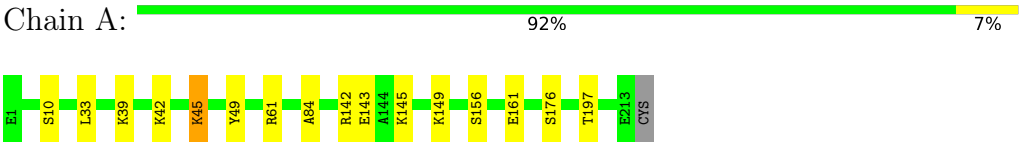
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	136	Total O 136 136	0	0
8	B	147	Total O 147 147	0	0
8	C	128	Total O 128 128	0	0
8	D	142	Total O 142 142	0	0
8	E	58	Total O 58 58	0	0
8	F	82	Total O 82 82	0	0
8	G	58	Total O 58 58	0	0
8	H	96	Total O 96 96	0	0
8	I	33	Total O 33 33	0	0
8	J	33	Total O 33 33	0	0
8	K	27	Total O 27 27	0	0
8	L	12	Total O 12 12	0	0

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.

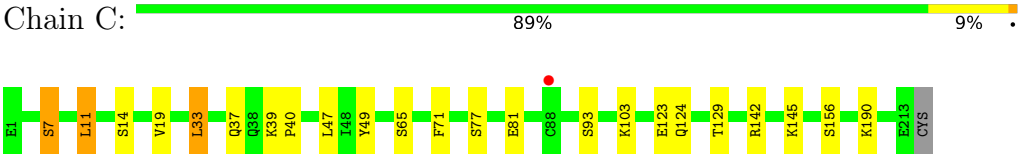
• Molecule 1: Centi-3FTX-D09 Fab light chain

Chain A:



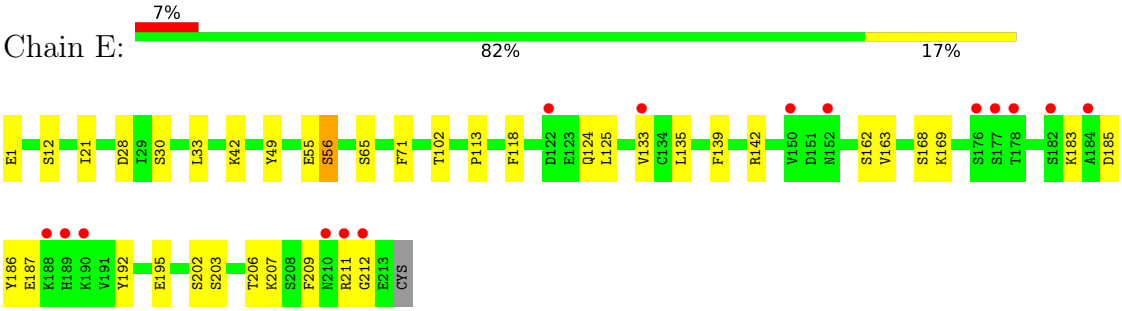
• Molecule 1: Centi-3FTX-D09 Fab light chain

Chain C:



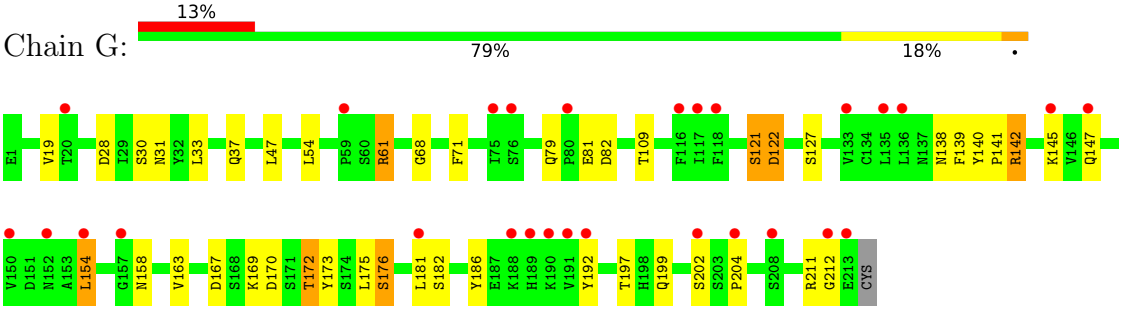
• Molecule 1: Centi-3FTX-D09 Fab light chain

Chain E:



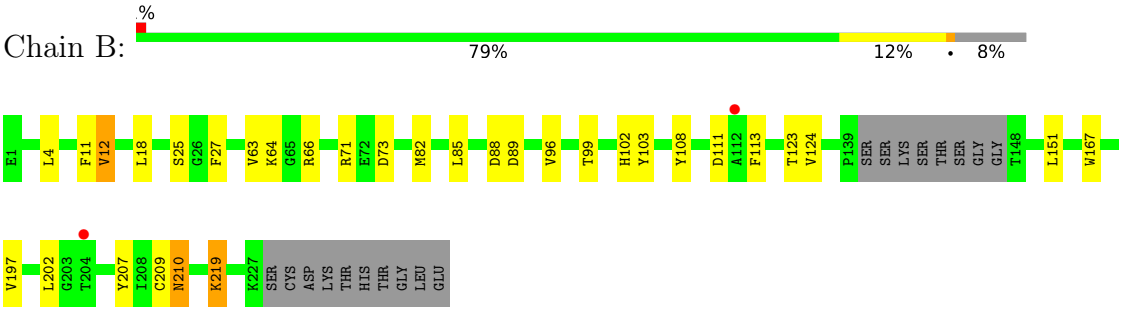
• Molecule 1: Centi-3FTX-D09 Fab light chain

Chain G:



