



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 14, 2024 – 04:19 am GMT

PDB ID : 6Y8K
Title : Crystal structure of CD137 in complex with the cyclic peptide BCY10916
Authors : Upadhyaya, P.; Kublin, J.; Dods, R.; Kristensson, J.; Lahdenranta, J.; Klyman, M.; Repash, E.; Ma, J.; Mudd, G.; Van Rietschoten, K.; Haines, E.; Harrison, H.; Beswick, P.; Chen, L.; McDonnell, K.; Battula, S.; Hurov, K.; Keen, N.
Deposited on : 2020-03-05
Resolution : 2.01 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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](#) ①) were used in the production of this report:

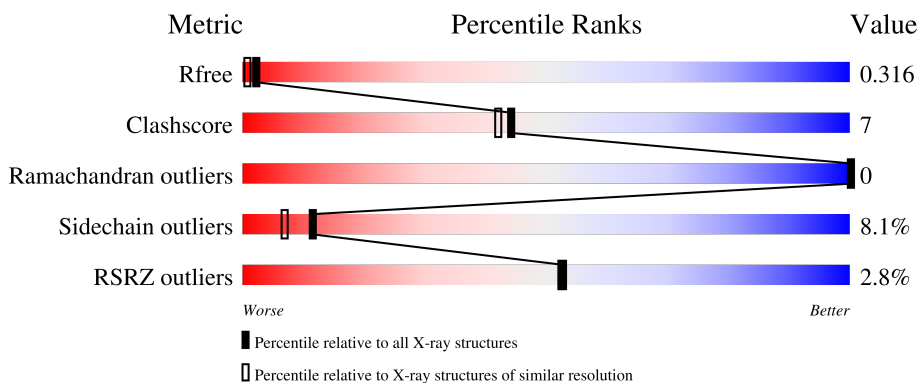
MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

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 2.01 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	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

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	AAA	165	
2	PPP	15	

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	EDO	AAA	202	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 2153 atoms, of which 1009 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 Tumor necrosis factor receptor superfamily member 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	AAA	130	1829	566	877	173	192	21	43	0	0

There are 31 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	4	MET	-	initiating methionine	UNP Q07011
AAA	5	VAL	-	expression tag	UNP Q07011
AAA	6	SER	-	expression tag	UNP Q07011
AAA	7	ALA	-	expression tag	UNP Q07011
AAA	8	ILE	-	expression tag	UNP Q07011
AAA	9	VAL	-	expression tag	UNP Q07011
AAA	10	LEU	-	expression tag	UNP Q07011
AAA	11	TYR	-	expression tag	UNP Q07011
AAA	12	VAL	-	expression tag	UNP Q07011
AAA	13	LEU	-	expression tag	UNP Q07011
AAA	14	LEU	-	expression tag	UNP Q07011
AAA	15	ALA	-	expression tag	UNP Q07011
AAA	16	ALA	-	expression tag	UNP Q07011
AAA	17	ALA	-	expression tag	UNP Q07011
AAA	18	ALA	-	expression tag	UNP Q07011
AAA	19	HIS	-	expression tag	UNP Q07011
AAA	20	SER	-	expression tag	UNP Q07011
AAA	21	ALA	-	expression tag	UNP Q07011
AAA	22	PHE	-	expression tag	UNP Q07011
AAA	23	ALA	-	expression tag	UNP Q07011
AAA	121	SER	CYS	conflict	UNP Q07011
AAA	138	ASP	ASN	conflict	UNP Q07011
AAA	149	ASP	ASN	conflict	UNP Q07011
AAA	161	GLY	-	expression tag	UNP Q07011
AAA	162	SER	-	expression tag	UNP Q07011
AAA	163	HIS	-	expression tag	UNP Q07011
AAA	164	HIS	-	expression tag	UNP Q07011

