



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:51 AM UTC

PDB ID : 8D6T / pdb_00008d6t
Title : Rana catesbeiana saxiphilin mutant - Y558I:STX (co-crystal)
Authors : Chen, Z.; Zakrzewska, S.; Minor, D.L.
Deposited on : 2022-06-06
Resolution : 2.15 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

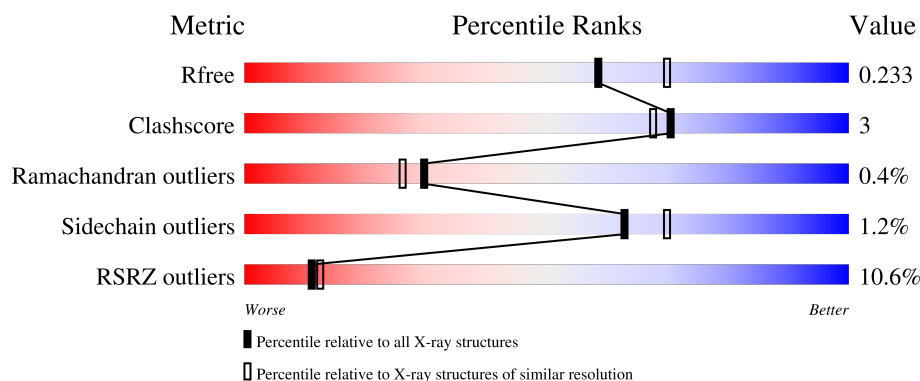
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	851	
1	B	851	

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
3	CAC	B	902	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13488 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.

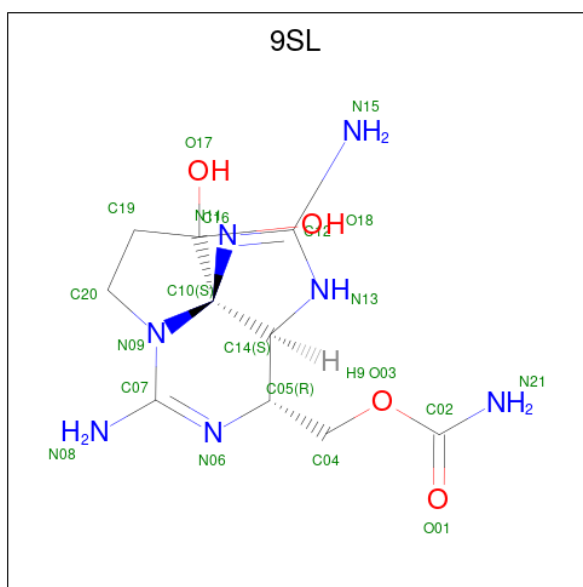
- Molecule 1 is a protein called Saxiphilin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	818	Total	C	N	O	S	0	0	0
			6311	3942	1090	1220	59			
1	A	818	Total	C	N	O	S	0	0	0
			6311	3942	1090	1220	59			

There are 16 discrepancies between the modelled and reference sequences:

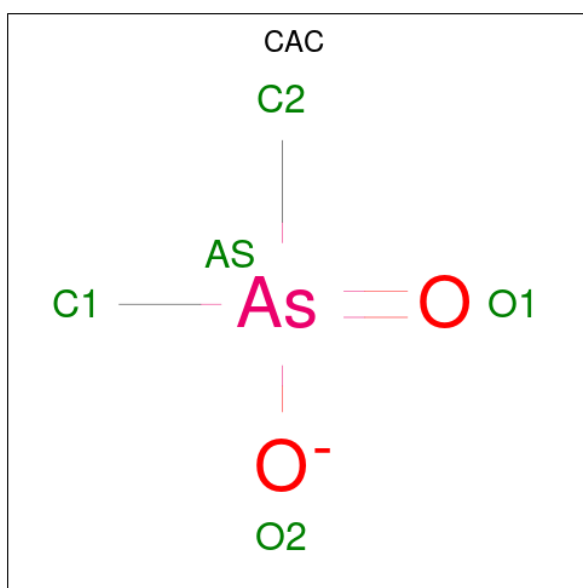
Chain	Residue	Modelled	Actual	Comment	Reference
B	558	ILE	TYR	engineered mutation	UNP P31226
B	826	SER	-	expression tag	UNP P31226
B	827	ASN	-	expression tag	UNP P31226
B	828	SER	-	expression tag	UNP P31226
B	829	LEU	-	expression tag	UNP P31226
B	830	GLU	-	expression tag	UNP P31226
B	831	VAL	-	expression tag	UNP P31226
B	832	LEU	-	expression tag	UNP P31226
A	558	ILE	TYR	engineered mutation	UNP P31226
A	826	SER	-	expression tag	UNP P31226
A	827	ASN	-	expression tag	UNP P31226
A	828	SER	-	expression tag	UNP P31226
A	829	LEU	-	expression tag	UNP P31226
A	830	GLU	-	expression tag	UNP P31226
A	831	VAL	-	expression tag	UNP P31226
A	832	LEU	-	expression tag	UNP P31226

- 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 (CCD ID: 9SL) (formula: C₁₀H₁₇N₇O₄) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is CACODYLATE ION (CCD ID: CAC) (formula: $C_2H_6AsO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	As	C	O	0	0
			5	1	2	2		
3	B	1	Total	As	C	O	0	0
			5	1	2	2		

