



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 25, 2022 – 10:26 AM EDT

PDB ID : 8D6M
Title : Nanorana parkeri saxiphilin:STX (co-crystal)
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Deposited on : 2022-06-06
Resolution : 2.00 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 : 2.31.2
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) : 2.31.2

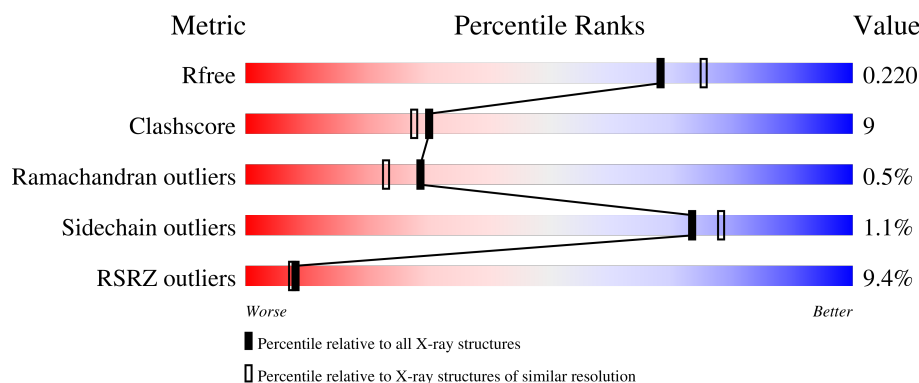
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	A	854	<div> <div>9%</div> <div>79%</div> <div>16%</div> <div>••</div> </div>

2 Entry composition [i](#)

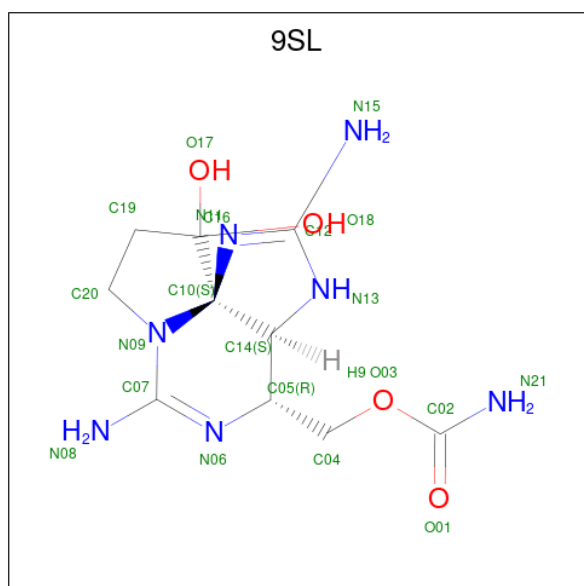
There are 4 unique types of molecules in this entry. The entry contains 6717 atoms, of which 22 are hydrogens and 0 are deuteriums.

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.

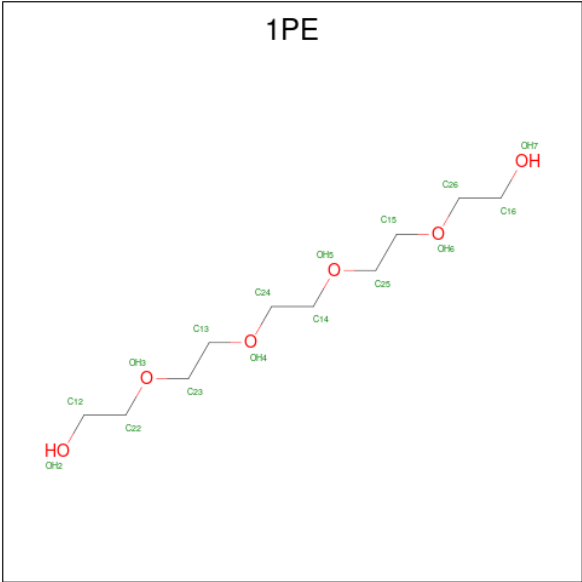
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	822	6371	3989	1100	1223	59	0	0	0

- Molecule 2 is [(3aS,4R,10aS)-2,6-diamino-10,10-dihydroxy-3a,4,9,10-tetrahydro-3H,8H-pyrrolo[1,2-c]purin-4-yl]methyl carbamate (three-letter code: 9SL) (formula: C₁₀H₁₇N₇O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	21	10	7	4	0	0