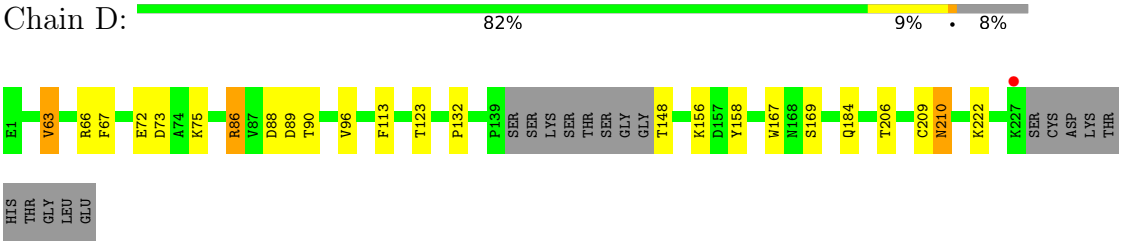
• Molecule 2: Centi-3FTX-D09 Fab heavy chain

Chain B:



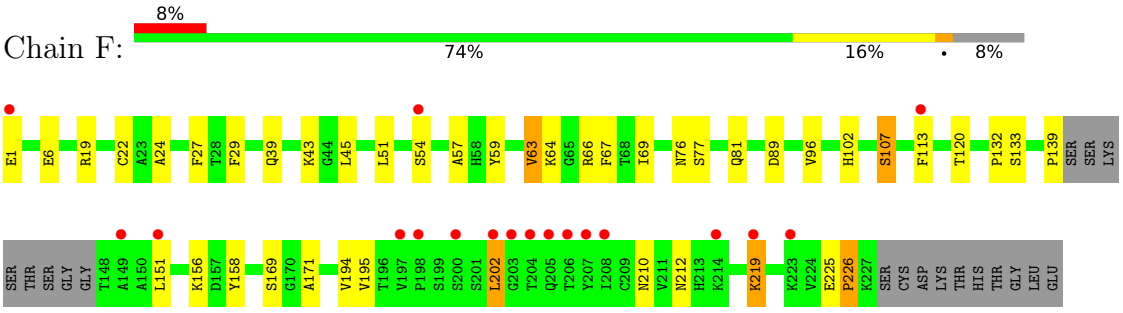
• Molecule 2: Centi-3FTX-D09 Fab heavy chain

Chain D:



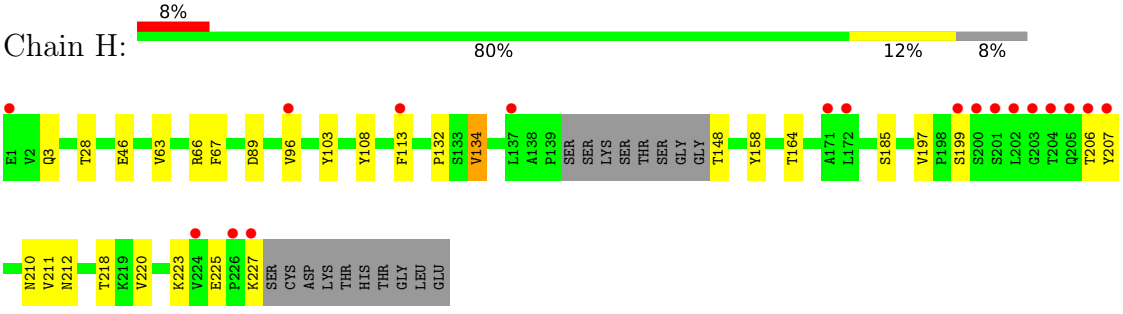
• Molecule 2: Centi-3FTX-D09 Fab heavy chain

Chain F:



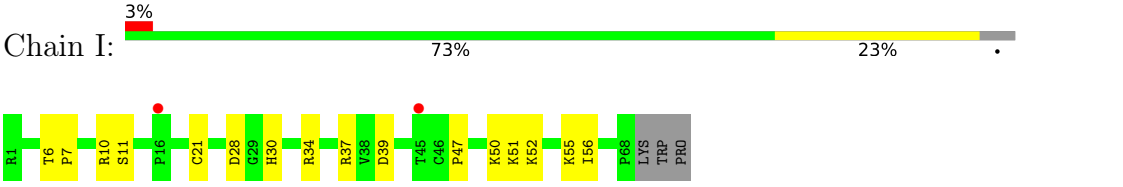
• Molecule 2: Centi-3FTX-D09 Fab heavy chain

Chain H:



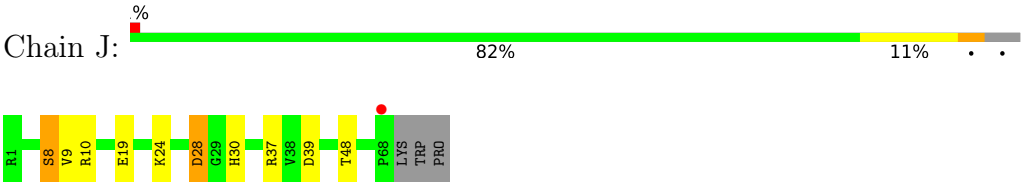
• Molecule 3: Long neurotoxin 1

Chain I:



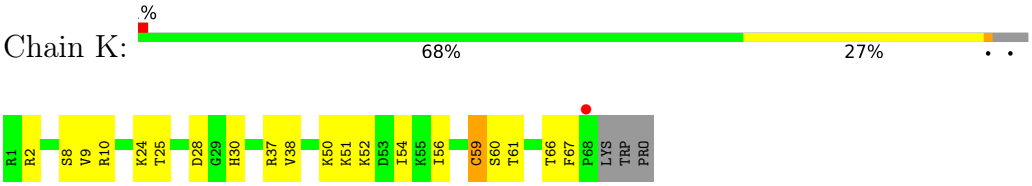
• Molecule 3: Long neurotoxin 1

Chain J:



