



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2020 – 09:57 PM BST

PDB ID : 5U8C
Title : CRYSTAL STRUCTURE OF GLUN1/GLUN2A LIGAND-BINDING DOMAIN IN COMPLEX WITH GLYCINE AND NVP-AAM077
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Deposited on : 2016-12-14
Resolution : 1.60 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 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 : **FAILED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.4.dev1

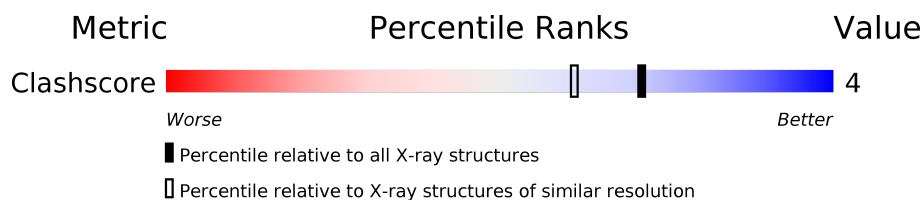
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 Å.

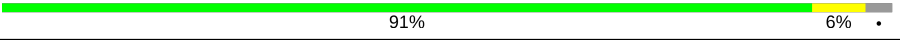
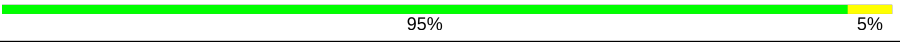
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3665 (1.60-1.60)

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 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 $\leq 5\%$

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	292	 91% 6% •
2	B	283	 95% 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
4	GOL	A	902	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4885 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 Glutamate receptor ionotropic, NMDA 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	284	2227	1419	380	412	16	0	0	0

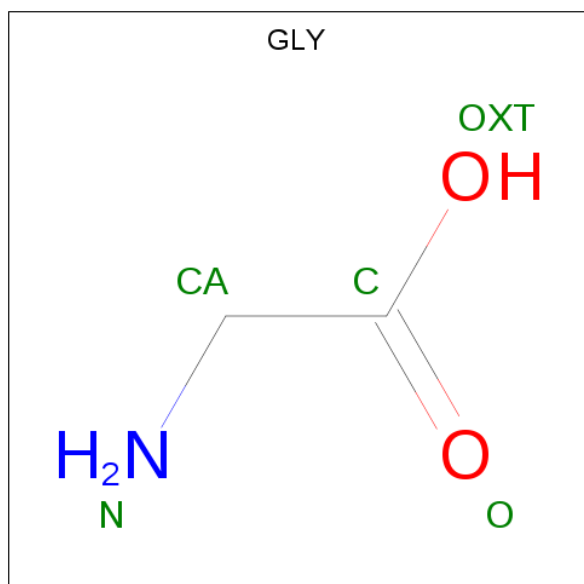
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P35439
A	153	GLY	-	linker	UNP P35439
A	154	THR	-	linker	UNP P35439

- Molecule 2 is a protein called GLUTAMATE RECEPTOR IONOTROPIC, NMDA 2A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	283	2188	1389	373	412	14	0	0	0

- Molecule 3 is GLYCINE (three-letter code: GLY) (formula: C₂H₅NO₂).



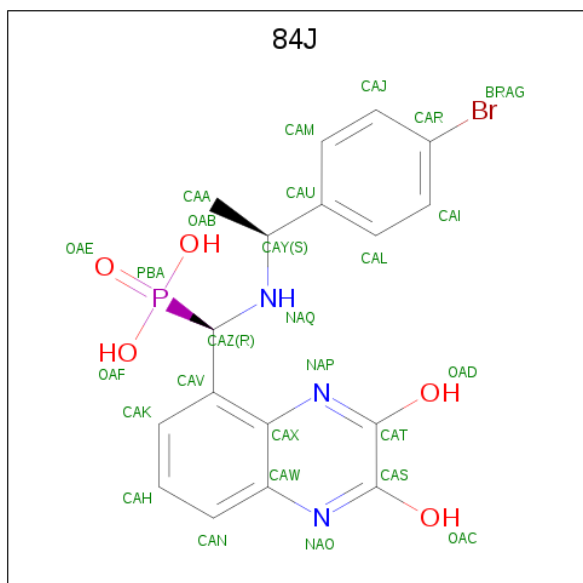
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			5	2	1	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is [(R)-{[(1S)-1-(4-bromophenyl)ethyl]amino}(2,3-dihydroxyquinoxalin-5-yl)methyl]phosphonic acid (three-letter code: 84J) (formula: $C_{17}H_{17}BrN_3O_5P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	B	1	Total 27	Br 1	C 17	N 3	O 5	P 1	0	0

- Molecule 6 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	201	Total 201	O 201	0	0
6	B	231	Total 231	O 231	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. 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. 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 failed to run properly.