- Molecule 3 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			38	10	22	6		

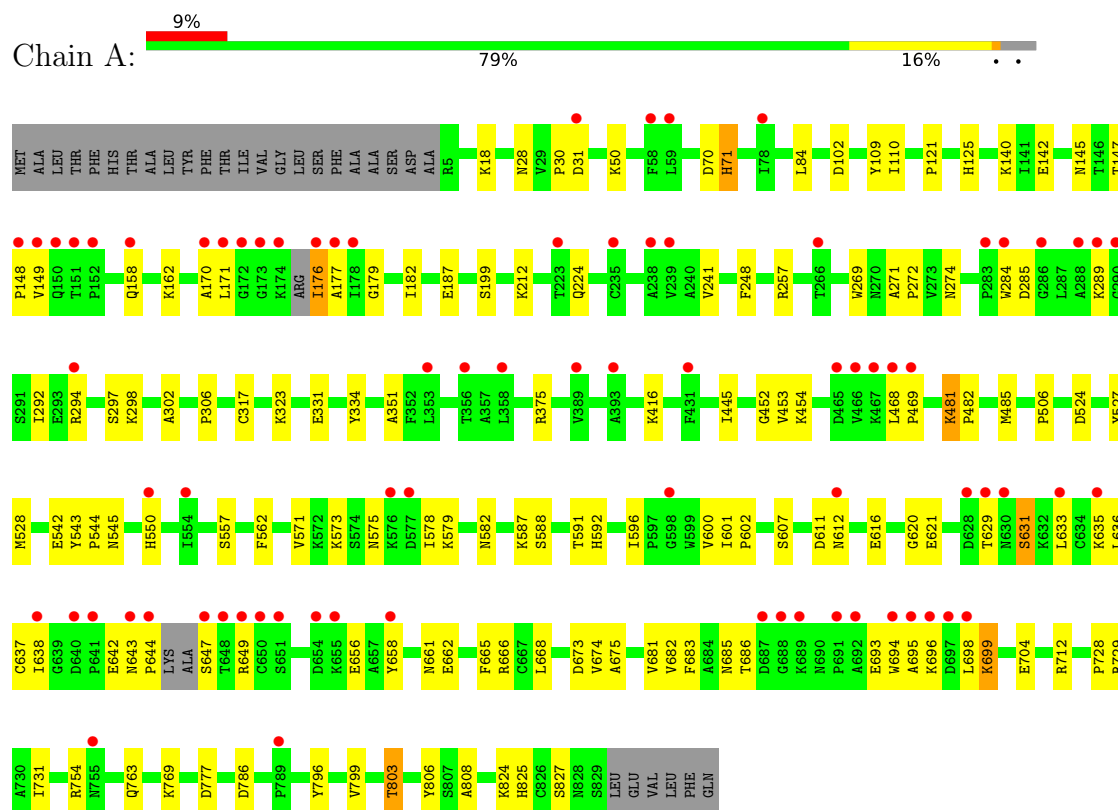
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	287	Total	O	0	0
			287	287		

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	228.85Å 228.85Å 67.22Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.55 – 2.00 42.55 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (42.55-2.00) 99.9 (42.55-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.192 , 0.221 0.191 , 0.220	Depositor DCC
R_{free} test set	4443 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	49.9	Xtriage
Anisotropy	0.328	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 55.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.011 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6717	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 1PE, 9SL

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	0.29	0/6515	0.49	0/8811

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	6371	0	6169	117	0
2	A	21	0	0	2	0
3	A	16	22	22	1	0
4	A	287	0	0	9	0
All	All	6695	22	6191	117	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 9.