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

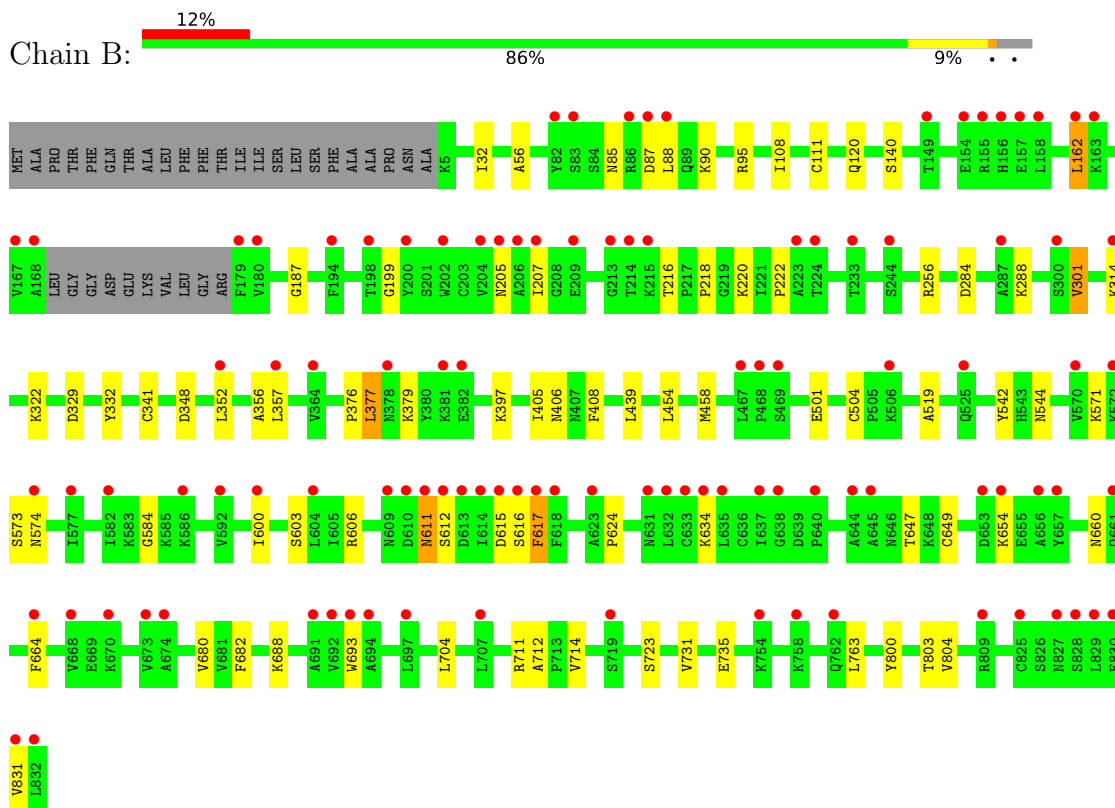
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	379	Total	O	0	0
			379	379		
4	A	415	Total	O	0	0
			415	415		

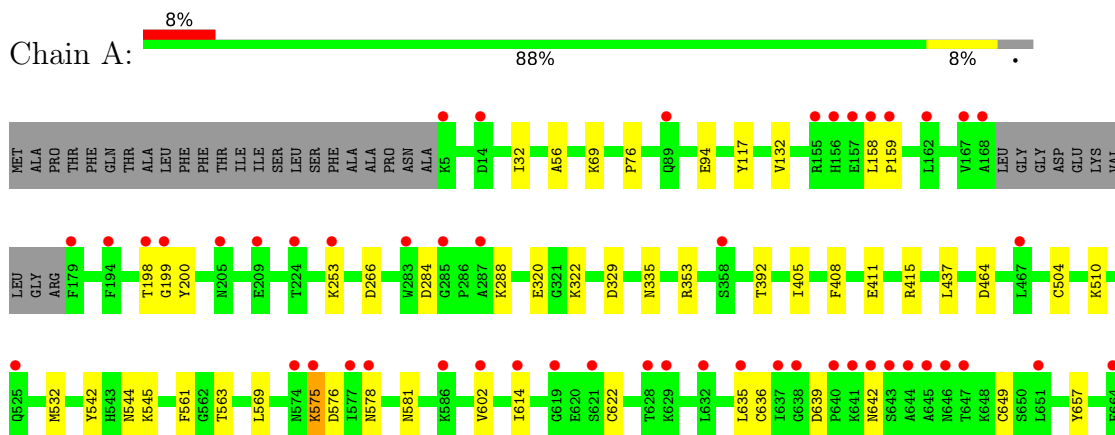
3 Residue-property plots [i](#)

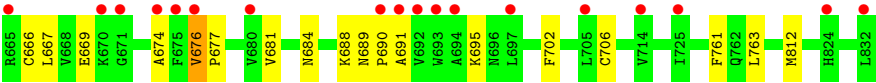
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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



• Molecule 1: Saxiphilin





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.03Å 107.81Å 253.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.50 – 2.15 47.50 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.4 (47.50-2.15) 99.4 (47.50-2.15)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.16Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.207 , 0.234 0.207 , 0.233	Depositor DCC
R_{free} test set	7104 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	44.0	Xtriage
Anisotropy	0.712	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 42.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13488	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% 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: 9SL, CAC

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	0.15	0/6436	0.36	0/8686
1	B	0.15	0/6436	0.34	0/8686
All	All	0.15	0/12872	0.35	0/17372

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	6311	0	6183	37	0
1	B	6311	0	6183	47	0
2	A	21	0	0	0	0
2	B	21	0	0	0	0
3	A	15	0	0	0	0
3	B	15	0	0	0	0
4	A	415	0	0	9	0
4	B	379	0	0	7	0
All	All	13488	0	12366	84	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 3.