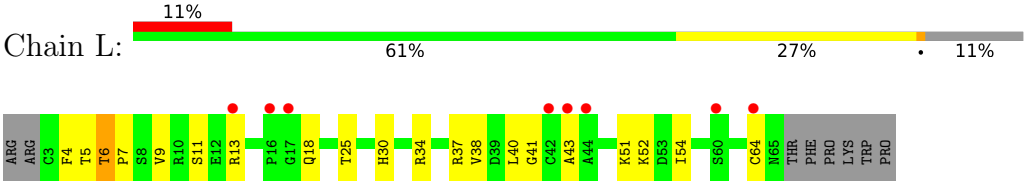
• Molecule 3: Long neurotoxin 1

Chain K:



• Molecule 3: Long neurotoxin 1

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	77.81Å 87.23Å 101.30Å 109.29° 104.26° 106.48°	Depositor
Resolution (Å)	29.54 – 2.20 29.54 – 2.20	Depositor EDS
% Data completeness (in resolution range)	86.6 (29.54-2.20) 86.7 (29.54-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.20	Depositor
R, R_{free}	0.209 , 0.262 0.206 , 0.257	Depositor DCC
R_{free} test set	1959 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å^2)	34.5	Xtriage
Anisotropy	0.741	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 51.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,h+k+l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16149	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: EPE, PG6, GOL, PG4

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	0.26	0/1670	0.51	0/2269
1	C	0.26	0/1670	0.49	0/2269
1	E	0.25	0/1670	0.50	0/2269
1	G	0.27	0/1670	0.56	0/2269
2	B	0.26	0/1688	0.52	0/2297
2	D	0.26	0/1688	0.52	0/2297
2	F	0.26	0/1688	0.53	0/2297
2	H	0.29	0/1688	0.53	0/2297
3	I	0.26	0/528	0.64	0/713
3	J	0.34	0/528	0.60	0/713
3	K	0.27	0/528	0.63	0/713
3	L	0.29	0/479	0.61	0/647
All	All	0.27	0/15495	0.53	0/21050

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

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	1635	0	1579	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1635	0	1579	13	0
1	E	1635	0	1579	22	0
1	G	1635	0	1579	24	0
2	B	1646	0	1589	16	0
2	D	1646	0	1589	13	0
2	F	1646	0	1589	25	0
2	H	1646	0	1589	17	0
3	I	517	0	506	14	0
3	J	517	0	506	6	0
3	K	517	0	506	11	0
3	L	470	0	454	15	0
4	A	15	0	17	1	0
5	C	18	0	26	0	0
6	J	13	0	18	1	0
7	K	6	0	8	1	0
8	A	136	0	0	3	0
8	B	147	0	0	1	0
8	C	128	0	0	6	0
8	D	142	0	0	1	0
8	E	58	0	0	5	0
8	F	82	0	0	1	0
8	G	58	0	0	1	0
8	H	96	0	0	1	0
8	I	33	0	0	4	0
8	J	33	0	0	1	0
8	K	27	0	0	0	0
8	L	12	0	0	1	0
All	All	16149	0	14713	170	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 6.

