



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:31 AM UTC

PDB ID : 8V68 / pdb_00008v68
Title : Nanorana parkeri saxiphilin:dcSTX (co-crystal)
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Deposited on : 2023-12-01
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

<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

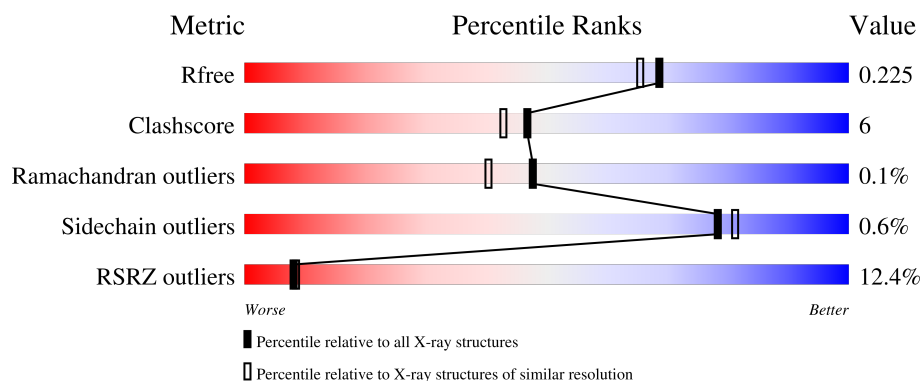
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (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 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	A	854	12% 84% 12% .

2 Entry composition [i](#)

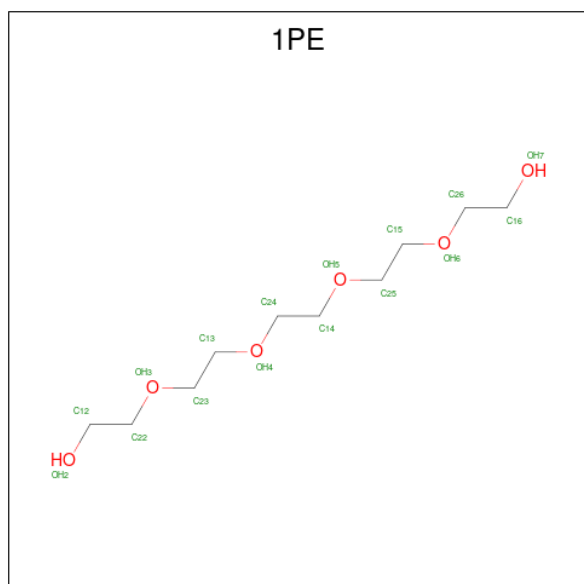
There are 4 unique types of molecules in this entry. The entry contains 6826 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Saxiphilin.

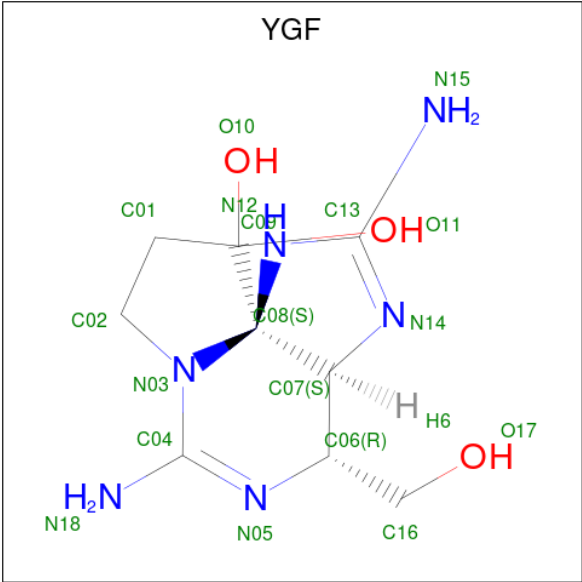
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	823	Total	C	N	O	S	0	1	0
			6392	4001	1107	1225	59			

