



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:43 PM GMT

PDB ID : 1GYG
Title : R32 CLOSED FORM OF ALPHA-TOXIN FROM CLOSTRIDIUM PERFRINGENS STRAIN CER89L43
Authors : Basak, A.K.; Eaton, J.T.; Titball, R.W.
Deposited on : 2002-04-23
Resolution : 1.90 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

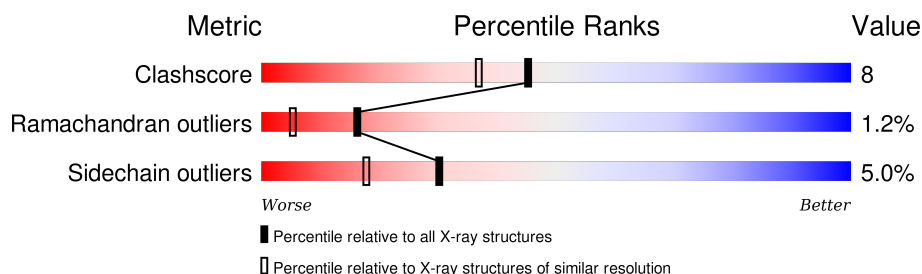
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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))
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	370	 82% 14% . .
1	B	370	 81% 16% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6232 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 PHOSPHOLIPASE C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	370	Total	C	N	O	S	0	0	0
			3001	1899	495	598	9			
1	B	370	Total	C	N	O	S	0	0	0
			3001	1899	495	598	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	167	VAL	ALA	VARIANT	UNP P15310
B	167	VAL	ALA	VARIANT	UNP P15310

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is water.

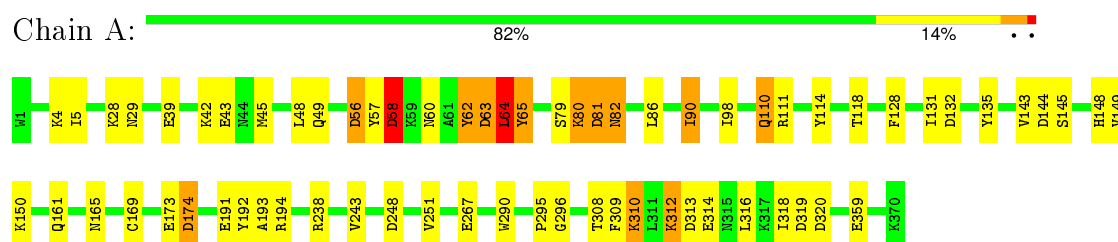
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	115	Total	O	0	0
			115	115		
3	B	111	Total	O	0	0
			111	111		

3 Residue-property plots

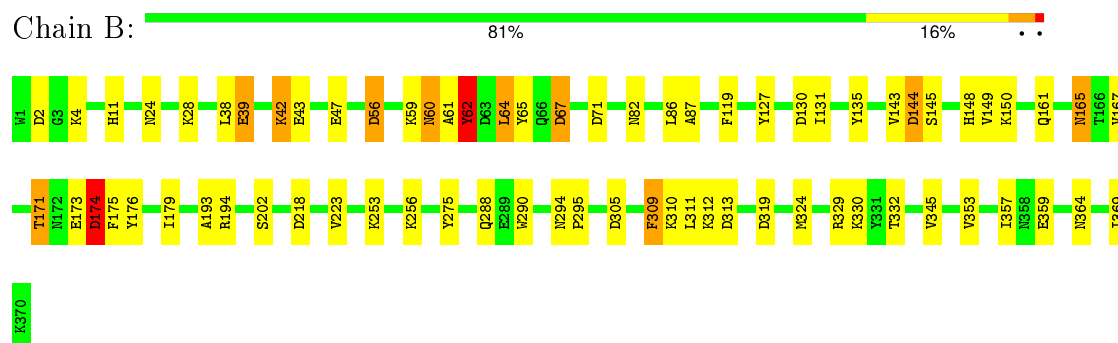
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

• Molecule 1: PHOSPHOLIPASE C



• Molecule 1: PHOSPHOLIPASE C



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	151.40 Å 151.40 Å 195.50 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 1.90	Depositor
% Data completeness (in resolution range)	87.5 (25.00-1.90)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 3.1	Depositor
R, R_{free}	0.208 , 0.254	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6232	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