All (170) 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)
2:B:102:HIS:NE2	3:I:7:PRO:O	2.07	0.87
1:E:186:TYR:O	1:E:192:TYR:OH	2.09	0.70
3:I:30:HIS:HB3	3:I:34:ARG:HG3	1.74	0.69
2:D:86:ARG:NH2	2:D:88:ASP:OD1	2.16	0.69
3:L:5:THR:HG23	3:L:41:GLY:HA2	1.72	0.69
2:D:169:SER:H	2:D:210:ASN:HD21	1.41	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:19:GLU:OE1	8:J:201:HOH:O	2.13	0.67
2:B:66:ARG:NH2	2:B:89:ASP:OD2	2.28	0.67
1:C:39:LYS:NZ	8:C:403:HOH:O	2.28	0.65
1:A:143:GLU:N	1:A:143:GLU:OE1	2.29	0.65
3:L:37:ARG:NH1	8:L:101:HOH:O	2.30	0.65
2:F:66:ARG:NH2	2:F:89:ASP:OD2	2.31	0.62
3:K:59:CYS:SG	3:K:60:SER:N	2.72	0.62
2:H:66:ARG:NH2	2:H:89:ASP:OD2	2.31	0.62
2:F:59:TYR:HB2	2:F:64:LYS:HG3	1.83	0.61
2:F:169:SER:OG	2:H:212:ASN:ND2	2.34	0.60
3:I:21:CYS:SG	8:I:110:HOH:O	2.56	0.60
2:D:148:THR:N	8:D:303:HOH:O	2.35	0.60
2:H:148:THR:N	2:H:199:SER:HG	2.00	0.60
3:L:18:GLN:HB2	3:L:43:ALA:O	2.01	0.60
1:C:142:ARG:NH2	8:C:408:HOH:O	2.35	0.59
2:F:51:LEU:HD22	2:F:69:ILE:HG23	1.84	0.59
2:H:46:GLU:HG3	8:H:301:HOH:O	2.03	0.59
3:J:28:ASP:HB3	3:J:30:HIS:H	1.68	0.59
3:K:28:ASP:HB3	3:K:30:HIS:H	1.68	0.59
1:E:169:LYS:HE2	8:E:301:HOH:O	2.01	0.58
2:F:132:PRO:HB3	2:F:158:TYR:HB3	1.85	0.58
2:D:66:ARG:NH2	2:D:89:ASP:OD2	2.36	0.58
1:E:42:LYS:HE3	8:E:346:HOH:O	2.04	0.58
1:C:7:SER:OG	8:C:401:HOH:O	2.17	0.58
1:G:140:TYR:CD1	1:G:141:PRO:HA	2.39	0.58
1:C:40:PRO:O	8:C:402:HOH:O	2.17	0.58
1:C:11:LEU:HD11	1:C:19:VAL:HG13	1.86	0.57
3:K:66:THR:HG21	7:K:101:GOL:H32	1.86	0.57
2:H:103:TYR:CE2	3:L:37:ARG:HG2	2.40	0.56
2:F:139:PRO:HG2	2:F:202:LEU:HD21	1.87	0.56
1:G:139:PHE:C	1:G:172:THR:HG1	2.09	0.56
3:I:47:PRO:HB2	3:I:56:ILE:HD13	1.88	0.56
1:G:28:ASP:OD2	1:G:68:GLY:HA2	2.06	0.56
1:G:81:GLU:N	1:G:81:GLU:OE2	2.39	0.55
2:F:27:PHE:CE1	2:F:29:PHE:HA	2.42	0.54
1:A:145:LYS:HB3	1:A:197:THR:HB	1.89	0.54
3:K:8:SER:O	3:K:10:ARG:N	2.40	0.54
2:F:24:ALA:O	2:F:76:ASN:ND2	2.34	0.54
1:E:135:LEU:HD22	2:F:194:VAL:HG11	1.91	0.53
1:E:21:ILE:HG12	1:E:102:THR:HG21	1.91	0.53
3:I:51:LYS:HB3	3:I:52:LYS:HG3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:223:LYS:NZ	2:H:225:GLU:OE1	2.34	0.53
2:F:63:VAL:HG13	2:F:67:PHE:HB2	1.90	0.52
1:G:121:SER:OG	1:G:122:ASP:N	2.42	0.52
1:G:169:LYS:HG3	1:G:170:ASP:N	2.24	0.52
1:E:118:PHE:HB2	1:E:133:VAL:HG13	1.90	0.52
1:E:187:GLU:HG2	1:E:211:ARG:HH21	1.73	0.52
1:G:172:THR:OG1	1:G:173:TYR:N	2.41	0.52
3:K:51:LYS:O	3:K:54:ILE:HG22	2.09	0.52
1:C:81:GLU:OE2	8:C:403:HOH:O	2.18	0.51
1:E:168:SER:N	8:E:301:HOH:O	2.42	0.51
1:G:211:ARG:HH11	1:G:212:GLY:HA3	1.75	0.51
3:K:25:THR:HG22	3:K:38:VAL:HG12	1.92	0.51
2:H:108:TYR:CZ	3:L:34:ARG:HD2	2.45	0.51
2:F:96:VAL:CG1	2:F:113:PHE:HB3	2.40	0.51
3:I:28:ASP:HB3	3:I:30:HIS:H	1.75	0.51
2:B:111:ASP:OD2	8:B:301:HOH:O	2.19	0.50
3:L:51:LYS:HG3	3:L:52:LYS:O	2.10	0.50
2:F:225:GLU:HB2	2:F:226:PRO:HD2	1.92	0.50
3:J:8:SER:O	3:J:10:ARG:N	2.37	0.50
2:D:72:GLU:HB3	2:D:75:LYS:HB2	1.94	0.50
1:E:124:GLN:NE2	8:E:308:HOH:O	2.43	0.50
3:J:24:LYS:HD3	6:J:101:PG4:H52	1.93	0.50
2:D:63:VAL:HG13	2:D:67:PHE:HB2	1.94	0.49
1:G:145:LYS:HB3	1:G:197:THR:HB	1.94	0.49
1:C:37:GLN:HB2	1:C:47:LEU:HD11	1.93	0.49
2:D:90:THR:HG23	2:D:123:THR:HA	1.94	0.49
1:A:39:LYS:HD3	1:A:84:ALA:HB2	1.94	0.49
2:F:139:PRO:HG2	2:F:202:LEU:CD2	2.43	0.49
2:H:63:VAL:HG13	2:H:67:PHE:HB2	1.94	0.48
1:E:207:LYS:HA	1:E:207:LYS:HD3	1.59	0.48
3:K:24:LYS:HD3	3:K:54:ILE:HD11	1.93	0.48
1:A:142:ARG:NH2	1:C:145:LYS:HE3	2.29	0.48
1:C:49:TYR:OH	3:J:28:ASP:OD1	2.27	0.48
1:E:142:ARG:NH1	1:E:163:VAL:HG21	2.29	0.48
1:G:30:SER:OG	1:G:31:ASN:N	2.44	0.48
1:G:139:PHE:N	1:G:172:THR:OG1	2.47	0.48
2:H:96:VAL:CG1	2:H:113:PHE:HB3	2.44	0.47
2:B:108:TYR:CZ	3:I:34:ARG:HD2	2.49	0.47
2:B:210:ASN:HB3	2:B:219:LYS:HZ1	1.78	0.47
2:F:96:VAL:HG11	2:F:113:PHE:HB3	1.97	0.47
2:B:11:PHE:CD2	2:B:123:THR:HB	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:10:ARG:NH2	8:I:106:HOH:O	2.48	0.47
2:B:11:PHE:HD2	2:B:123:THR:HB	1.80	0.46
2:D:132:PRO:HB3	2:D:158:TYR:HB3	1.97	0.46
1:G:37:GLN:HB2	1:G:47:LEU:HD11	1.97	0.46