- Molecule 2 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			16	10	6		

- Molecule 3 is (3aS,4R,7R,10aS)-2,6-diamino-4-(hydroxymethyl)-3a,4,8,9-tetrahydro-1H,10H-pyrrolo[1,2-c]purine-10,10-diol (CCD ID: YGF) (formula: $C_9H_{16}N_6O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			18	9	6	3		

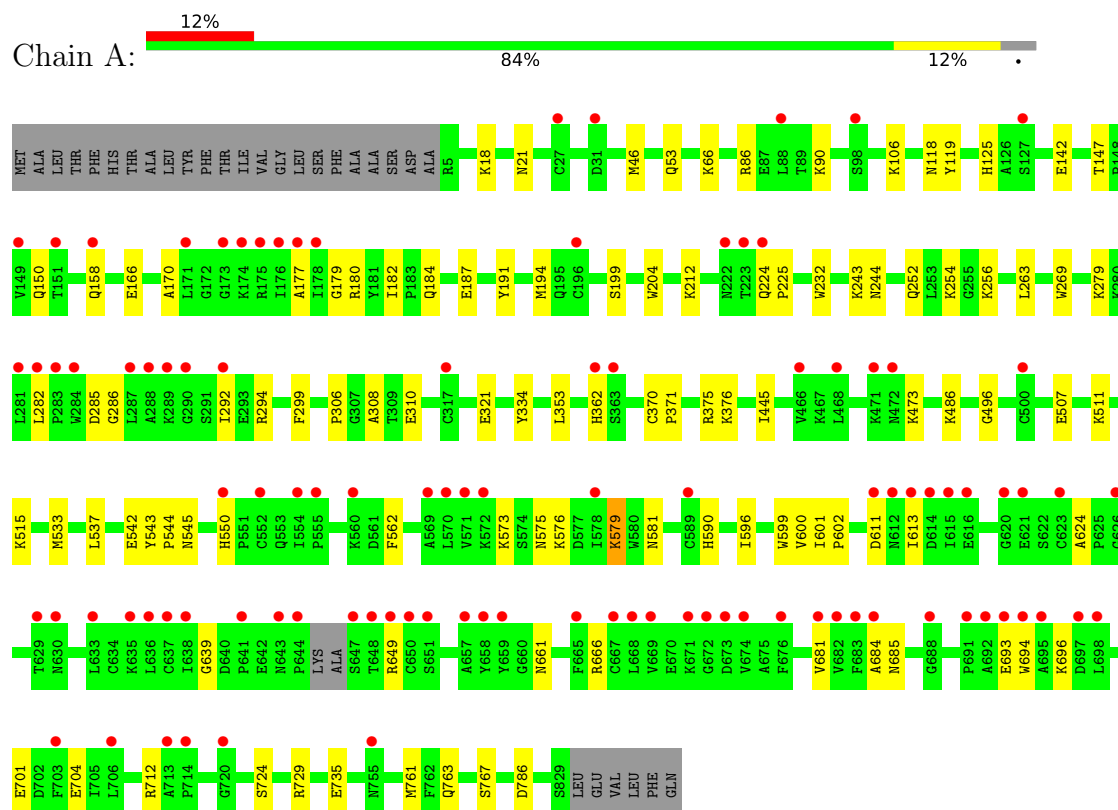
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	400	Total	O	0	0
			400	400		

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: Saxiphilin



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	229.47Å 229.47Å 67.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.37 – 1.90 43.37 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (43.37-1.90) 99.6 (43.37-1.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 1.89Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.197 , 0.225 0.197 , 0.225	Depositor DCC
R_{free} test set	1997 reflections (1.91%)	wwPDB-VP
Wilson B-factor (Å ²)	43.5	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6826	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 3.55% 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: 1PE, YGF