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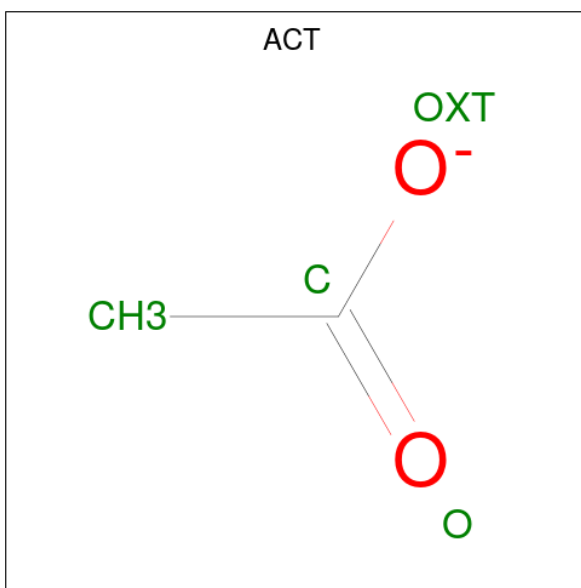
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Chain	Residue	Modelled	Actual	Comment	Reference
AAA	165	HIS	-	expression tag	UNP Q07011
AAA	166	HIS	-	expression tag	UNP Q07011
AAA	167	HIS	-	expression tag	UNP Q07011
AAA	168	HIS	-	expression tag	UNP Q07011

- Molecule 2 is a protein called BCY10916.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
2	PPP	15	225	77	105	16	24	3	4	0	0

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
3	AAA	1	7	2	3	2	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	AAA	1	10	2	6	2	1	0

- Molecule 5 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).

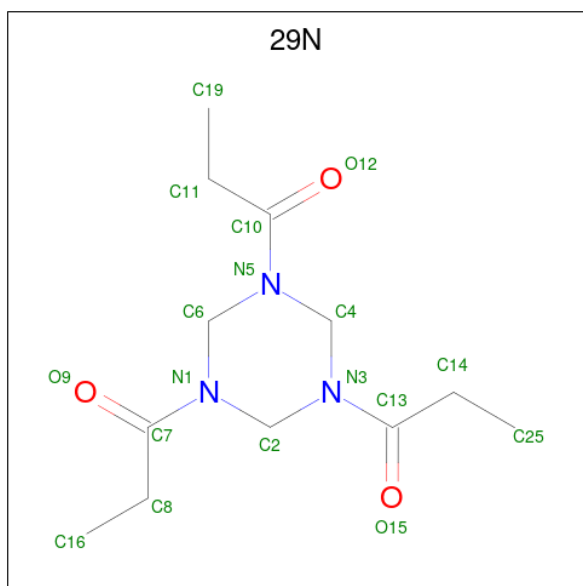


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
5	AAA	1	5	4	1	0	0
5	AAA	1	5	4	1	0	0
5	AAA	1	5	4	1	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	AAA	1	Total Na 1 1	0	0

- Molecule 7 is 1,1',1''-(1,3,5-triazinane-1,3,5-triyl)tripropan-1-one (three-letter code: 29N) (formula: C₁₂H₂₁N₃O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	PPP	1	Total C H N O 36 12 18 3 3	0	0

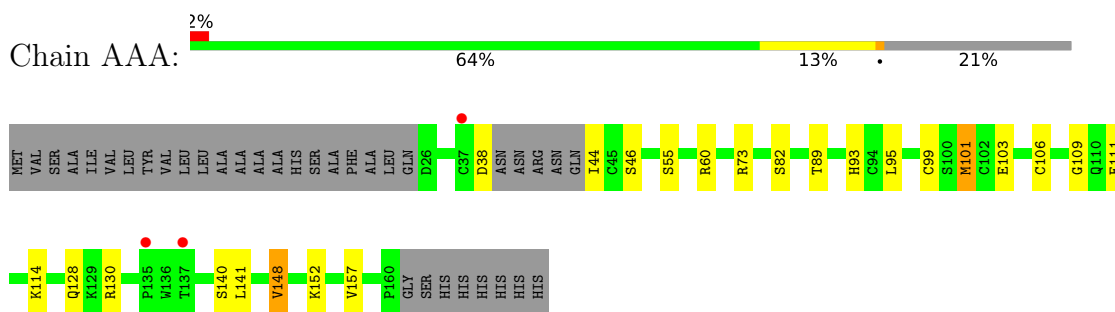
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	AAA	28	Total O 28 28	0	0
8	PPP	2	Total O 2 2	0	0

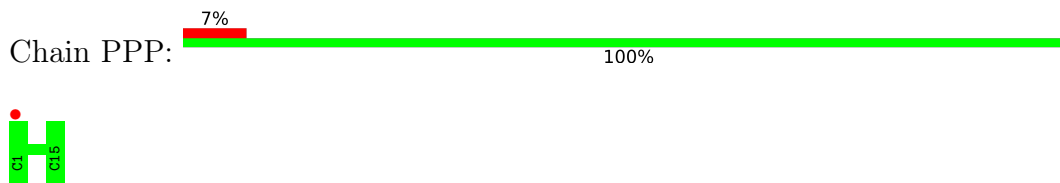
3 Residue-property plots [i](#)