2:B:71:ARG:HD2	2:B:73:ASP:OD1	2.15	0.46
2:B:82:MET:HB3	2:B:85:LEU:HD21	1.97	0.46
3:K:25:THR:HA	3:K:37:ARG:O	2.15	0.46
1:G:202:SER:N	8:G:308:HOH:O	2.48	0.46
2:H:132:PRO:HB3	2:H:158:TYR:HB3	1.98	0.46
3:K:24:LYS:HG2	3:K:56:ILE:HG12	1.96	0.46
2:D:156:LYS:NZ	2:D:184:GLN:HE22	2.13	0.46
1:G:175:LEU:HD23	1:G:176:SER:N	2.31	0.46
4:A:301:EPE:H32	8:A:513:HOH:O	2.16	0.46
1:G:61:ARG:NH1	1:G:82:ASP:OD1	2.47	0.45
1:A:45:LYS:HD3	8:A:470:HOH:O	2.16	0.45
2:H:206:THR:HB	2:H:223:LYS:HE2	1.97	0.45
1:A:61:ARG:NH2	8:A:419:HOH:O	2.48	0.45
2:B:167:TRP:CZ3	2:B:209:CYS:HB3	2.51	0.45
1:G:147:GLN:OE1	1:G:154:LEU:HD12	2.17	0.45
1:E:55:GLU:HG3	1:E:56:SER:N	2.31	0.45
2:H:108:TYR:CE2	3:L:34:ARG:HD2	2.51	0.45
2:B:108:TYR:CE2	3:I:34:ARG:HD2	2.52	0.45
1:E:169:LYS:N	8:E:301:HOH:O	2.20	0.45
1:G:158:ASN:ND2	1:G:181:LEU:HD21	2.31	0.45
1:G:167:ASP:HB3	1:G:170:ASP:OD1	2.16	0.45
2:D:167:TRP:CZ3	2:D:209:CYS:HB3	2.52	0.44
1:E:192:TYR:HD1	1:E:209:PHE:CE1	2.36	0.44
1:G:158:ASN:HD22	1:G:181:LEU:HD21	1.81	0.44
2:F:6:GLU:HB2	2:F:120:THR:OG1	2.17	0.44
1:G:197:THR:HG23	1:G:204:PRO:HG3	2.00	0.44
2:F:102:HIS:NE2	2:F:107:SER:OG	2.50	0.44
1:E:49:TYR:OH	3:K:28:ASP:OD1	2.30	0.43
3:L:30:HIS:HB3	3:L:34:ARG:HG3	1.99	0.43
2:F:19:ARG:HB2	2:F:81:GLN:OE1	2.18	0.43
2:H:218:THR:HG22	2:H:220:VAL:HG23	1.99	0.43
2:F:39:GLN:HB2	2:F:45:LEU:HD23	1.99	0.43
3:I:6:THR:HG21	3:I:39:ASP:HA	2.01	0.43
3:L:7:PRO:O	3:L:9:VAL:HG23	2.19	0.43
2:B:4:LEU:HD21	2:B:27:PHE:HZ	1.82	0.43
2:F:171:ALA:HA	2:H:164:THR:HG21	2.00	0.43
2:F:212:ASN:HD22	2:F:219:LYS:HG3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:197:VAL:HG11	2:H:207:TYR:CZ	2.54	0.43
1:C:190:LYS:NZ	8:C:419:HOH:O	2.51	0.43
1:E:169:LYS:HE2	1:E:169:LYS:HB2	1.92	0.43
3:I:55:LYS:NZ	8:I:107:HOH:O	2.50	0.43
3:L:6:THR:HB	3:L:40:LEU:H	1.84	0.43
3:L:25:THR:HG22	3:L:38:VAL:HG12	2.01	0.43
1:G:142:ARG:NH2	1:G:163:VAL:HG11	2.33	0.42
3:K:66:THR:HG22	3:K:67:PHE:O	2.19	0.42
2:D:96:VAL:CG1	2:D:113:PHE:HB3	2.50	0.42
3:L:4:PHE:CD1	3:L:11:SER:HB2	2.54	0.42
3:L:51:LYS:O	3:L:54:ILE:HG22	2.19	0.42
2:B:96:VAL:CG1	2:B:113:PHE:HB3	2.49	0.42
2:D:88:ASP:OD2	2:D:88:ASP:N	2.37	0.42
1:E:187:GLU:HA	1:E:211:ARG:NE	2.34	0.42
2:F:156:LYS:NZ	8:F:316:HOH:O	2.53	0.42
1:A:49:TYR:OH	3:I:28:ASP:OD2	2.37	0.42
1:C:49:TYR:OH	3:J:37:ARG:NH1	2.53	0.42
1:G:186:TYR:HA	1:G:192:TYR:OH	2.20	0.42
1:C:124:GLN:HG2	1:C:129:THR:O	2.20	0.41
3:I:10:ARG:HB2	8:I:103:HOH:O	2.20	0.41
2:B:103:TYR:CE2	3:I:37:ARG:HG2	2.55	0.41
1:E:209:PHE:C	1:E:209:PHE:CD1	2.94	0.41
2:F:151:LEU:HD12	2:F:195:VAL:HG13	2.02	0.41
3:L:52:LYS:HE2	3:L:52:LYS:HB2	1.93	0.41
1:C:33:LEU:HD22	1:C:71:PHE:CG	2.56	0.41
2:H:134:VAL:HG11	2:H:211:VAL:HG21	2.03	0.41
1:A:161:GLU:HA	1:A:176:SER:O	2.21	0.41
2:F:22:CYS:O	2:F:77:SER:HA	2.20	0.41
2:B:197:VAL:HG11	2:B:207:TYR:CE1	2.56	0.41
2:D:169:SER:N	2:D:210:ASN:HD21	2.14	0.41
2:F:51:LEU:HD13	2:F:57:ALA:HB2	2.03	0.41
2:F:212:ASN:ND2	2:F:219:LYS:HD2	2.36	0.41
2:H:96:VAL:HG11	2:H:113:PHE:HB3	2.03	0.41
1:E:33:LEU:HD22	1:E:71:PHE:CG	2.56	0.41
3:L:51:LYS:HD3	3:L:52:LYS:H	1.86	0.41
1:E:125:LEU:O	1:E:183:LYS:HD2	2.20	0.40
1:E:113:PRO:HB3	1:E:139:PHE:HB3	2.03	0.40
1:G:33:LEU:HD22	1:G:71:PHE:CG	2.57	0.40
1:E:195:GLU:HG3	1:E:206:THR:HG22	2.02	0.40
2:B:12:VAL:O	2:B:124:VAL:HA	2.21	0.40
1:G:61:ARG:NH1	1:G:79:GLN:HB2	2.36	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	A	211/214 (99%)	205 (97%)	6 (3%)	0	100 100
1	C	211/214 (99%)	205 (97%)	6 (3%)	0	100 100
1	E	211/214 (99%)	200 (95%)	10 (5%)	1 (0%)	29 31
1	G	211/214 (99%)	196 (93%)	13 (6%)	2 (1%)	17 16
2	B	215/237 (91%)	211 (98%)	4 (2%)	0	100 100
2	D	215/237 (91%)	209 (97%)	6 (3%)	0	100 100
2	F	215/237 (91%)	209 (97%)	5 (2%)	1 (0%)	29 31
2	H	215/237 (91%)	211 (98%)	4 (2%)	0	100 100
3	I	66/71 (93%)	62 (94%)	4 (6%)	0	100 100
3	J	66/71 (93%)	65 (98%)	0	1 (2%)	10 8
3	K	66/71 (93%)	62 (94%)	2 (3%)	2 (3%)	4 2
3	L	61/71 (86%)	58 (95%)	3 (5%)	0	100 100
All	All	1963/2088 (94%)	1893 (96%)	63 (3%)	7 (0%)	34 37