- Molecule 1: Glutamate receptor ionotropic, NMDA 1

Chain A:  91% 6% .



- Molecule 2: GLUTAMATE RECEPTOR IONOTROPIC, NMDA 2A

Chain B:  95% 5%



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.55Å 84.23Å 121.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.20 – 1.60	Depositor
% Data completeness (in resolution range)	89.4 (49.20-1.60)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 1.60Å)	Xtriage
Refinement program	PHENIX 1.10_2155	Depositor
R, R_{free}	0.189 , 0.204	Depositor
Wilson B-factor (Å ²)	19.7	Xtriage
Anisotropy	0.148	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4885	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.33% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 84J

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	0.39	0/2274	0.59	1/3074 (0.0%)
2	B	0.42	0/2231	0.57	0/3023
All	All	0.41	0/4505	0.58	1/6097 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	76	ARG	NE-CZ-NH1	5.34	122.97	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	A	2227	0	2153	19	0
2	B	2188	0	2135	14	0
3	A	5	0	2	1	0
4	A	6	0	8	4	0
5	B	27	0	0	0	0
6	A	201	0	0	2	0
6	B	231	0	0	6	0
All	All	4885	0	4298	31	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 4.

All (31) 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:287:TYR:HD1	1:A:288:GLN:H	1.10	0.92
1:A:287:TYR:HD1	1:A:288:GLN:N	1.79	0.80
1:A:197:HIS:HD1	4:A:902:GOL:H31	1.46	0.78
2:B:256:LYS:NZ	6:B:403:HOH:O	2.17	0.76
2:B:133:GLU:OE2	6:B:401:HOH:O	2.06	0.73
2:B:131:PHE:CD1	2:B:132:VAL:HG23	2.33	0.64
1:A:287:TYR:CD1	1:A:288:GLN:N	2.65	0.59
1:A:197:HIS:HD1	4:A:902:GOL:C3	2.16	0.59
1:A:271:SER:HB3	1:A:277:MET:CE	2.35	0.57
2:B:131:PHE:HD1	2:B:132:VAL:HG23	1.69	0.57
2:B:205:LYS:HE2	2:B:226:ASP:OD1	2.08	0.53
1:A:126:THR:HG1	3:A:901:GLY:N	2.08	0.52
1:A:281:ASP:HB2	6:A:1067:HOH:O	2.09	0.52
1:A:177:LYS:HG2	1:A:202:ASN:HB3	1.91	0.51
2:B:11:ILE:HD13	2:B:110:MET:HE2	1.92	0.51
2:B:158:HIS:HD2	6:B:612:HOH:O	1.95	0.49
2:B:79:ASP:HB3	6:B:584:HOH:O	2.12	0.49
1:A:247:ARG:NH2	6:A:1004:HOH:O	2.44	0.49
1:A:247:ARG:HH22	2:B:276:GLU:CD	2.15	0.48
2:B:40:ARG:NH1	6:B:414:HOH:O	2.47	0.48
1:A:247:ARG:NH2	2:B:276:GLU:OE1	2.44	0.47
1:A:197:HIS:ND1	4:A:902:GOL:H31	2.22	0.46
1:A:210:ILE:HD13	1:A:231:GLU:HG3	1.98	0.45
2:B:42:PHE:HB3	2:B:84:THR:HG21	1.99	0.45
1:A:101:SER:OG	1:A:102:ASN:N	2.49	0.45
1:A:149:LEU:HD21	1:A:238:LEU:HD13	1.99	0.43
1:A:197:HIS:HA	4:A:902:GOL:H11	2.00	0.43
1:A:214:ARG:HG2	1:A:238:LEU:HD21	2.01	0.43
2:B:226:ASP:HA	6:B:404:HOH:O	2.20	0.41
2:B:272:MET:O	2:B:276:GLU:HG3	2.21	0.41
1:A:76:ARG:HG2	1:A:76:ARG:HH11	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	$\# Z > 2$
3	GLY	A	901	-	1,4,4	0.03	0	0,4,4	0.00	-
5	84J	B	301	-	29,29,29	1.38	4 (13%)	36,43,43	1.68	8 (22%)
4	GOL	A	902	-	5,5,5	0.37	0	5,5,5	0.73	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
3	GLY	A	901	-	-	0/0/2/2	-
5	84J	B	301	-	-	3/18/18/18	0/3/3/3
4	GOL	A	902	-	-	2/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	301	84J	PBA-CAZ	-3.02	1.79	1.83
5	B	301	84J	PBA-OAB	-2.47	1.50	1.54
5	B	301	84J	CAV-CAX	-2.33	1.39	1.43
5	B	301	84J	CAS-CAT	-2.05	1.35	1.42