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: Tumor necrosis factor receptor superfamily member 9



- Molecule 2: BCY10916



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 3 2	Depositor
Cell constants a, b, c, α , β , γ	122.47Å 122.47Å 122.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.86 – 2.01 40.82 – 2.01	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.86-2.01) 99.9 (40.82-2.01)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 2.01Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.283 , 0.314 0.291 , 0.316	Depositor DCC
R_{free} test set	1070 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	58.6	Xtrriage
Anisotropy	0.000	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 50.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2153	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% 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: NLE, EDO, SO4, 29N, ACT, NA

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	AAA	0.75	0/967	0.98	0/1298
2	PPP	0.63	0/114	0.95	0/152
All	All	0.74	0/1081	0.98	0/1450

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 [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	AAA	952	877	872	14	0
2	PPP	120	105	101	0	0
3	AAA	4	3	3	0	0
4	AAA	4	6	6	7	0
5	AAA	15	0	0	0	0
6	AAA	1	0	0	0	0
7	PPP	18	18	17	0	0
8	AAA	28	0	0	0	1
8	PPP	2	0	0	0	0
All	All	1144	1009	999	14	1

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 7.

The worst 5 of 14 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:AAA:106:CYS:HB2	4:AAA:202:EDO:C1	2.16	0.74
1:AAA:130:ARG:C	4:AAA:202:EDO:H22	2.11	0.70
1:AAA:106:CYS:HB2	4:AAA:202:EDO:H12	1.77	0.67
1:AAA:106:CYS:HB2	4:AAA:202:EDO:H11	1.79	0.63
1:AAA:148:VAL:HG13	1:AAA:157:VAL:HB	1.82	0.61

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AAA:302:HOH:O	8:AAA:302:HOH:O[18_554]	1.44	0.76

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	AAA	126/165 (76%)	116 (92%)	10 (8%)	0	100	100
2	PPP	12/15 (80%)	12 (100%)	0	0	100	100
All	All	138/180 (77%)	128 (93%)	10 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	AAA	111/139 (80%)	101 (91%)	10 (9%)	9	5
2	PPP	12/12 (100%)	12 (100%)	0	100	100
All	All	123/151 (82%)	113 (92%)	10 (8%)	11	7

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	114	LYS
1	AAA	140	SER
1	AAA	148	VAL
1	AAA	73	ARG
1	AAA	82	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
2	NLE	PPP	14	2	6,7,8	0.53	0	2,7,9	0.32	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
2	NLE	PPP	14	2	-	0/5/6/8	-

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.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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$
4	EDO	AAA	202	-	3,3,3	0.31	0	2,2,2	0.69	0
7	29N	PPP	101	2	18,18,18	0.45	0	24,24,24	1.63	4 (16%)
5	SO4	AAA	204	-	4,4,4	0.34	0	6,6,6	0.10	0
3	ACT	AAA	201	-	3,3,3	1.04	0	3,3,3	0.80	0
5	SO4	AAA	205	-	4,4,4	0.34	0	6,6,6	0.08	0
5	SO4	AAA	203	-	4,4,4	0.32	0	6,6,6	0.12	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	EDO	AAA	202	-	-	1/1/1/1	-
7	29N	PPP	101	2	-	1/18/30/30	0/0/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
7	PPP	101	29N	N3-C2-N1	-5.14	102.79	110.77
7	PPP	101	29N	C25-C14-C13	3.20	118.63	112.72
7	PPP	101	29N	N5-C4-N3	-2.34	107.14	110.77
7	PPP	101	29N	C6-N5-C4	-2.08	106.85	111.73

There are no chirality outliers.