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	0.11	0/6538	0.31	0/8843

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	A	6392	0	6189	71	0
2	A	16	0	22	0	0
3	A	18	0	0	1	0
4	A	400	0	0	17	0
All	All	6826	0	6211	72	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 (72) 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:244:ASN:ND2	4:A:1001:HOH:O	1.81	1.04
1:A:507:GLU:OE1	4:A:1003:HOH:O	2.05	0.73
1:A:763:GLN:OE1	4:A:1005:HOH:O	2.06	0.73
1:A:212:LYS:HE2	4:A:1337:HOH:O	1.90	0.71
3:A:902:YGF:O17	4:A:1007:HOH:O	2.10	0.68
1:A:170:ALA:O	1:A:180:ARG:NH2	2.32	0.62
1:A:177:ALA:HB3	1:A:182:ILE:HD11	1.80	0.62
1:A:177:ALA:HB1	1:A:180:ARG:HE	1.65	0.61
1:A:639:GLY:HA3	1:A:649:ARG:HG2	1.82	0.60
1:A:225:PRO:HG3	1:A:362:HIS:ND1	2.18	0.59
1:A:147:THR:H	1:A:150:GLN:NE2	2.01	0.58
1:A:252:GLN:O	1:A:256:LYS:NZ	2.32	0.57
1:A:661:ASN:HB3	1:A:681:VAL:HG22	1.86	0.57
1:A:579:LYS:NZ	1:A:581:ASN:OD1	2.37	0.56
1:A:639:GLY:HA2	1:A:649:ARG:HA	1.86	0.56
1:A:533:MET:HE2	4:A:1062:HOH:O	2.04	0.56
1:A:573:LYS:NZ	1:A:701:GLU:O	2.39	0.56
1:A:666:ARG:HH11	1:A:694:TRP:CD1	2.25	0.55
1:A:106:LYS:NZ	4:A:1009:HOH:O	2.25	0.54
1:A:90:LYS:NZ	4:A:1027:HOH:O	2.40	0.54
1:A:166:GLU:OE1	1:A:191:TYR:OH	2.12	0.54
1:A:86:ARG:HG3	1:A:232:TRP:NE1	2.23	0.53
1:A:90:LYS:HG3	1:A:119:TYR:HE2	1.73	0.53
1:A:590:HIS:HD2	1:A:624:ALA:HB2	1.73	0.52
1:A:46:MET:HE1	1:A:66:LYS:HG2	1.91	0.52
1:A:542:GLU:OE1	4:A:1008:HOH:O	2.19	0.52
1:A:596:ILE:HA	1:A:600:VAL:HB	1.93	0.51
1:A:575:ASN:C	1:A:575:ASN:HD22	2.18	0.50
1:A:590:HIS:CD2	1:A:624:ALA:HB2	2.47	0.50
1:A:321:GLU:HA	1:A:321:GLU:OE1	2.11	0.50
1:A:601:ILE:HD13	1:A:724:SER:HB3	1.94	0.49
1:A:786:ASP:OD1	1:A:786:ASP:N	2.41	0.49
1:A:182:ILE:O	1:A:184:GLN:NE2	2.44	0.48
1:A:53:GLN:NE2	4:A:1004:HOH:O	2.05	0.48