All (84) 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:636:CYS:SG	4:A:1328:HOH:O	2.36	0.83
1:A:602:VAL:HG23	1:A:614:ILE:HG13	1.68	0.75
1:A:649:CYS:SG	4:A:1328:HOH:O	2.46	0.73
1:B:501:GLU:OE1	4:B:1001:HOH:O	2.13	0.67
1:A:253:LYS:NZ	4:A:1002:HOH:O	2.16	0.65
1:B:140:SER:HB3	1:B:831:VAL:HG12	1.78	0.64
1:B:600:ILE:HD13	1:B:723:SER:HB3	1.79	0.64
1:A:411:GLU:OE1	1:A:415:ARG:NH1	2.32	0.63
1:A:94:GLU:OE1	4:A:1001:HOH:O	2.15	0.63
1:B:504:CYS:SG	4:B:1286:HOH:O	2.55	0.60
1:A:32:ILE:HG21	1:A:408:PHE:HB2	1.83	0.60
1:B:205:ASN:O	1:B:207:ILE:N	2.32	0.60
1:A:284:ASP:HB3	1:A:288:LYS:HD2	1.83	0.59
1:B:199:GLY:HA3	1:B:218:PRO:HB3	1.85	0.58
1:A:76:PRO:HB3	1:A:392:THR:HG21	1.86	0.58
1:B:85:ASN:HA	1:B:88:LEU:HD13	1.86	0.58
1:B:647:THR:HB	1:B:654:LYS:HB3	1.86	0.57
1:B:322:LYS:HD3	1:B:329:ASP:HB3	1.86	0.57
1:B:301:VAL:HG12	1:B:314:LYS:HD2	1.86	0.56
1:A:667:LEU:HB2	1:A:674:ALA:HB2	1.88	0.56
1:A:691:ALA:HB1	1:A:695:LYS:HE3	1.88	0.55
1:A:335:ASN:ND2	4:A:1013:HOH:O	2.38	0.54
1:B:120:GLN:NE2	4:B:1015:HOH:O	2.42	0.53
1:B:87:ASP:HA	1:B:90:LYS:HB2	1.91	0.53
1:B:256:ARG:NH1	1:B:348:ASP:OD1	2.41	0.52
1:B:284:ASP:HB3	1:B:288:LYS:HD2	1.92	0.51
1:B:603:SER:OG	1:B:803:THR:O	2.27	0.51
1:B:314:LYS:NZ	4:B:1004:HOH:O	2.27	0.51
1:A:569:LEU:HD22	1:A:681:VAL:HG22	1.91	0.50
1:B:216:THR:HG21	1:B:222:PRO:HA	1.93	0.50
1:A:504:CYS:SG	4:A:1343:HOH:O	2.59	0.50
1:A:437:LEU:HD13	4:A:1354:HOH:O	2.11	0.49
1:B:612:SER:HB2	1:B:616:SER:HB2	1.93	0.49
1:A:94:GLU:OE1	1:A:117:TYR:OH	2.30	0.49
1:B:571:LYS:O	1:B:573:SER:N	2.41	0.49
1:B:574:ASN:O	1:B:711:ARG:NH2	2.46	0.49
1:B:664:PHE:HD2	1:B:693:TRP:HZ3	1.61	0.49
1:A:691:ALA:HA	1:A:695:LYS:HG3	1.95	0.49
1:B:32:ILE:HG21	1:B:408:PHE:HB2	1.95	0.48
1:A:761:PHE:HE2	1:A:763:LEU:HD23	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:712:ALA:HB3	4:B:1278:HOH:O	2.13	0.47
1:A:622:CYS:HB2	1:A:635:LEU:HD12	1.96	0.47
1:A:676:VAL:HG12	1:A:677:PRO:HD2	1.96	0.47
1:B:357:LEU:HG	1:B:377:LEU:HG	1.98	0.46
1:B:624:PRO:HA	1:B:649:CYS:HA	1.98	0.46
1:A:569:LEU:HD11	1:A:702:PHE:HB3	1.98	0.45
1:A:322:LYS:HD2	1:A:329:ASP:HB3	1.99	0.45
1:B:584:GLY:N	1:B:617:PHE:O	2.47	0.44
1:A:159:PRO:HA	4:A:1286:HOH:O	2.17	0.44
1:A:657:TYR:OH	1:A:669:GLU:OE1	2.32	0.44
1:B:332:TYR:CG	1:B:341:CYS:HB2	2.53	0.44
1:A:510:LYS:NZ	4:A:1027:HOH:O	2.50	0.44
1:A:575:LYS:H	1:A:575:LYS:HG3	1.62	0.44
1:B:704:LEU:HD13	1:B:714:VAL:HG12	2.00	0.43
1:B:542:TYR:CZ	1:B:544:ASN:HB3	2.53	0.43
1:A:578:ASN:HB2	1:A:581:ASN:ND2	2.33	0.43
1:B:454:LEU:HD11	1:B:458:MET:HE2	2.01	0.43
1:A:198:THR:O	1:A:200:TYR:N	2.52	0.42
1:B:647:THR:HG21	1:B:654:LYS:HE2	2.01	0.42
1:B:660:ASN:HB3	1:B:680:VAL:HG22	2.01	0.42
1:A:266:ASP:OD2	1:A:353:ARG:HB2	2.20	0.42
1:A:69:LYS:NZ	1:A:464:ASP:OD2	2.36	0.42
1:B:56:ALA:HB2	1:B:405:ILE:HD13	2.02	0.42
1:A:532:MET:HE2	1:A:532:MET:HB2	1.95	0.42
1:B:220:LYS:HE3	1:B:220:LYS:HB3	1.85	0.42
1:B:606:ARG:HG2	1:B:611:ASN:HA	2.02	0.42
1:B:95:ARG:HG3	1:B:108:ILE:HG22	2.02	0.41
1:B:406:ASN:OD1	1:B:439:LEU:HB2	2.21	0.41
1:B:501:GLU:HG3	4:B:1162:HOH:O	2.20	0.41
1:A:542:TYR:CZ	1:A:544:ASN:HB3	2.56	0.41
1:B:376:PRO:HD2	1:B:379:LYS:HG3	2.02	0.41
1:B:162:LEU:HD13	1:B:187:GLY:HA2	2.02	0.41
1:B:397:LYS:HE2	4:B:1321:HOH:O	2.19	0.41
1:B:800:TYR:CE1	1:B:804:VAL:HG21	2.56	0.41
1:A:561:PHE:HB3	1:A:563:THR:HG23	2.03	0.41
1:A:684:ASN:C	1:A:689:ASN:HB3	2.45	0.41
1:B:352:LEU:HD12	1:B:356:ALA:HB3	2.03	0.41
1:B:603:SER:OG	1:B:804:VAL:HA	2.21	0.41
1:A:545:LYS:HB3	1:A:545:LYS:HE2	1.84	0.41
1:B:682:PHE:O	1:B:688:LYS:HD2	2.21	0.40
1:B:519:ALA:HA	1:B:731:VAL:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:654:LYS:HD2	1:B:654:LYS:HA	1.95	0.40
1:A:657:TYR:CG	1:A:666:CYS:HB2	2.56	0.40
1:A:56:ALA:HB2	1:A:405:ILE:HD13	2.02	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	814/851 (96%)	778 (96%)	33 (4%)	3 (0%)	30	26
1	B	814/851 (96%)	774 (95%)	37 (4%)	3 (0%)	30	26
All	All	1628/1702 (96%)	1552 (95%)	70 (4%)	6 (0%)	30	26