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	301	84J	PBA-CAZ-CAV	4.45	118.71	111.52
5	B	301	84J	CAN-CAW-NAO	3.79	124.47	118.69
5	B	301	84J	CAK-CAV-CAZ	-3.53	116.72	121.00
5	B	301	84J	CAX-CAW-NAO	-3.52	116.53	121.22
5	B	301	84J	CAT-NAP-CAX	2.57	120.90	116.27
5	B	301	84J	CAU-CAY-NAQ	-2.48	105.79	111.77
5	B	301	84J	OAE-PBA-CAZ	-2.42	106.95	111.07
5	B	301	84J	CAK-CAV-CAX	2.24	122.09	117.75

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	301	84J	CAK-CAV-CAZ-NAQ
5	B	301	84J	CAM-CAU-CAY-CAA
5	B	301	84J	CAL-CAU-CAY-CAA
4	A	902	GOL	O1-C1-C2-C3
4	A	902	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 5 short contacts:

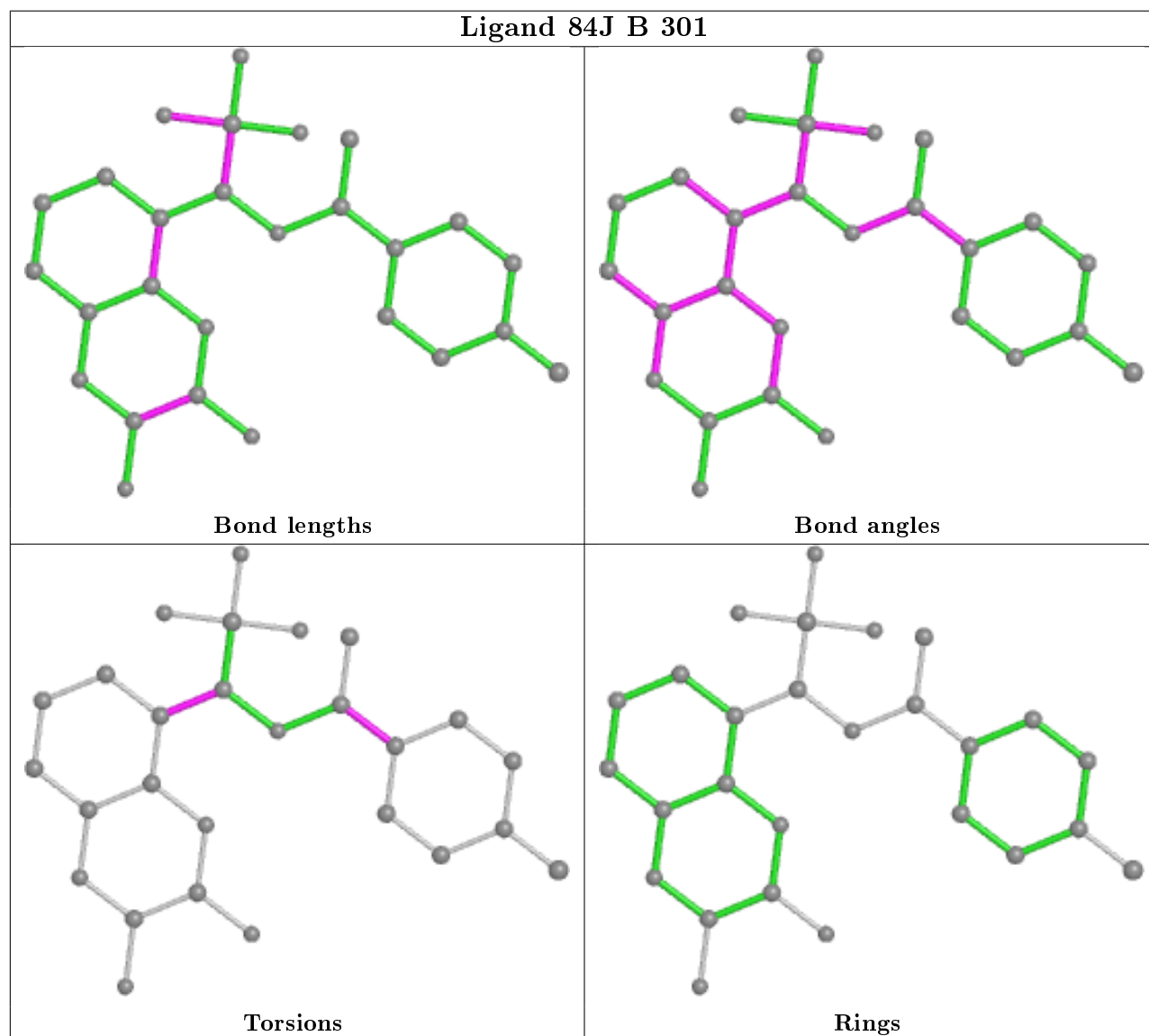
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	GLY	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	902	GOL	4	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section is therefore empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section is therefore empty.