1:A:118:ASN:ND2	4:A:1006:HOH:O	2.08	0.47
1:A:142:GLU:HG3	4:A:1353:HOH:O	2.13	0.47
1:A:294:ARG:HG3	1:A:310:GLU:OE2	2.14	0.46
1:A:473:LYS:HG3	1:A:496:GLY:O	2.16	0.46
1:A:684:ALA:C	1:A:685:ASN:HD22	2.24	0.46
1:A:599:TRP:C	1:A:602:PRO:HD2	2.41	0.46
1:A:704:GLU:OE2	1:A:712:ARG:NH2	2.43	0.45
1:A:18:LYS:HE2	1:A:18:LYS:HB2	1.73	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:GLU:OE1	1:A:729:ARG:HD3	2.16	0.44
1:A:761:MET:HB3	1:A:761:MET:HE3	1.71	0.44
1:A:158:GLN:HG2	4:A:1255:HOH:O	2.17	0.44
1:A:511:LYS:NZ	4:A:1043:HOH:O	2.50	0.44
1:A:544:PRO:HD2	1:A:562:PHE:O	2.18	0.44
1:A:187:GLU:OE2	1:A:187:GLU:HA	2.18	0.43
1:A:21:ASN:ND2	4:A:1041:HOH:O	2.49	0.43
1:A:90:LYS:HG3	1:A:119:TYR:CE2	2.54	0.43
1:A:179:GLY:HA2	1:A:199:SER:OG	2.19	0.43
1:A:666:ARG:HD3	1:A:694:TRP:CG	2.54	0.43
1:A:515:LYS:NZ	4:A:1032:HOH:O	2.44	0.42
1:A:263:LEU:HD22	1:A:308:ALA:HA	2.01	0.42
1:A:486:LYS:HD2	1:A:767:SER:HB2	2.01	0.42
1:A:543:TYR:CZ	1:A:545:ASN:HB3	2.55	0.42
1:A:243:LYS:O	1:A:375:ARG:NH2	2.53	0.42
1:A:254:LYS:NZ	4:A:1048:HOH:O	2.52	0.42
1:A:269:TRP:HZ2	1:A:292:ILE:HG23	1.84	0.42
1:A:282:LEU:HD23	1:A:282:LEU:HA	1.86	0.42
1:A:306:PRO:HG2	1:A:334:TYR:HA	2.02	0.42
1:A:285:ASP:OD1	1:A:286:GLY:N	2.53	0.41
1:A:576:LYS:H	1:A:576:LYS:HG2	1.52	0.41
1:A:370:CYS:SG	1:A:376:LYS:HG3	2.60	0.41
1:A:194:MET:HG3	1:A:224:GLN:OE1	2.21	0.41
1:A:204:TRP:NE1	1:A:212:LYS:HE3	2.35	0.41
1:A:282:LEU:HD21	1:A:299:PHE:HB2	2.03	0.41
1:A:537:LEU:HD12	1:A:735:GLU:HG3	2.03	0.41
1:A:550:HIS:CD2	1:A:550:HIS:C	2.99	0.41
1:A:125:HIS:ND1	1:A:611:ASP:OD1	2.45	0.40
1:A:279:LYS:HE3	1:A:371:PRO:O	2.21	0.40
1:A:693:GLU:OE1	1:A:693:GLU:N	2.31	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	820/854 (96%)	795 (97%)	24 (3%)	1 (0%)	48	40