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	639	ASP
1	B	301	VAL
1	A	199	GLY
1	B	611	ASN
1	B	617	PHE
1	A	690	PRO

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	A	704/729 (97%)	694 (99%)	10 (1%)	59	66
1	B	704/729 (97%)	697 (99%)	7 (1%)	68	75
All	All	1408/1458 (97%)	1391 (99%)	17 (1%)	63	70

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	111	CYS
1	B	162	LEU
1	B	377	LEU
1	B	615	ASP
1	B	634	LYS
1	B	735	GLU
1	B	763	LEU
1	A	132	VAL
1	A	158	LEU
1	A	320	GLU
1	A	575	LYS
1	A	576	ASP
1	A	642	ASN
1	A	676	VAL
1	A	688	LYS
1	A	706	CYS
1	A	812	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	73	ASN
1	B	106	HIS
1	B	156	HIS
1	B	226	GLN
1	B	248	GLN
1	B	315	GLN
1	A	73	ASN
1	A	192	GLN
1	A	228	HIS
1	A	248	GLN
1	A	315	GLN
1	A	378	ASN
1	A	574	ASN

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Mol	Chain	Res	Type
1	A	609	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 ⓘ

8 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	CAC	A	903	-	2,4,4	2.68	2 (100%)	4,6,6	1.73	1 (25%)
2	9SL	A	901	-	17,23,23	3.42	9 (52%)	14,37,37	2.82	6 (42%)
3	CAC	B	902	-	2,4,4	2.76	2 (100%)	4,6,6	1.97	2 (50%)
3	CAC	B	904	-	2,4,4	2.70	2 (100%)	4,6,6	1.44	0
3	CAC	A	902	-	2,4,4	2.74	2 (100%)	4,6,6	1.57	1 (25%)
3	CAC	B	903	-	2,4,4	2.65	2 (100%)	4,6,6	1.28	0
3	CAC	A	904	-	2,4,4	2.71	2 (100%)	4,6,6	1.41	0
2	9SL	B	901	-	17,23,23	3.47	8 (47%)	14,37,37	3.01	5 (35%)

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	B	901	-	-	4/5/53/53	0/3/3/3
2	9SL	A	901	-	-	2/5/53/53	0/3/3/3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	9SL	C02-N21	6.85	1.45	1.33
2	A	901	9SL	C02-N21	6.81	1.45	1.33
2	B	901	9SL	C12-N13	6.81	1.45	1.35
2	A	901	9SL	C12-N13	6.77	1.45	1.35
2	A	901	9SL	C07-N08	6.41	1.45	1.34
2	B	901	9SL	C07-N08	6.40	1.45	1.34
2	B	901	9SL	C12-N15	4.90	1.45	1.34
2	A	901	9SL	C12-N15	4.75	1.45	1.34
2	B	901	9SL	O03-C02	3.90	1.41	1.35
2	A	901	9SL	O03-C02	3.58	1.40	1.35
2	B	901	9SL	C05-C14	3.12	1.59	1.52
2	A	901	9SL	C05-C14	3.10	1.58	1.52
3	A	902	CAC	AS-C2	2.79	1.96	1.90
3	B	903	CAC	AS-C1	2.78	1.96	1.90
3	B	902	CAC	AS-C1	2.76	1.96	1.90
3	B	902	CAC	AS-C2	2.76	1.96	1.90
3	A	904	CAC	AS-C1	2.72	1.96	1.90
3	B	904	CAC	AS-C2	2.71	1.96	1.90
3	A	904	CAC	AS-C2	2.71	1.96	1.90
3	B	904	CAC	AS-C1	2.70	1.96	1.90
3	A	902	CAC	AS-C1	2.70	1.96	1.90
3	A	903	CAC	AS-C1	2.69	1.96	1.90
3	A	903	CAC	AS-C2	2.66	1.96	1.90
3	B	903	CAC	AS-C2	2.51	1.96	1.90
2	B	901	9SL	C07-N09	2.30	1.39	1.35
2	A	901	9SL	C07-N09	2.17	1.39	1.35
2	B	901	9SL	C05-N06	-2.05	1.44	1.47
2	A	901	9SL	C05-N06	-2.02	1.44	1.47
2	A	901	9SL	O03-C04	-2.01	1.40	1.45