All (117) 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:102:ASP:H	1:A:803:THR:HG21	1.09	1.07
1:A:454:LYS:NZ	4:A:1001:HOH:O	1.80	1.06
1:A:631:SER:OG	1:A:633:LEU:HD12	1.66	0.95
1:A:284:TRP:HA	1:A:289:LYS:HD3	1.49	0.94
1:A:298:LYS:HE3	1:A:298:LYS:HA	1.51	0.90
1:A:452:GLY:HA3	4:A:1001:HOH:O	1.72	0.89
1:A:661:ASN:HB3	1:A:681:VAL:HG22	1.52	0.89
1:A:481:LYS:H	1:A:481:LYS:HE2	1.37	0.88
1:A:693:GLU:OE1	1:A:693:GLU:N	2.11	0.84
1:A:799:VAL:O	1:A:803:THR:HG23	1.79	0.82
1:A:102:ASP:N	1:A:803:THR:HG21	1.92	0.81
1:A:621:GLU:HB3	1:A:636:LEU:HD13	1.63	0.79
1:A:621:GLU:HB3	1:A:636:LEU:CD1	2.13	0.78
1:A:661:ASN:HB3	1:A:681:VAL:CG2	2.17	0.75
1:A:187:GLU:OE2	1:A:187:GLU:HA	1.85	0.75
1:A:638:ILE:HG13	1:A:658:TYR:CE2	2.25	0.71
1:A:179:GLY:HA2	1:A:199:SER:OG	1.93	0.68
1:A:662:GLU:HG3	1:A:685:ASN:ND2	2.09	0.68
1:A:644:PRO:HG3	1:A:647:SER:N	2.09	0.68
1:A:616:GLU:HB3	1:A:633:LEU:HD11	1.75	0.68
1:A:481:LYS:H	1:A:481:LYS:CE	2.07	0.67
1:A:662:GLU:HG3	1:A:685:ASN:HD21	1.60	0.67
1:A:587:LYS:HG3	1:A:673:ASP:OD2	1.96	0.66
1:A:125:HIS:ND1	1:A:611:ASP:OD1	2.27	0.66
1:A:294:ARG:O	1:A:297:SER:OG	2.12	0.65
1:A:682:VAL:O	1:A:686:THR:HG23	1.96	0.65
1:A:140:LYS:HD3	1:A:145:ASN:HD21	1.62	0.64
1:A:298:LYS:HE3	1:A:298:LYS:CA	2.23	0.63
1:A:631:SER:HG	1:A:633:LEU:HD12	1.63	0.62
1:A:453:VAL:HG13	1:A:454:LYS:HD3	1.80	0.62
1:A:649:ARG:HA	1:A:656:GLU:OE1	2.02	0.60
1:A:694:TRP:O	1:A:698:LEU:HD21	2.01	0.60
1:A:30:PRO:O	1:A:31:ASP:HB2	2.02	0.60
1:A:84:LEU:HD22	1:A:824:LYS:HE2	1.82	0.60
1:A:573:LYS:HD2	1:A:704:GLU:CD	2.23	0.59
1:A:274:ASN:HB3	3:A:902:1PE:H141	1.83	0.59
1:A:50:LYS:HE2	1:A:71:HIS:O	2.03	0.58
1:A:375:ARG:NH1	4:A:1002:HOH:O	1.94	0.58
1:A:695:ALA:C	1:A:698:LEU:HD23	2.24	0.58
1:A:147:THR:HB	1:A:148:PRO:HD2	1.87	0.57
1:A:596:ILE:HA	1:A:600:VAL:HB	1.87	0.57
1:A:607:SER:OG	1:A:612:ASN:HA	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:643:ASN:HB2	1:A:644:PRO:HD2	1.87	0.56
1:A:109:TYR:O	1:A:110:ILE:HD13	2.05	0.56
1:A:728:PRO:HD2	2:A:901:9SL:N08	2.22	0.54
1:A:224:GLN:HA	1:A:224:GLN:OE1	2.06	0.54
1:A:616:GLU:HA	1:A:633:LEU:HD21	1.90	0.54
1:A:601:ILE:HB	1:A:602:PRO:HD3	1.90	0.54
1:A:587:LYS:HA	1:A:621:GLU:O	2.08	0.53
1:A:542:GLU:OE1	1:A:729:ARG:HD3	2.08	0.53
1:A:298:LYS:HA	1:A:298:LYS:CE	2.31	0.52
1:A:121:PRO:HG3	1:A:158:GLN:HG3	1.91	0.52
1:A:637:CYS:HA	1:A:658:TYR:HD2	1.75	0.52
1:A:638:ILE:O	1:A:649:ARG:HG3	2.10	0.52
1:A:28:ASN:O	1:A:416:LYS:HE2	2.10	0.51
1:A:550:HIS:HE1	1:A:557:SER:CB	2.24	0.51
1:A:171:LEU:HD23	1:A:182:ILE:HD13	1.92	0.51
1:A:453:VAL:CG1	1:A:454:LYS:HD3	2.42	0.50
1:A:763:GLN:NE2	4:A:1019:HOH:O	2.44	0.50