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	696	LYS

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	708/731 (97%)	704 (99%)	4 (1%)	78	81

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	353	LEU
1	A	445	ILE
1	A	579	LYS
1	A	613	ILE

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

Mol	Chain	Res	Type
1	A	44	ASN
1	A	120	HIS
1	A	150	GLN
1	A	188	GLN
1	A	228	GLN
1	A	249	GLN
1	A	379	ASN
1	A	553	GLN
1	A	575	ASN

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Mol	Chain	Res	Type
1	A	722	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 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	YGF	A	902	-	15,20,20	0.57	0	8,33,33	1.38	1 (12%)
2	1PE	A	901	-	15,15,15	0.12	0	14,14,14	0.09	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	YGF	A	902	-	-	1/2/50/50	0/3/3/3
2	1PE	A	901	-	-	4/13/13/13	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	902	YGF	N03-C04-N05	-3.19	120.98	125.42

There are no chirality outliers.

All (5) torsion outliers are listed below:

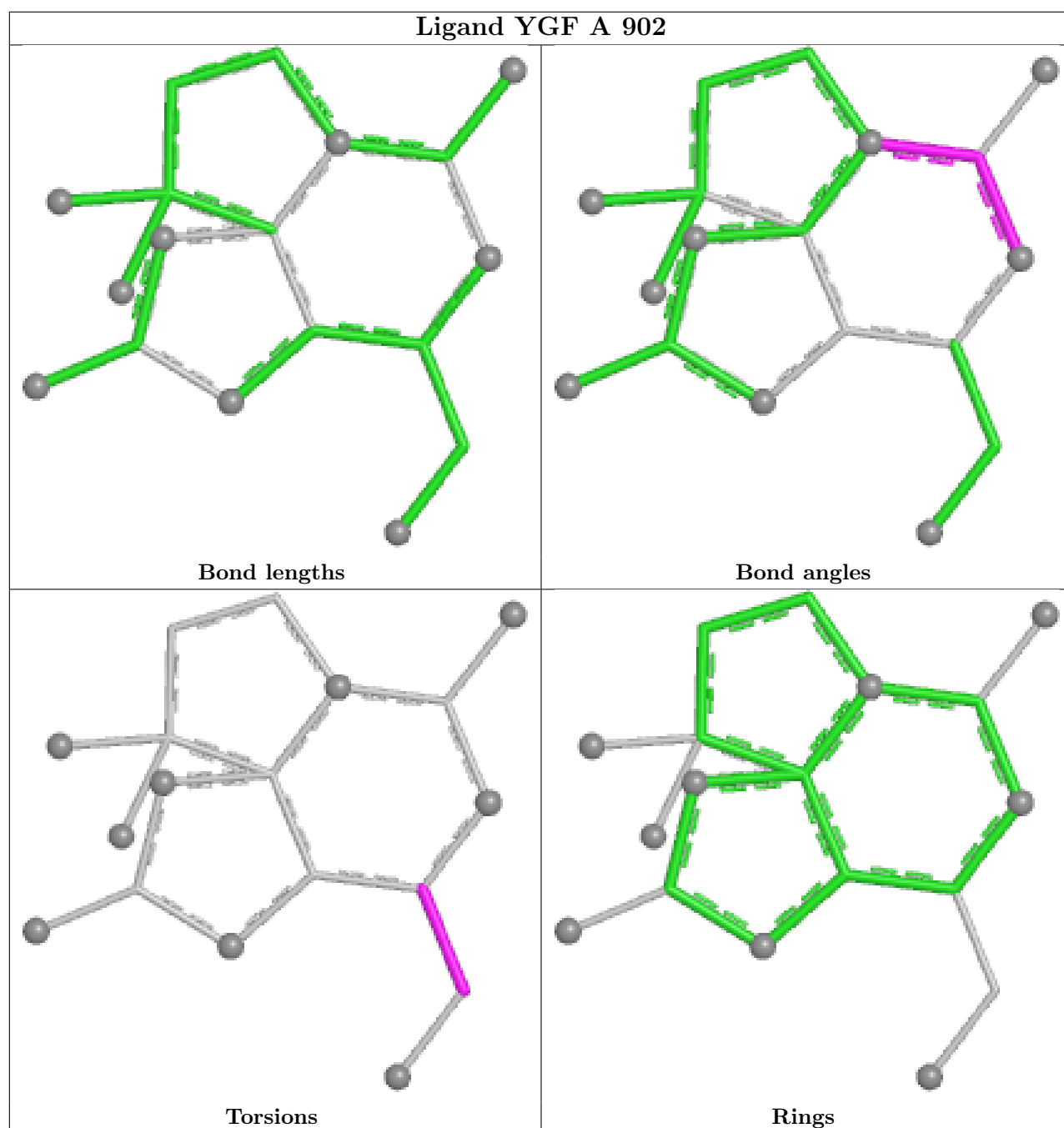
Mol	Chain	Res	Type	Atoms
2	A	901	1PE	OH7-C16-C26-OH6
3	A	902	YGF	N05-C06-C16-O17
2	A	901	1PE	C25-C15-OH6-C26
2	A	901	1PE	OH4-C13-C23-OH3
2	A	901	1PE	C14-C24-OH4-C13