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	9SL	O03-C02-N21	7.77	120.77	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	9SL	O03-C02-N21	7.11	119.96	111.11
2	B	901	9SL	N09-C07-N06	-4.27	119.48	125.42
2	A	901	9SL	N09-C07-N06	-4.05	119.79	125.42
2	B	901	9SL	O01-C02-N21	-3.99	119.28	125.58
2	A	901	9SL	O01-C02-N21	-3.56	119.97	125.58
2	B	901	9SL	O03-C02-O01	-3.43	119.92	123.08
2	A	901	9SL	O03-C02-O01	-3.26	120.08	123.08
2	B	901	9SL	C14-C05-N06	2.90	119.13	111.22
2	A	901	9SL	C14-C05-N06	2.79	118.83	111.22
3	B	902	CAC	O1-AS-C1	-2.34	108.59	111.50
3	A	903	CAC	O2-AS-C1	2.27	111.34	105.84
3	B	902	CAC	O1-AS-C2	-2.19	108.78	111.50
3	A	902	CAC	O1-AS-C2	-2.08	108.91	111.50
2	A	901	9SL	C14-N13-C12	-2.04	105.44	109.36

There are no chirality outliers.

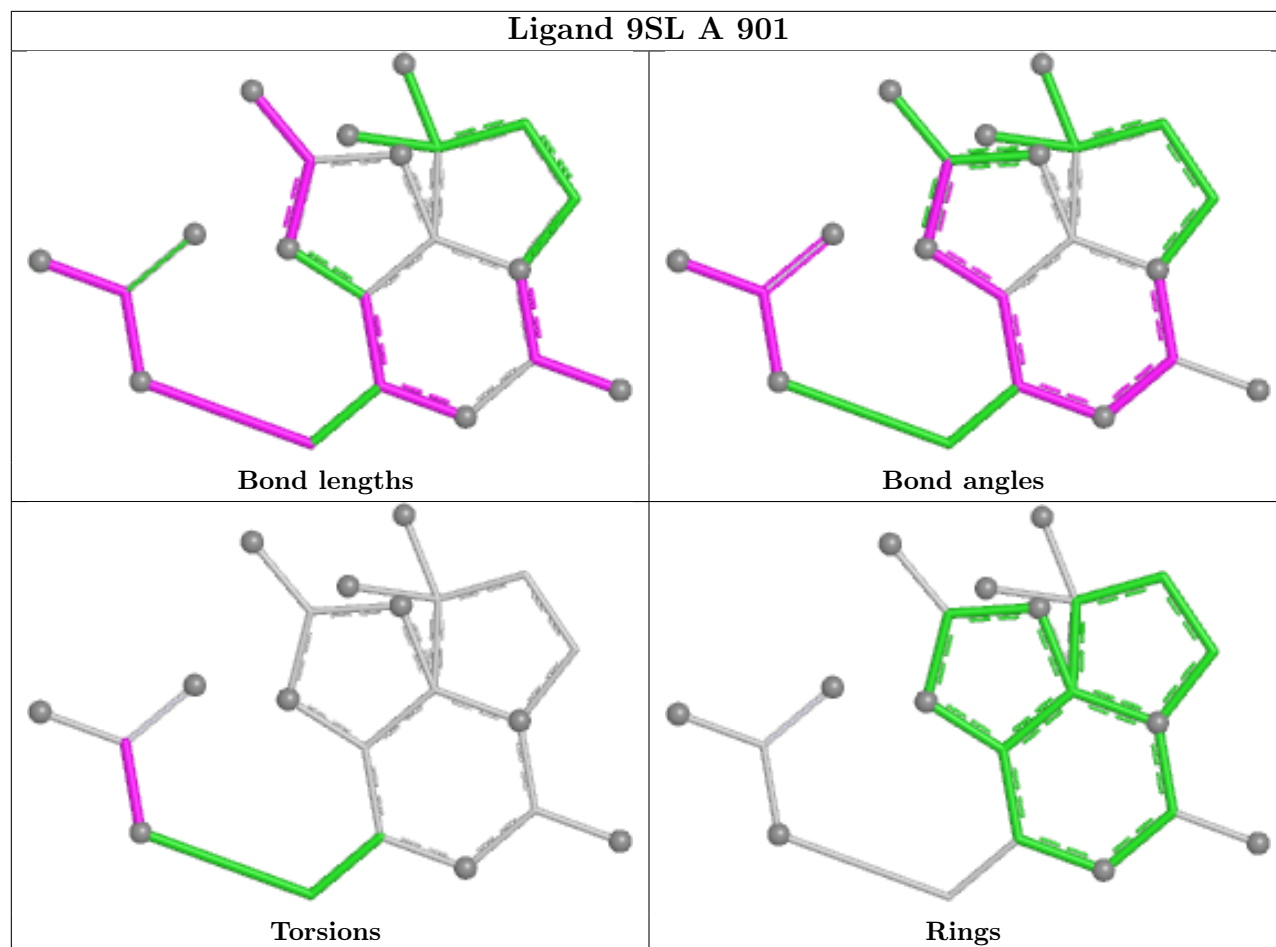
All (6) torsion outliers are listed below:

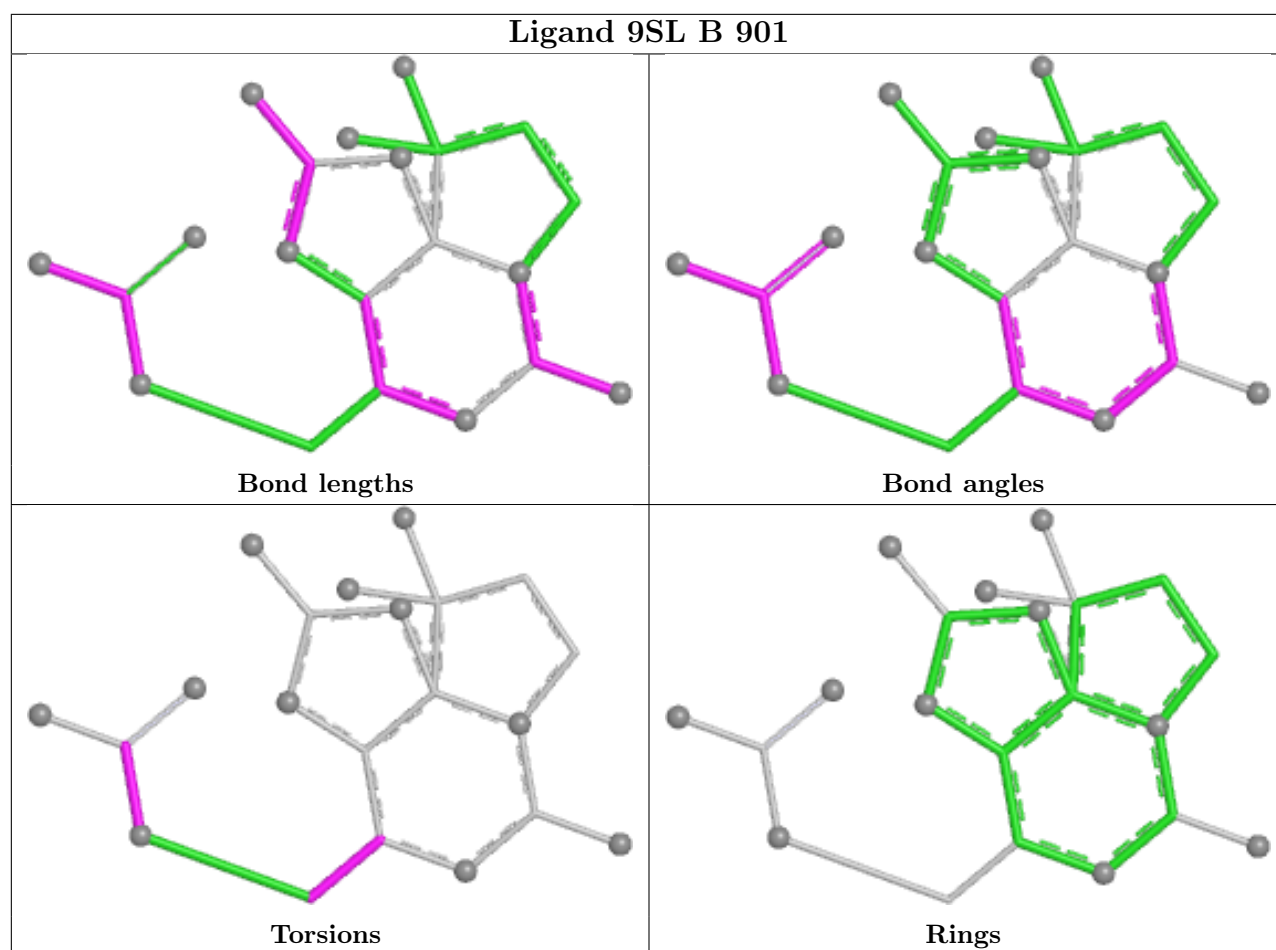
Mol	Chain	Res	Type	Atoms
2	B	901	9SL	O01-C02-O03-C04
2	B	901	9SL	N21-C02-O03-C04
2	B	901	9SL	O03-C04-C05-N06
2	B	901	9SL	O03-C04-C05-C14
2	A	901	9SL	O01-C02-O03-C04
2	A	901	9SL	N21-C02-O03-C04

There are no ring outliers.

No monomer is involved in short contacts.

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	818/851 (96%)	0.44	68 (8%)	17 19	36, 56, 115, 166	0
1	B	818/851 (96%)	0.69	105 (12%)	7 8	39, 64, 133, 191	0
All	All	1636/1702 (96%)	0.57	173 (10%)	11 12	36, 60, 124, 191	0