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	121	SER
3	K	52	LYS
3	J	9	VAL
3	K	9	VAL
1	G	138	ASN
1	E	212	GLY
2	F	226	PRO

5.3.2 Protein sidechains (i)

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	187/188 (100%)	181 (97%)	6 (3%)	39	50
1	C	187/188 (100%)	177 (95%)	10 (5%)	22	27
1	E	187/188 (100%)	177 (95%)	10 (5%)	22	27
1	G	187/188 (100%)	175 (94%)	12 (6%)	17	20
2	B	183/198 (92%)	172 (94%)	11 (6%)	19	22
2	D	183/198 (92%)	177 (97%)	6 (3%)	38	49
2	F	183/198 (92%)	174 (95%)	9 (5%)	25	31
2	H	183/198 (92%)	177 (97%)	6 (3%)	38	49
3	I	60/63 (95%)	58 (97%)	2 (3%)	38	49
3	J	60/63 (95%)	56 (93%)	4 (7%)	16	18
3	K	60/63 (95%)	56 (93%)	4 (7%)	16	18
3	L	55/63 (87%)	52 (94%)	3 (6%)	21	26
All	All	1715/1796 (96%)	1632 (95%)	83 (5%)	25	32

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	SER
1	A	33	LEU
1	A	42	LYS
1	A	45	LYS
1	A	149	LYS
1	A	156	SER
2	B	12	VAL
2	B	18	LEU
2	B	25	SER
2	B	63	VAL
2	B	64	LYS
2	B	88	ASP
2	B	99	THR
2	B	151	LEU

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Mol	Chain	Res	Type
2	B	202	LEU
2	B	210	ASN
2	B	219	LYS
1	C	7	SER
1	C	11	LEU
1	C	14	SER
1	C	33	LEU
1	C	65	SER
1	C	77	SER
1	C	93	SER
1	C	103	LYS
1	C	123	GLU
1	C	156	SER
2	D	63	VAL
2	D	73	ASP
2	D	86	ARG
2	D	206	THR
2	D	210	ASN
2	D	222	LYS
1	E	1	GLU
1	E	12	SER
1	E	28	ASP
1	E	30	SER
1	E	56	SER
1	E	65	SER
1	E	162	SER
1	E	185	ASP
1	E	202	SER
1	E	203	SER
2	F	1	GLU
2	F	43	LYS
2	F	54	SER
2	F	63	VAL
2	F	107	SER
2	F	133	SER
2	F	202	LEU
2	F	210	ASN
2	F	219	LYS
1	G	19	VAL
1	G	54	LEU
1	G	61	ARG
1	G	109	THR

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Mol	Chain	Res	Type
1	G	122	ASP
1	G	127	SER
1	G	142	ARG
1	G	154	LEU
1	G	172	THR
1	G	176	SER
1	G	182	SER
1	G	199	GLN
2	H	3	GLN
2	H	28	THR
2	H	134	VAL
2	H	185	SER
2	H	210	ASN
2	H	227	LYS
3	I	11	SER
3	I	50	LYS
3	J	8	SER
3	J	28	ASP
3	J	39	ASP
3	J	48	THR
3	K	2	ARG
3	K	50	LYS
3	K	59	CYS
3	K	61	THR
3	L	6	THR
3	L	13	ARG
3	L	64	CYS

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

Mol	Chain	Res	Type
2	D	184	GLN
2	D	210	ASN
2	F	212	ASN
2	H	31	ASN
2	H	212	ASN

5.3.3 RNA

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are 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	$\#\|Z\| > 2$
4	EPE	A	301	-	15,15,15	0.95	1 (6%)	18,20,20	1.74	5 (27%)
5	PG6	C	301	-	17,17,17	0.29	0	16,16,16	0.18	0
7	GOL	K	101	-	5,5,5	0.91	0	5,5,5	1.00	0
6	PG4	J	101	-	12,12,12	0.14	0	11,11,11	0.60	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
4	EPE	A	301	-	-	4/9/19/19	0/1/1/1
5	PG6	C	301	-	-	5/15/15/15	-
7	GOL	K	101	-	-	2/4/4/4	-
6	PG4	J	101	-	-	7/10/10/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	301	EPE	C10-S	3.26	1.82	1.77