1:A:481:LYS:N	1:A:481:LYS:HD3	2.26	0.50
1:A:621:GLU:HG2	1:A:635:LYS:HB2	1.93	0.49
1:A:285:ASP:OD1	1:A:289:LYS:HD2	2.12	0.49
1:A:481:LYS:N	1:A:481:LYS:CD	2.75	0.49
1:A:145:ASN:H	1:A:145:ASN:HD22	1.60	0.49
1:A:682:VAL:HG13	1:A:683:PHE:N	2.27	0.49
1:A:142:GLU:OE1	1:A:142:GLU:HA	2.12	0.49
1:A:524:ASP:HB3	4:A:1200:HOH:O	2.13	0.49
1:A:171:LEU:CD2	1:A:182:ILE:HD13	2.44	0.48
1:A:481:LYS:H	1:A:481:LYS:CD	2.27	0.48
1:A:317:CYS:HB3	1:A:331:GLU:OE1	2.14	0.47
1:A:109:TYR:C	1:A:110:ILE:HD13	2.35	0.47
1:A:629:THR:HG22	1:A:649:ARG:HH21	1.80	0.47
1:A:257:ARG:HA	1:A:302:ALA:O	2.16	0.46
1:A:665:PHE:CD2	1:A:685:ASN:HB2	2.49	0.46
1:A:825:HIS:CG	4:A:1001:HOH:O	2.69	0.46
1:A:18:LYS:HB2	1:A:18:LYS:HE2	1.67	0.46
1:A:171:LEU:HD22	1:A:176:ILE:HA	1.97	0.46
1:A:269:TRP:HZ2	1:A:292:ILE:HG22	1.81	0.46
1:A:588:SER:HA	1:A:674:VAL:O	2.16	0.46
1:A:693:GLU:HG2	1:A:694:TRP:N	2.31	0.46
1:A:485:MET:HE3	1:A:769:LYS:HD3	1.98	0.45
1:A:271:ALA:HB3	1:A:272:PRO:HD3	1.98	0.45
1:A:571:VAL:HG12	1:A:673:ASP:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:ALA:O	1:A:177:ALA:HB2	2.16	0.45
1:A:666:ARG:HG2	1:A:694:TRP:CE2	2.52	0.45
1:A:806:TYR:OH	4:A:1003:HOH:O	2.20	0.45
1:A:323:LYS:HA	1:A:323:LYS:HD3	1.82	0.44
1:A:731:ILE:HD12	1:A:731:ILE:N	2.32	0.44
1:A:543:TYR:CZ	1:A:545:ASN:HB3	2.52	0.44
1:A:803:THR:HG22	1:A:808:ALA:HB2	1.97	0.44
1:A:578:ILE:O	1:A:712:ARG:NH1	2.50	0.44
1:A:454:LYS:HE2	1:A:454:LYS:HB2	1.63	0.44
1:A:579:LYS:H	1:A:582:ASN:HD21	1.66	0.44
1:A:140:LYS:NZ	4:A:1006:HOH:O	2.28	0.44
1:A:241:VAL:CG1	1:A:351:ALA:HB3	2.49	0.43
1:A:506:PRO:HG2	1:A:527:TYR:CE2	2.53	0.43
1:A:269:TRP:CZ2	1:A:292:ILE:HG22	2.53	0.43
1:A:269:TRP:O	1:A:272:PRO:HD2	2.19	0.43
1:A:306:PRO:HG2	1:A:334:TYR:HA	2.00	0.42
1:A:248:PHE:O	1:A:375:ARG:NH1	2.53	0.42
1:A:544:PRO:HD2	1:A:562:PHE:O	2.19	0.42
1:A:481:LYS:N	1:A:482:PRO:HD2	2.34	0.42
1:A:591:THR:O	1:A:592:HIS:HB3	2.19	0.42
1:A:803:THR:HA	1:A:808:ALA:N	2.35	0.41
1:A:147:THR:OG1	1:A:149:VAL:HG22	2.20	0.41
1:A:454:LYS:HE3	1:A:827:SER:CB	2.50	0.41
1:A:212:LYS:HE2	4:A:1259:HOH:O	2.20	0.41
1:A:528:MET:HG3	1:A:796:TYR:CZ	2.56	0.41
1:A:698:LEU:O	1:A:699:LYS:HB2	2.21	0.41
1:A:754:ARG:NH2	1:A:777:ASP:O	2.54	0.41
1:A:696:LYS:HE2	1:A:696:LYS:HB3	1.82	0.40
1:A:786:ASP:O	2:A:901:9SL:N15	2.53	0.40
1:A:686:THR:HB	1:A:699:LYS:C	2.41	0.40
1:A:298:LYS:CA	1:A:298:LYS:CE	2.92	0.40
1:A:647:SER:C	1:A:649:ARG:H	2.24	0.40
1:A:468:LEU:HA	1:A:469:PRO:HD3	1.92	0.40
1:A:668:LEU:HB2	1:A:675:ALA:HB2	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	816/854 (96%)	781 (96%)	31 (4%)	4 (0%)	29	23