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: 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	A	0.51	1/3079 (0.0%)	1.41	10/4165 (0.2%)
1	B	0.50	2/3078 (0.1%)	1.09	14/4162 (0.3%)
All	All	0.51	3/6157 (0.0%)	1.26	24/8327 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8
1	B	0	5
All	All	0	13

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	58	ASP	C-N	9.33	1.55	1.34
1	B	59	LYS	C-N	-6.71	1.18	1.34
1	B	60	ASN	N-CA	-6.42	1.33	1.46

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	ASP	O-C-N	-37.00	63.50	122.70
1	A	64	LEU	C-N-CA	-30.90	44.45	121.70
1	A	64	LEU	CA-C-N	-30.78	49.49	117.20
1	A	58	ASP	CA-C-N	20.64	162.61	117.20
1	B	130	ASP	CB-CG-OD2	12.49	129.54	118.30
1	A	58	ASP	C-N-CA	10.84	148.80	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	TYR	O-C-N	-7.48	110.73	122.70
1	B	60	ASN	N-CA-CB	-7.34	97.38	110.60
1	B	194	ARG	NE-CZ-NH1	6.97	123.79	120.30
1	B	2	ASP	CB-CG-OD2	-6.48	112.47	118.30
1	A	132	ASP	CB-CG-OD2	6.45	124.10	118.30
1	B	67	ASP	CB-CG-OD1	6.36	124.02	118.30
1	B	144	ASP	CB-CG-OD1	5.97	123.68	118.30
1	B	305	ASP	CB-CG-OD2	5.92	123.62	118.30
1	B	62	TYR	CB-CG-CD2	5.65	124.39	121.00
1	B	313	ASP	CB-CG-OD2	5.48	123.23	118.30
1	B	223	VAL	N-CA-CB	-5.45	99.52	111.50
1	B	127	TYR	CB-CG-CD2	-5.33	117.81	121.00
1	B	11	HIS	CA-CB-CG	-5.27	104.65	113.60
1	B	56	ASP	CB-CG-OD2	5.26	123.04	118.30
1	A	64	LEU	O-C-N	5.16	130.96	122.70
1	B	218	ASP	CB-CG-OD1	5.16	122.94	118.30
1	A	192	TYR	CA-CB-CG	5.14	123.16	113.40
1	A	238	ARG	NE-CZ-NH2	5.08	122.84	120.30

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	29	ASN	Mainchain
1	A	320	ASP	Mainchain
1	A	56	ASP	Mainchain
1	A	58	ASP	Mainchain,Peptide
1	A	64	LEU	Mainchain,Peptide
1	A	90	ILE	Mainchain
1	B	171	THR	Mainchain
1	B	256	LYS	Mainchain
1	B	309	PHE	Mainchain
1	B	364	ASN	Mainchain
1	B	82	ASN	Mainchain

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	3001	0	2803	49	0
1	B	3001	0	2802	48	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	115	0	0	4	0
3	B	111	0	0	10	0
All	All	6232	0	5605	90	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 8.