All (173) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	832	LEU	7.6
1	B	832	LEU	7.5
1	A	637	ILE	7.4
1	B	168	ALA	5.7
1	A	640	PRO	5.5
1	B	614	ILE	5.5
1	B	167	VAL	5.1
1	B	613	ASP	5.0
1	B	179	PHE	4.8
1	B	830	GLU	4.8
1	A	5	LYS	4.7
1	B	205	ASN	4.7
1	B	831	VAL	4.6
1	A	199	GLY	4.5
1	A	644	ALA	4.5
1	B	467	LEU	4.4
1	A	692	VAL	4.1
1	B	180	VAL	4.0
1	A	167	VAL	4.0
1	A	467	LEU	3.9
1	A	635	LEU	3.9
1	B	233	THR	3.9
1	A	159	PRO	3.9
1	B	88	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	602	VAL	3.8
1	B	206	ALA	3.8
1	B	635	LEU	3.8
1	B	758	LYS	3.8
1	A	691	ALA	3.7
1	A	162	LEU	3.7
1	A	670	LYS	3.7
1	B	207	ILE	3.7
1	B	829	LEU	3.6
1	B	156	HIS	3.6
1	B	707	LEU	3.6
1	B	82	TYR	3.6
1	A	693	TRP	3.4
1	B	640	PRO	3.4
1	B	314	LYS	3.4
1	B	87	ASP	3.4
1	A	614	ILE	3.4
1	B	202	TRP	3.3
1	A	824	HIS	3.3
1	B	645	ALA	3.3
1	B	657	TYR	3.3
1	A	676	VAL	3.3
1	A	157	GLU	3.3
1	A	283	TRP	3.2
1	B	525	GLN	3.2
1	A	287	ALA	3.1
1	B	637	ILE	3.1
1	B	612	SER	3.1
1	B	213	GLY	3.0
1	B	357	LEU	3.0
1	B	223	ALA	3.0
1	A	155	ARG	3.0
1	B	615	ASP	3.0
1	A	690	PRO	3.0
1	B	616	SER	2.9
1	A	675	PHE	2.9
1	A	651	LEU	2.9
1	A	647	THR	2.9
1	A	205	ASN	2.9
1	B	352	LEU	2.9
1	A	224	THR	2.9
1	B	215	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	572	LYS	2.9
1	A	629	LYS	2.9
1	A	645	ALA	2.8
1	B	194	PHE	2.8
1	B	668	VAL	2.8
1	B	692	VAL	2.8
1	B	825	CYS	2.8
1	A	168	ALA	2.8
1	A	714	VAL	2.8
1	A	89	GLN	2.7
1	B	83	SER	2.7
1	A	156	HIS	2.7
1	B	506	LYS	2.7
1	A	641	LYS	2.7
1	B	827	ASN	2.7
1	B	618	PHE	2.7
1	B	204	VAL	2.7
1	A	285	GLY	2.7
1	B	570	VAL	2.6
1	A	253	LYS	2.6
1	B	644	ALA	2.6
1	A	198	THR	2.6
1	B	200	TYR	2.6
1	B	154	GLU	2.6
1	B	828	SER	2.6
1	A	643	SER	2.6
1	B	664	PHE	2.5
1	B	364	VAL	2.5
1	B	198	THR	2.5
1	B	468	PRO	2.5
1	B	609	ASN	2.5
1	B	224	THR	2.5
1	A	632	LEU	2.5
1	B	617	PHE	2.5
1	A	665	ARG	2.5
1	A	628	THR	2.4
1	B	592	VAL	2.4
1	B	86	ARG	2.4
1	B	694	ALA	2.4
1	A	674	ALA	2.4
1	B	604	LEU	2.4
1	A	638	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	577	ILE	2.4
1	B	300	SER	2.4
1	B	381	LYS	2.4
1	B	209	GLU	2.4
1	A	179	PHE	2.4
1	B	244	SER	2.4
1	B	586	LYS	2.4
1	B	611	ASN	2.3
1	B	653	ASP	2.3
1	A	664	PHE	2.3
1	B	674	ALA	2.3
1	A	574	ASN	2.3
1	B	162	LEU	2.3
1	B	638	GLY	2.3
1	B	155	ARG	2.3
1	B	661	GLN	2.3
1	B	631	ASN	2.3
1	B	287	ALA	2.3
1	B	157	GLU	2.3
1	A	194	PHE	2.3
1	B	582	ILE	2.3
1	B	634	LYS	2.3
1	B	654	LYS	2.3
1	B	691	ALA	2.3
1	B	762	GLN	2.2
1	B	600	ILE	2.2
1	A	642	ASN	2.2
1	A	158	LEU	2.2
1	A	586	LYS	2.2
1	A	646	ASN	2.2
1	B	610	ASP	2.2
1	A	671	GLY	2.2
1	B	632	LEU	2.2
1	B	158	LEU	2.2
1	B	469	SER	2.2
1	B	809	ARG	2.2
1	B	693	TRP	2.2
1	B	149	THR	2.2
1	A	680	VAL	2.1
1	B	378	ASN	2.1
1	A	525	GLN	2.1
1	B	656	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	694	ALA	2.1
1	A	697	LEU	2.1
1	A	14	ASP	2.1
1	B	577	ILE	2.1
1	A	725	ILE	2.1
1	B	670	LYS	2.1
1	A	575	LYS	2.1
1	B	623	ALA	2.1
1	A	705	LEU	2.1
1	A	209	GLU	2.1
1	A	578	ASN	2.1
1	A	619	GLY	2.1
1	B	754	LYS	2.1
1	B	673	VAL	2.1
1	A	358	SER	2.1
1	A	621	SER	2.1
1	B	574	ASN	2.0
1	B	633	CYS	2.0
1	B	163	LYS	2.0
1	B	382	GLU	2.0
1	B	719	SER	2.0
1	B	697	LEU	2.0
1	B	214	THR	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 [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.