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	575	ASN
1	A	642	GLU
1	A	699	LYS
1	A	620	GLY

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	706/731 (97%)	698 (99%)	8 (1%)	73	78

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	ASP
1	A	71	HIS
1	A	162	LYS
1	A	176	ILE
1	A	445	ILE
1	A	481	LYS
1	A	631	SER

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Mol	Chain	Res	Type
1	A	803	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	ASN
1	A	550	HIS
1	A	685	ASN
1	A	763	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
2	9SL	A	901	-	17,23,23	3.44	11 (64%)	13,37,37	3.65	5 (38%)
3	1PE	A	902	-	15,15,15	0.53	0	14,14,14	0.21	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	9SL	A	901	-	-	2/5/53/53	0/3/3/3
3	1PE	A	902	-	-	6/13/13/13	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	9SL	C12-N13	6.96	1.46	1.35
2	A	901	9SL	C02-N21	6.37	1.45	1.33
2	A	901	9SL	C07-N08	6.27	1.45	1.34
2	A	901	9SL	C12-N15	4.82	1.45	1.34
2	A	901	9SL	O03-C02	3.24	1.40	1.35
2	A	901	9SL	C19-C20	2.44	1.57	1.52
2	A	901	9SL	O01-C02	-2.44	1.18	1.21
2	A	901	9SL	C19-C16	2.42	1.57	1.52
2	A	901	9SL	C05-C14	2.38	1.58	1.52
2	A	901	9SL	O03-C04	-2.34	1.39	1.45
2	A	901	9SL	C05-N06	-2.12	1.44	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	9SL	O03-C02-N21	8.69	121.87	111.08
2	A	901	9SL	O03-C02-O01	-5.52	117.85	123.07
2	A	901	9SL	N09-C07-N06	-5.43	117.86	125.42
2	A	901	9SL	C19-C20-N09	-4.66	98.55	103.83
2	A	901	9SL	O01-C02-N21	-3.18	120.27	125.51

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	9SL	O01-C02-O03-C04
2	A	901	9SL	N21-C02-O03-C04
3	A	902	1PE	OH5-C14-C24-OH4
3	A	902	1PE	OH6-C15-C25-OH5
3	A	902	1PE	C25-C15-OH6-C26
3	A	902	1PE	C15-C25-OH5-C14