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	301	EPE	C5-N4-C3	3.70	117.17	108.83
4	A	301	EPE	C7-N4-C5	3.03	118.99	111.23
4	A	301	EPE	O3S-S-C10	2.88	110.42	105.77
4	A	301	EPE	C7-N4-C3	2.35	117.25	111.23
4	A	301	EPE	O1S-S-C10	2.15	109.50	106.92

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	301	EPE	S-C10-C9-N1
5	C	301	PG6	O2-C4-C5-O3
6	J	101	PG4	O3-C5-C6-O4
5	C	301	PG6	O1-C2-C3-O2
5	C	301	PG6	O5-C10-C11-O6
6	J	101	PG4	O2-C3-C4-O3
4	A	301	EPE	C9-C10-S-O3S
7	K	101	GOL	O2-C2-C3-O3
6	J	101	PG4	C3-C4-O3-C5
6	J	101	PG4	C5-C6-O4-C7
7	K	101	GOL	C1-C2-C3-O3
5	C	301	PG6	C6-C7-O4-C8
4	A	301	EPE	C9-C10-S-O1S
4	A	301	EPE	C9-C10-S-O2S
5	C	301	PG6	C3-C2-O1-C1
6	J	101	PG4	C6-C5-O3-C4
6	J	101	PG4	C4-C3-O2-C2
6	J	101	PG4	O4-C7-C8-O5

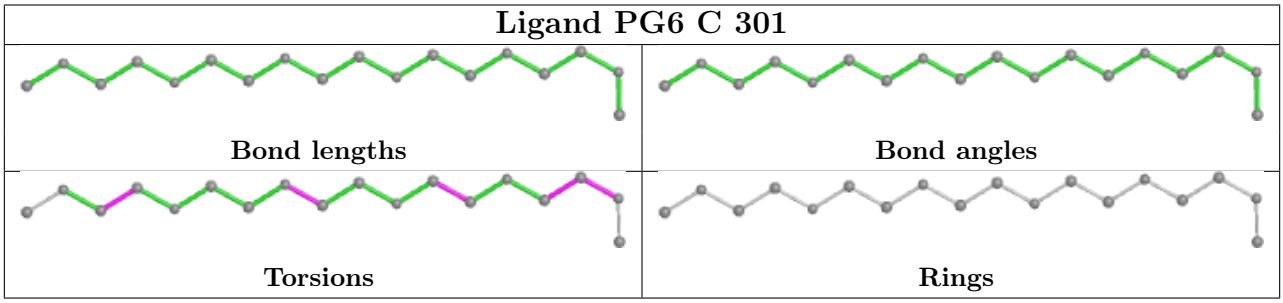
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	301	EPE	1	0
7	K	101	GOL	1	0
6	J	101	PG4	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.



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, 95^{th} 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	213/214 (99%)	-0.53	0 100 100	24, 38, 55, 82	0
1	C	213/214 (99%)	-0.44	1 (0%) 91 90	28, 40, 57, 68	0
1	E	213/214 (99%)	0.30	15 (7%) 16 15	32, 63, 103, 115	0
1	G	213/214 (99%)	0.45	28 (13%) 3 3	36, 74, 114, 129	0
2	B	219/237 (92%)	-0.44	2 (0%) 84 83	22, 35, 59, 78	0
2	D	219/237 (92%)	-0.39	1 (0%) 91 90	26, 40, 65, 81	0
2	F	219/237 (92%)	0.14	18 (8%) 11 10	28, 52, 97, 121	0
2	H	219/237 (92%)	0.21	18 (8%) 11 10	27, 47, 101, 116	0
3	I	68/71 (95%)	0.07	2 (2%) 51 49	36, 49, 82, 99	0
3	J	68/71 (95%)	-0.17	1 (1%) 73 72	35, 48, 74, 91	0
3	K	68/71 (95%)	-0.23	1 (1%) 73 72	36, 47, 75, 94	0
3	L	63/71 (88%)	0.40	8 (12%) 3 3	39, 67, 103, 116	0
All	All	1995/2088 (95%)	-0.07	95 (4%) 30 29	22, 46, 94, 129	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	203	GLY	6.8
3	L	17	GLY	6.1
2	F	204	THR	5.4
2	H	203	GLY	5.0
2	F	197	VAL	4.6
2	H	204	THR	4.3
2	H	206	THR	4.3
2	F	200	SER	4.2
1	G	191	VAL	4.0
1	G	133	VAL	3.9
2	H	199	SER	3.8