All (2) torsion outliers are listed below:

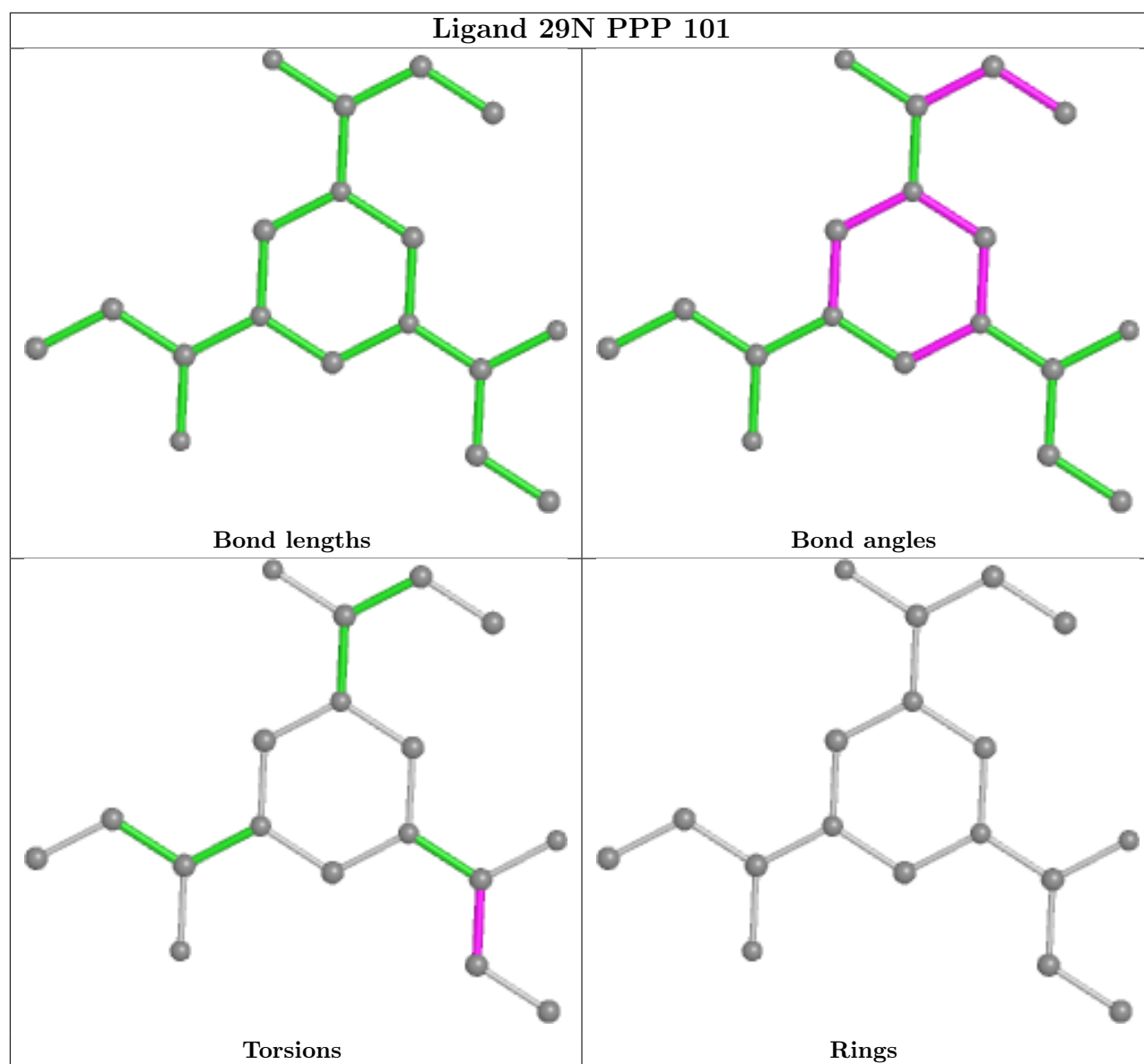
Mol	Chain	Res	Type	Atoms
7	PPP	101	29N	O12-C10-C11-C19
4	AAA	202	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	AAA	202	EDO	7	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	AAA	130/165 (78%)	0.47	3 (2%) 60 59	47, 64, 95, 112	0
2	PPP	14/15 (93%)	0.54	1 (7%) 16 15	58, 64, 70, 81	0
All	All	144/180 (80%)	0.48	4 (2%) 53 52	47, 64, 92, 112	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	PPP	1	CYS	3.4
1	AAA	135	PRO	2.3
1	AAA	37	CYS	2.1
1	AAA	137	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
2	NLE	PPP	14	8/9	0.95	0.14	52,57,61,63	0