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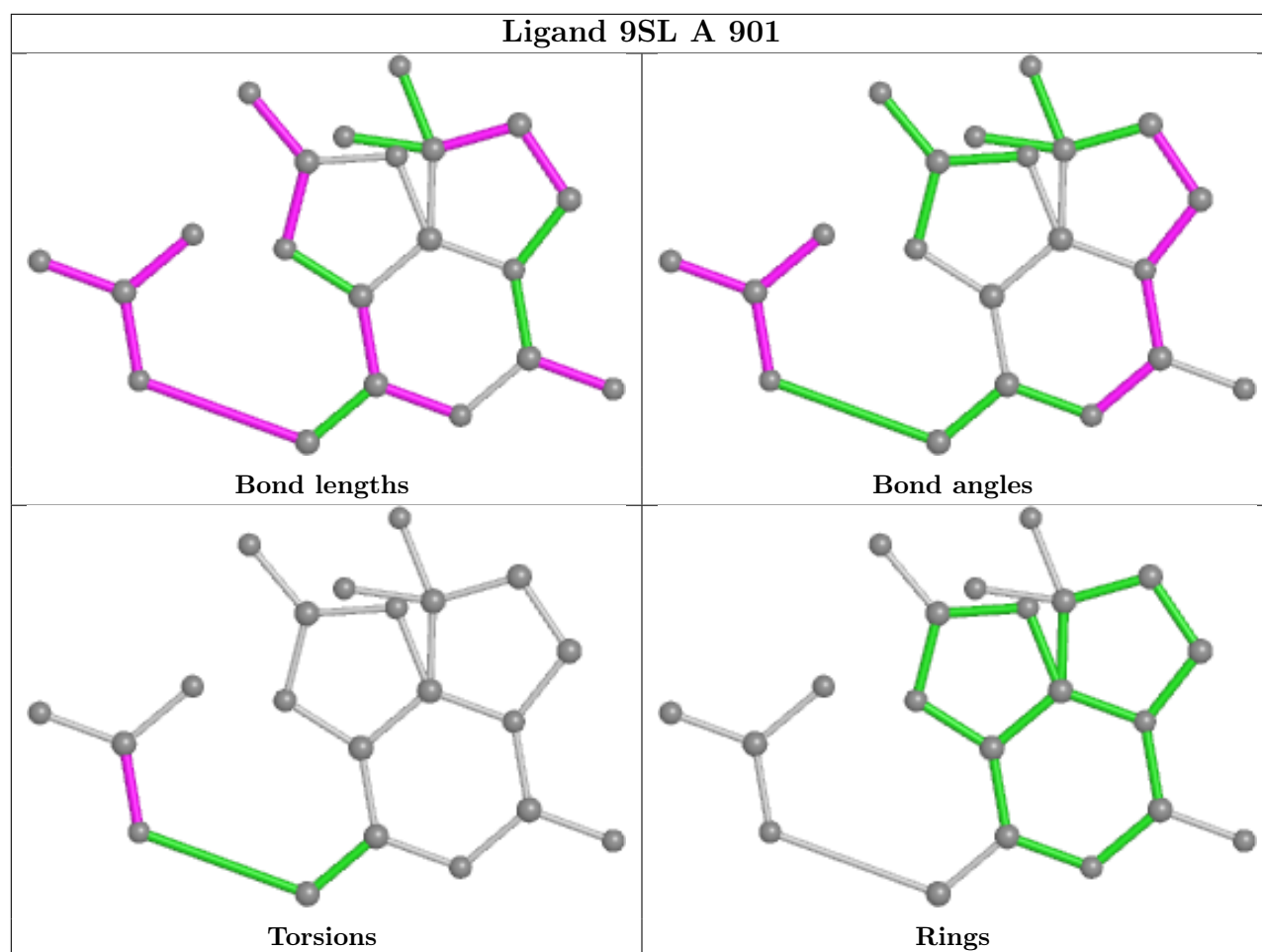
Mol	Chain	Res	Type	Atoms
3	A	902	1PE	C14-C24-OH4-C13
3	A	902	1PE	OH7-C16-C26-OH6