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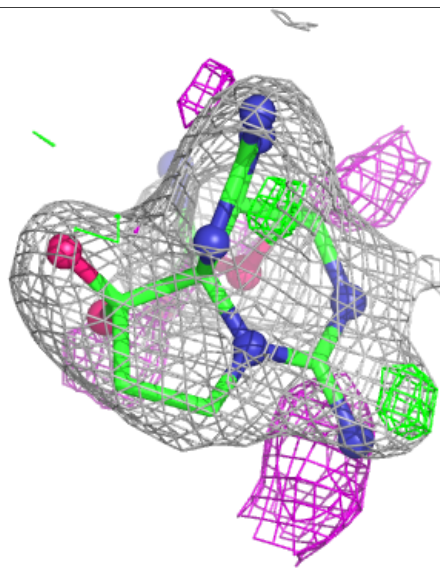
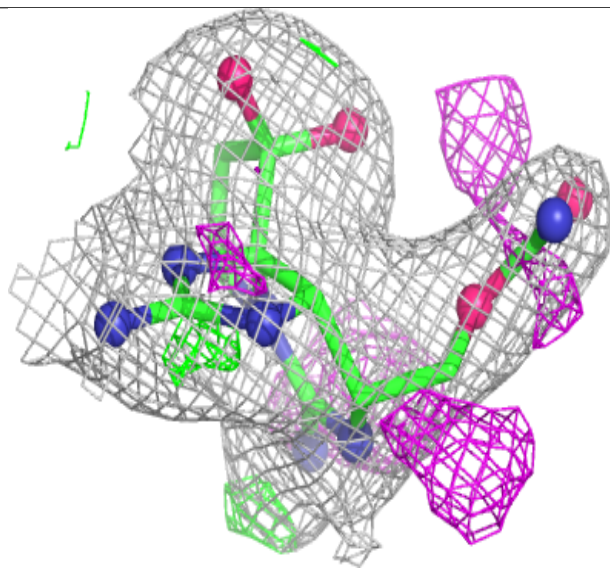
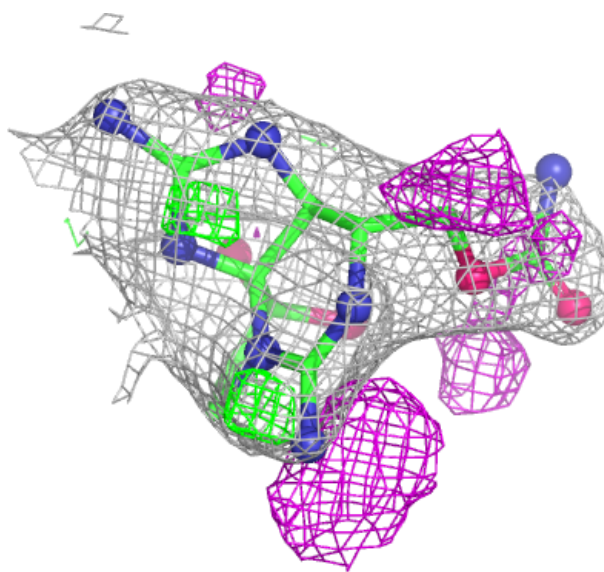
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CAC	A	904	5/5	0.61	0.22	107,109,116,186	0
3	CAC	B	902	5/5	0.78	0.25	85,94,128,154	0
3	CAC	B	903	5/5	0.80	0.22	69,73,93,173	0
3	CAC	B	904	5/5	0.81	0.23	108,114,124,177	0
3	CAC	A	902	5/5	0.82	0.23	86,89,129,158	0
3	CAC	A	903	5/5	0.86	0.21	66,85,109,162	0
2	9SL	A	901	21/21	0.87	0.12	60,68,76,79	0
2	9SL	B	901	21/21	0.93	0.10	61,70,75,76	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.

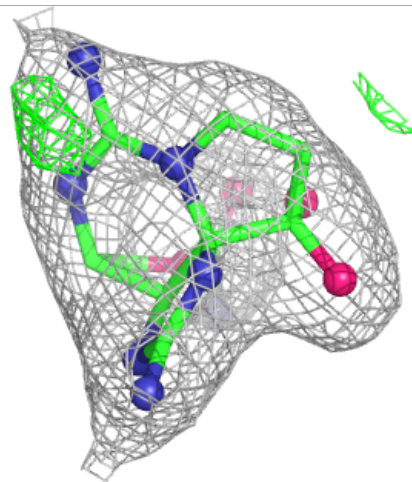
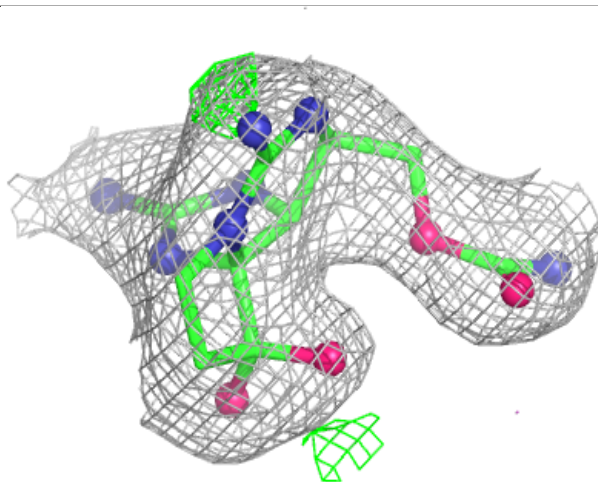
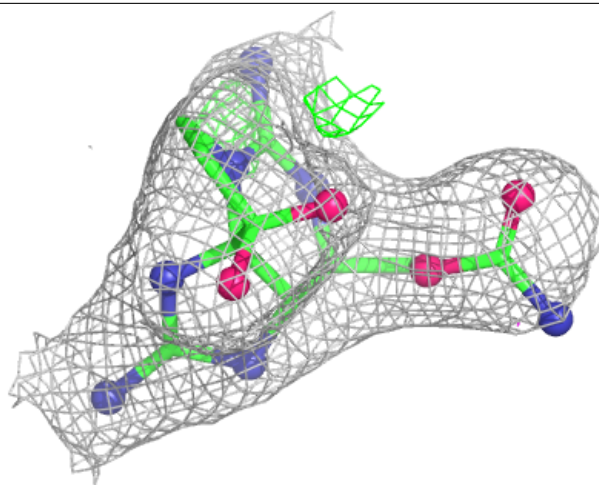
Electron density around 9SL A 901:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 9SL B 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.