6.3 Carbohydrates [i](#)

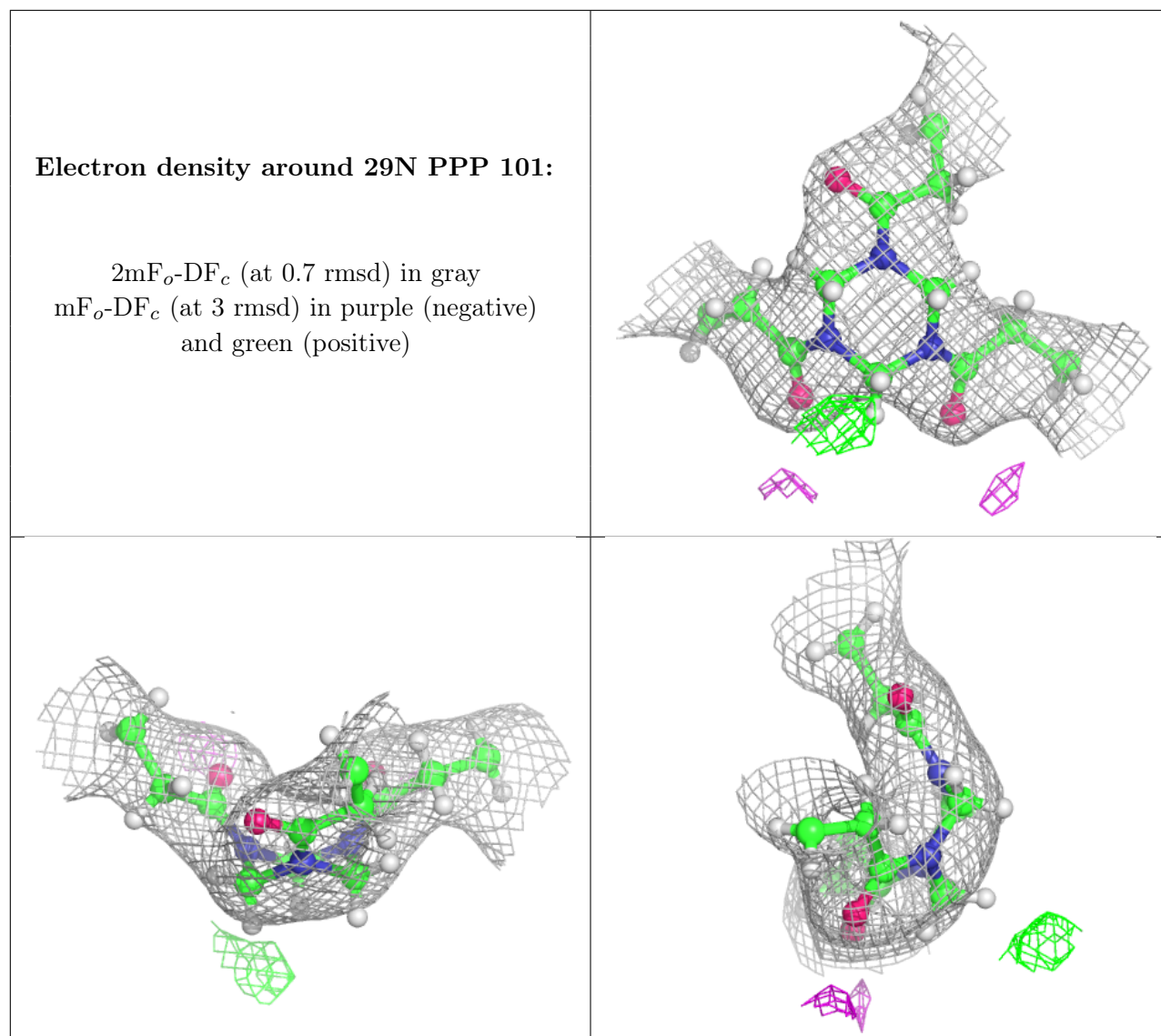
There are no monosaccharides in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	SO4	AAA	204	5/5	0.69	0.20	130,130,139,142	0
5	SO4	AAA	205	5/5	0.74	0.26	119,126,139,161	0
6	NA	AAA	206	1/1	0.82	0.40	53,53,53,53	1
4	EDO	AAA	202	4/4	0.83	0.38	49,50,56,56	1
3	ACT	AAA	201	4/4	0.86	0.20	76,81,81,83	0
5	SO4	AAA	203	5/5	0.92	0.12	84,96,105,122	0
7	29N	PPP	101	18/18	0.94	0.13	60,65,80,80	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.



6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.