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	9SL	2	0
3	A	902	1PE	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	822/854 (96%)	0.50	77 (9%) 8 8	39, 58, 111, 158	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	149	VAL	8.5
1	A	176	ILE	7.4
1	A	649	ARG	7.1
1	A	288	ALA	7.1
1	A	290	GLY	6.4
1	A	691	PRO	6.2
1	A	651	SER	6.2
1	A	174	LYS	6.1
1	A	647	SER	5.9
1	A	466	VAL	5.6
1	A	638	ILE	5.4
1	A	696	LYS	5.3
1	A	644	PRO	4.9
1	A	688	GLY	4.9
1	A	650	CYS	4.7
1	A	629	THR	4.7
1	A	640	ASP	4.5
1	A	648	THR	4.5
1	A	641	PRO	4.3
1	A	697	ASP	4.2
1	A	177	ALA	4.1
1	A	630	ASN	3.9
1	A	178	ILE	3.8
1	A	148	PRO	3.8
1	A	173	GLY	3.8
1	A	577	ASP	3.8
1	A	171	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	31	ASP	3.6
1	A	172	GLY	3.5
1	A	465	ASP	3.5
1	A	289	LYS	3.5
1	A	628	ASP	3.4
1	A	612	ASN	3.4
1	A	283	PRO	3.3
1	A	550	HIS	3.3
1	A	150	GLN	3.3
1	A	655	LYS	3.2
1	A	695	ALA	3.2
1	A	468	LEU	3.2
1	A	151	THR	3.0
1	A	356	THR	3.0
1	A	658	TYR	2.9
1	A	469	PRO	2.9
1	A	576	LYS	2.9
1	A	654	ASP	2.9
1	A	694	TRP	2.8
1	A	643	ASN	2.8
1	A	284	TRP	2.8
1	A	286	GLY	2.7
1	A	389	VAL	2.7
1	A	223	THR	2.7
1	A	353	LEU	2.7
1	A	58	PHE	2.6
1	A	687	ASP	2.5
1	A	755	ASN	2.4
1	A	152	PRO	2.4
1	A	467	LYS	2.3
1	A	358	LEU	2.3
1	A	633	LEU	2.3
1	A	431	PHE	2.3
1	A	78	ILE	2.2
1	A	266	THR	2.2
1	A	59	LEU	2.2
1	A	239	VAL	2.2
1	A	692	ALA	2.1
1	A	698	LEU	2.1
1	A	238	ALA	2.1
1	A	689	LYS	2.1
1	A	635	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	235	CYS	2.1
1	A	598	GLY	2.1
1	A	554	ILE	2.1
1	A	158	GLN	2.0
1	A	294	ARG	2.0
1	A	170	ALA	2.0
1	A	393	ALA	2.0
1	A	789	PRO	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](#)

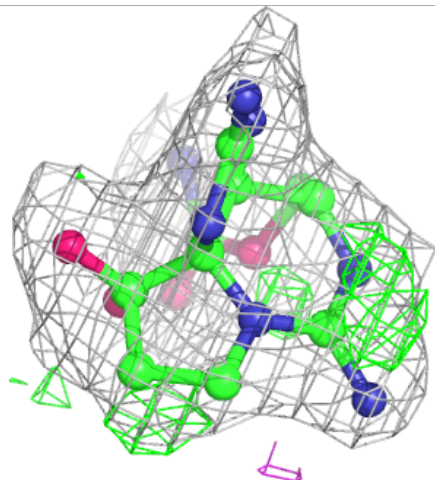
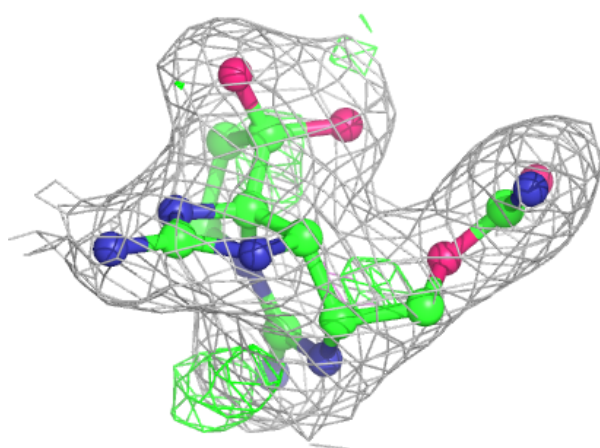
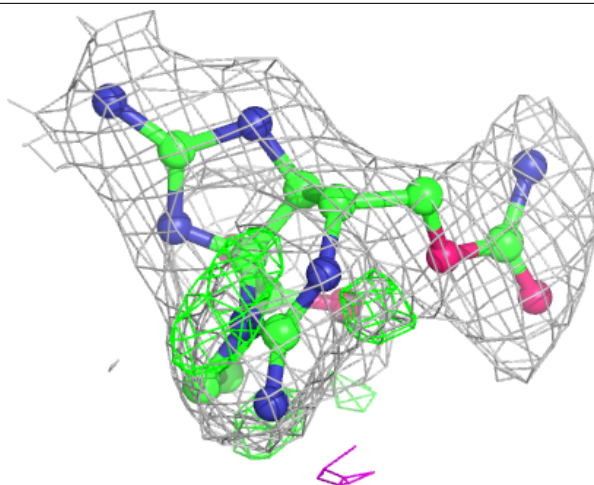
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	1PE	A	902	16/16	0.72	0.23	73,96,107,113	0
2	9SL	A	901	21/21	0.93	0.12	46,58,67,77	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 9SL A 901:

$2mF_o-DF_c$ (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.