All (90) 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:A:143:VAL:O	1:B:64:LEU:CD1	1.85	1.23
1:A:143:VAL:O	1:B:64:LEU:HD12	1.09	1.23
1:A:62:TYR:CE1	1:A:295:PRO:HD2	1.75	1.19
1:A:62:TYR:HE1	1:A:295:PRO:HD2	1.05	1.11
1:B:64:LEU:HD22	1:B:64:LEU:O	1.59	0.99
1:A:63:ASP:O	1:A:64:LEU:HB2	1.64	0.97
1:A:60:ASN:HB3	3:A:2012:HOH:O	1.71	0.91
1:A:143:VAL:C	1:B:64:LEU:HD12	1.91	0.91
1:B:64:LEU:O	1:B:64:LEU:CD2	2.24	0.85
1:A:62:TYR:CE1	1:A:295:PRO:CD	2.61	0.80
1:B:61:ALA:O	1:B:62:TYR:C	2.17	0.80
1:B:61:ALA:O	1:B:62:TYR:O	2.01	0.78
1:A:143:VAL:C	1:B:64:LEU:CD1	2.50	0.78
1:B:71:ASP:OD1	3:B:2020:HOH:O	2.02	0.77
1:B:67:ASP:CG	3:B:2015:HOH:O	2.23	0.77
1:B:143:VAL:HG11	1:B:150:LYS:HG3	1.67	0.76
1:B:64:LEU:C	1:B:64:LEU:CD2	2.55	0.74
1:A:110:GLN:HE22	1:A:243:VAL:HA	1.54	0.72
1:A:145:SER:HB2	1:B:145:SER:HB2	1.74	0.70
1:B:64:LEU:C	1:B:64:LEU:HD23	2.12	0.69
1:B:288:GLN:HE22	1:B:312:LYS:H	1.40	0.69
1:B:39:GLU:O	1:B:43:GLU:HG3	1.93	0.68
1:B:202:SER:O	3:B:2077:HOH:O	2.11	0.67
1:B:324:MET:HE3	1:B:369:ILE:HD11	1.77	0.66
1:A:79:SER:HB3	3:A:2023:HOH:O	1.95	0.65
1:B:175:PHE:O	3:B:2070:HOH:O	2.15	0.64
1:B:56:ASP:OD2	1:B:148:HIS:HE1	1.82	0.62
1:A:56:ASP:OD2	1:A:148:HIS:HE1	1.83	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:TYR:O	1:A:63:ASP:C	2.36	0.61
1:A:63:ASP:O	1:A:64:LEU:CB	2.38	0.60
1:A:81:ASP:O	1:A:82:ASN:HB2	2.01	0.60
1:A:62:TYR:O	1:A:63:ASP:O	2.18	0.60
1:B:288:GLN:NE2	1:B:312:LYS:H	2.01	0.58
1:B:324:MET:CE	1:B:353:VAL:HG21	2.33	0.57
1:B:144:ASP:OD2	1:B:148:HIS:HD2	1.87	0.57
1:A:86:LEU:HD12	1:A:312:LYS:HG3	1.86	0.57
1:B:87:ALA:N	3:B:2031:HOH:O	2.33	0.57
1:A:63:ASP:O	1:A:63:ASP:OD2	2.22	0.56
1:B:143:VAL:HG11	1:B:150:LYS:CG	2.35	0.56
1:B:4:LYS:HE2	3:B:2001:HOH:O	2.06	0.55
1:A:144:ASP:OD2	1:A:148:HIS:HD2	1.90	0.55
1:A:60:ASN:CB	3:A:2012:HOH:O	2.41	0.55
1:A:62:TYR:HA	1:A:296:GLY:HA3	1.90	0.54
1:A:290:TRP:CE2	1:A:309:PHE:HB3	2.43	0.54
1:B:179:ILE:HG13	3:B:2070:HOH:O	2.07	0.53
1:A:62:TYR:CA	1:A:296:GLY:HA3	2.39	0.53
1:A:45:MET:HE2	1:A:49:GLN:HG3	1.92	0.51
1:A:80:LYS:O	1:A:81:ASP:HB3	2.10	0.51
1:A:114:TYR:O	1:A:118:THR:HG23	2.09	0.51
1:A:191:GLU:OE1	1:A:194:ARG:NH1	2.44	0.50
1:A:39:GLU:O	1:A:43:GLU:HG3	2.12	0.50
1:B:62:TYR:CE1	1:B:295:PRO:HD2	2.47	0.50
1:B:290:TRP:CE2	1:B:309:PHE:HB3	2.47	0.50
1:B:275:TYR:HB2	1:B:329:ARG:HB3	1.95	0.49
1:A:86:LEU:HD22	1:A:310:LYS:HB3	1.95	0.49
1:A:143:VAL:C	1:B:64:LEU:HD11	2.31	0.48
1:A:60:ASN:HA	3:A:2012:HOH:O	2.12	0.48
1:B:324:MET:HE1	1:B:353:VAL:HG21	1.94	0.48
1:B:24:ASN:ND2	1:B:165:ASN:OD1	2.46	0.48
1:A:143:VAL:HG11	1:A:150:LYS:HG3	1.96	0.48
1:B:67:ASP:OD2	3:B:2015:HOH:O	2.20	0.47
1:A:45:MET:HE1	1:A:48:LEU:HD23	1.96	0.47
1:A:248:ASP:HB3	1:A:251:VAL:HG13	1.97	0.47
1:A:80:LYS:O	1:A:81:ASP:CB	2.63	0.47
1:A:64:LEU:HD13	1:A:65:TYR:O	2.15	0.46
1:A:4:LYS:HD3	1:A:4:LYS:HA	1.80	0.46
1:A:135:TYR:CE1	1:A:149:VAL:HG11	2.50	0.46
1:B:324:MET:HE2	1:B:353:VAL:HG21	1.96	0.46
1:A:45:MET:CE	1:A:48:LEU:HD23	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:MET:HE1	1:B:345:VAL:HG21	1.97	0.45
1:A:313:ASP:OD1	1:A:316:LEU:HG	2.17	0.45
1:B:135:TYR:CE1	1:B:149:VAL:HG11	2.51	0.45
1:A:63:ASP:OD2	1:A:63:ASP:C	2.56	0.44
1:A:5:ILE:HD12	1:A:57:TYR:HB3	1.99	0.44
1:B:173:GLU:HB3	1:B:174:ASP:OD2	2.18	0.44
1:A:131:ILE:HD11	1:A:193:ALA:HB1	1.99	0.44
1:A:144:ASP:HA	1:B:64:LEU:HD12	2.00	0.43
1:B:86:LEU:HG	3:B:2029:HOH:O	2.18	0.43
1:A:169:CYS:HB2	1:A:173:GLU:HG3	1.99	0.43
1:B:357:ILE:HG22	1:B:359:GLU:H	1.83	0.43
1:B:171:THR:HA	1:B:176:TYR:CD1	2.54	0.43
1:B:294:ASN:O	3:B:2097:HOH:O	2.21	0.43
1:B:131:ILE:HD11	1:B:193:ALA:HB1	2.01	0.42
1:B:64:LEU:HA	1:B:65:TYR:HD1	1.47	0.42
1:B:144:ASP:OD2	1:B:148:HIS:CD2	2.71	0.42
1:A:45:MET:CE	1:A:49:GLN:HG3	2.50	0.41
1:B:38:LEU:O	1:B:42:LYS:HG3	2.20	0.41
1:B:47:GLU:HG3	1:B:119:PHE:HB2	2.01	0.41
1:A:98:ILE:HD11	1:A:128:PHE:HA	2.03	0.41
1:A:90:ILE:HB	1:A:308:THR:HB	2.03	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	366/370 (99%)	353 (96%)	7 (2%)	6 (2%)	12	3
1	B	364/370 (98%)	352 (97%)	9 (2%)	3 (1%)	24	11
All	All	730/740 (99%)	705 (97%)	16 (2%)	9 (1%)	16	5