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	902	YGF	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 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 ⓘ

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	A	823/854 (96%)	0.84	102 (12%) 8 8	24, 52, 107, 144	1 (0%)

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	176	ILE	7.4
1	A	698	LEU	5.6
1	A	638	ILE	5.6
1	A	641	PRO	5.1
1	A	613	ILE	4.9
1	A	466	VAL	4.4
1	A	284	TRP	4.4
1	A	178	ILE	4.2
1	A	635	LYS	4.0
1	A	665	PHE	4.0
1	A	224	GLN	3.9
1	A	554	ILE	3.9
1	A	177	ALA	3.8
1	A	468	LEU	3.7
1	A	697	ASP	3.6
1	A	695	ALA	3.6
1	A	283	PRO	3.4
1	A	650	CYS	3.4
1	A	287	LEU	3.4
1	A	644	PRO	3.4
1	A	648	THR	3.4
1	A	362	HIS	3.3
1	A	694	TRP	3.3
1	A	629	THR	3.2
1	A	614	ASP	3.1
1	A	173	GLY	3.1
1	A	158	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	623	CYS	3.1
1	A	714	PRO	3.1
1	A	672	GLY	3.1
1	A	682	VAL	3.0
1	A	174	LYS	3.0
1	A	681	VAL	3.0
1	A	571	VAL	3.0
1	A	647	SER	3.0
1	A	692	ALA	2.9
1	A	223	THR	2.9
1	A	688	GLY	2.9
1	A	552	CYS	2.9
1	A	703	PHE	2.8
1	A	570	LEU	2.8
1	A	637	CYS	2.8
1	A	569	ALA	2.8
1	A	589	CYS	2.8
1	A	471	LYS	2.7
1	A	612	ASN	2.7
1	A	676	PHE	2.6
1	A	88	LEU	2.6
1	A	363	SER	2.6
1	A	683	PHE	2.6
1	A	282	LEU	2.6
1	A	472	ASN	2.6
1	A	706	LEU	2.6
1	A	713	ALA	2.6
1	A	500	CYS	2.5
1	A	649	ARG	2.5
1	A	659	TYR	2.5
1	A	281	LEU	2.5
1	A	636	LEU	2.5
1	A	651	SER	2.5
1	A	616	GLU	2.5
1	A	669	VAL	2.5
1	A	657	ALA	2.4
1	A	658	TYR	2.4
1	A	668	LEU	2.4
1	A	572	LYS	2.4
1	A	620	GLY	2.4
1	A	196	CYS	2.4
1	A	222	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	643	ASN	2.3
1	A	667	CYS	2.3
1	A	684	ALA	2.3
1	A	290	GLY	2.3
1	A	292	ILE	2.3
1	A	578	ILE	2.3
1	A	171	LEU	2.3
1	A	674	VAL	2.2
1	A	691	PRO	2.2
1	A	289	LYS	2.2
1	A	630	ASN	2.2
1	A	611	ASP	2.2
1	A	560	LYS	2.2
1	A	673	ASP	2.1
1	A	127	SER	2.1
1	A	27	CYS	2.1
1	A	555	PRO	2.1
1	A	288	ALA	2.1
1	A	615	ILE	2.1
1	A	31	ASP	2.1
1	A	693	GLU	2.1
1	A	626	GLY	2.1
1	A	633	LEU	2.1
1	A	621	GLU	2.0
1	A	98	SER	2.0
1	A	671	LYS	2.0
1	A	151	THR	2.0
1	A	550	HIS	2.0
1	A	755	ASN	2.0
1	A	149	VAL	2.0
1	A	317	CYS	2.0
1	A	175	ARG	2.0
1	A	720	GLY	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](#)