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Mol	Chain	Res	Type	RSRZ
2	F	198	PRO	3.8
1	E	150	VAL	3.7
1	G	157	GLY	3.7
1	G	208	SER	3.6
1	G	213	GLU	3.6
1	G	75	ILE	3.6
2	F	206	THR	3.5
1	E	189	HIS	3.4
3	L	42	CYS	3.4
1	G	80	PRO	3.4
2	H	200	SER	3.4
1	G	135	LEU	3.4
2	F	149	ALA	3.3
3	L	64	CYS	3.3
1	G	212	GLY	3.3
1	E	182	SER	3.2
2	H	226	PRO	3.2
3	L	16	PRO	3.2
2	F	219	LYS	3.2
2	H	137	LEU	3.1
2	F	205	GLN	3.1
2	H	1	GLU	3.1
1	E	212	GLY	3.1
3	L	13	ARG	3.0
2	H	207	TYR	3.0
1	G	20	THR	3.0
1	E	190	LYS	2.9
2	H	227	LYS	2.9
2	H	96	VAL	2.9
1	E	177	SER	2.8
2	H	201	SER	2.8
2	F	202	LEU	2.8
1	E	188	LYS	2.8
1	G	189	HIS	2.7
2	H	113	PHE	2.7
2	H	202	LEU	2.7
3	I	16	PRO	2.7
1	C	88	CYS	2.6
2	F	208	ILE	2.6
3	L	44	ALA	2.6
1	G	150	VAL	2.6
1	G	152	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
2	H	205	GLN	2.6
1	G	204	PRO	2.5
1	G	118	PHE	2.5
1	G	192	TYR	2.5
1	E	211	ARG	2.4
2	F	214	LYS	2.4
1	G	188	LYS	2.4
1	E	210	ASN	2.4
2	H	171	ALA	2.4
1	E	133	VAL	2.4
2	F	207	TYR	2.4
1	E	152	ASN	2.4
2	F	223	LYS	2.3
3	J	68	PRO	2.3
1	G	76	SER	2.3
1	G	190	LYS	2.3
1	G	117	ILE	2.3
2	F	151	LEU	2.3
1	G	181	LEU	2.2
2	B	204	THR	2.2
2	F	54	SER	2.2
2	B	112	ALA	2.2
2	D	227	LYS	2.2
1	G	116	PHE	2.2
3	I	45	THR	2.2
1	E	178	THR	2.2
3	K	68	PRO	2.2
1	E	176	SER	2.2
3	L	43	ALA	2.1
1	E	122	ASP	2.1
1	G	147	GLN	2.1
2	F	1	GLU	2.1
1	G	59	PRO	2.1
2	H	224	VAL	2.1
1	G	202	SER	2.1
1	G	136	LEU	2.0
2	H	172	LEU	2.0
1	G	145	LYS	2.0
1	G	154	LEU	2.0
1	E	184	ALA	2.0
2	F	113	PHE	2.0
3	L	60	SER	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 monosaccharides in this entry.

6.4 Ligands (i)

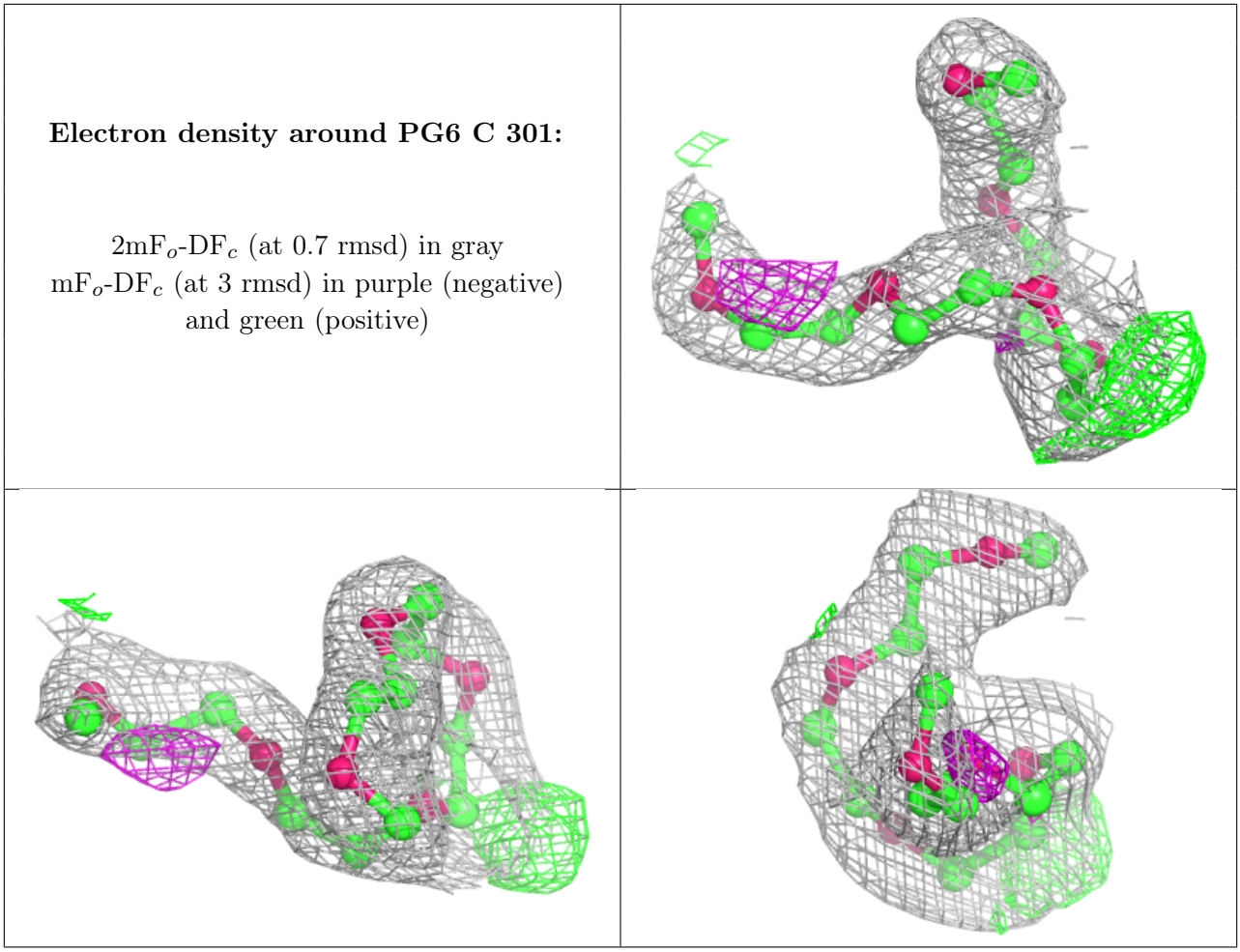
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
7	GOL	K	101	6/6	0.78	0.16	72,75,79,79	0
5	PG6	C	301	18/18	0.83	0.21	45,56,67,68	0
6	PG4	J	101	13/13	0.84	0.16	45,53,62,63	0
4	EPE	A	301	15/15	0.84	0.18	42,61,119,121	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 PG6 C 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.