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	ASP
1	A	64	LEU
1	A	82	ASN
1	A	174	ASP
1	B	174	ASP
1	A	58	ASP
1	B	60	ASN
1	B	62	TYR
1	A	81	ASP

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	318/320 (99%)	301 (95%)	17 (5%)	28	16
1	B	318/320 (99%)	303 (95%)	15 (5%)	32	20
All	All	636/640 (99%)	604 (95%)	32 (5%)	30	18

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LYS
1	A	42	LYS
1	A	64	LEU
1	A	65	TYR
1	A	80	LYS
1	A	110	GLN
1	A	111	ARG
1	A	161	GLN
1	A	165	ASN
1	A	174	ASP
1	A	267	GLU
1	A	310	LYS
1	A	312	LYS
1	A	314	GLU

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Mol	Chain	Res	Type
1	A	318	ILE
1	A	319	ASP
1	A	359	GLU
1	B	28	LYS
1	B	39	GLU
1	B	42	LYS
1	B	62	TYR
1	B	64	LEU
1	B	161	GLN
1	B	165	ASN
1	B	167	VAL
1	B	174	ASP
1	B	253	LYS
1	B	310	LYS
1	B	311	LEU
1	B	319	ASP
1	B	330	LYS
1	B	332	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	77	ASN
1	A	148	HIS
1	A	165	ASN
1	A	186	ASN
1	A	297	ASN
1	B	24	ASN
1	B	49	GLN
1	B	77	ASN
1	B	148	HIS
1	B	165	ASN
1	B	186	ASN
1	B	207	HIS
1	B	212	HIS
1	B	254	ASN
1	B	288	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.