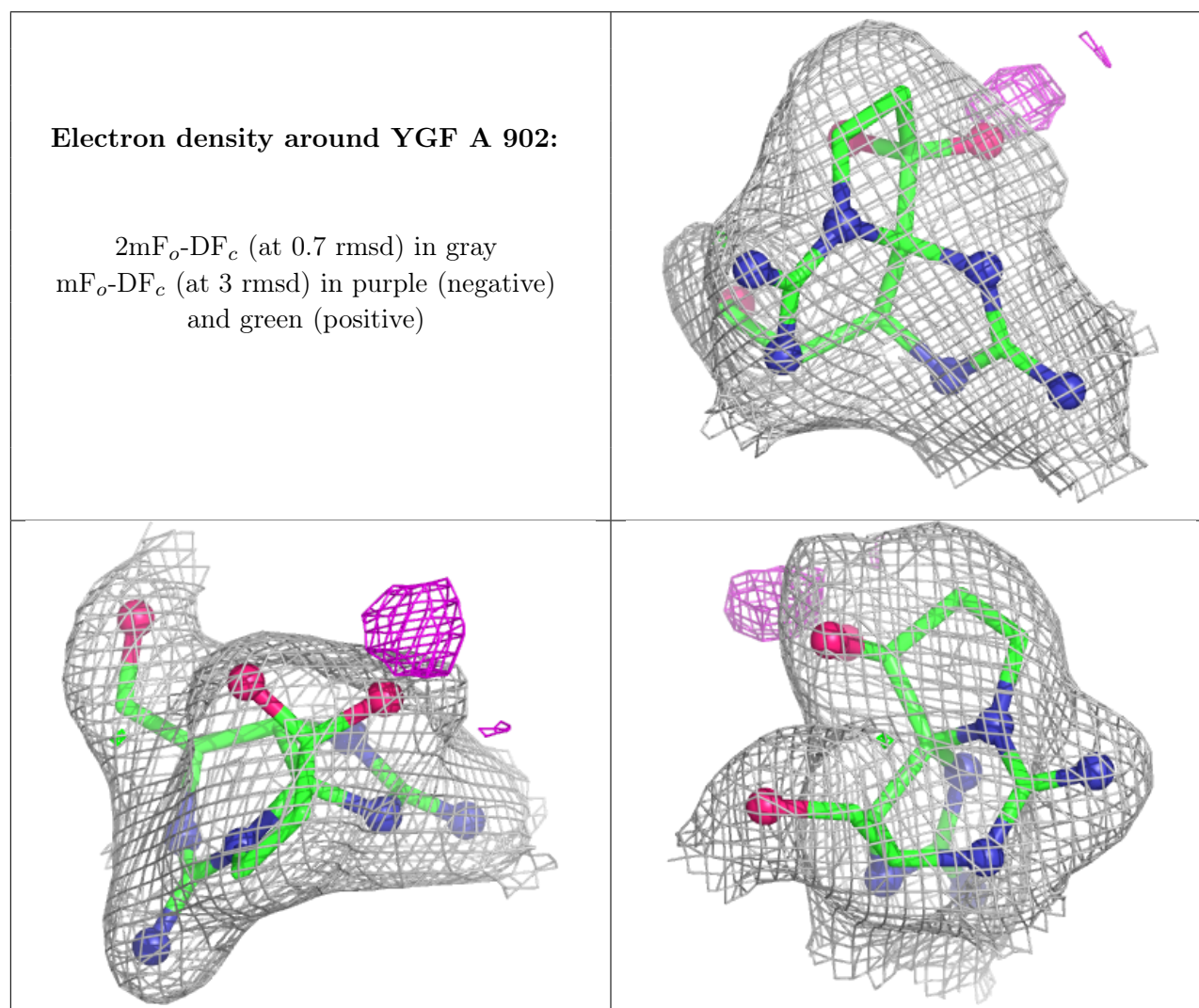
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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	1PE	A	901	16/16	0.88	0.15	62,73,82,83	0
3	YGF	A	902	18/18	0.91	0.10	46,57,68,68	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.