



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 15, 2024 – 10:30 PM EST

PDB ID : 6O0F
Title : Saxiphilin:STX complex, co-crystal
Authors : Yen, T.J.; Lolicato, M.; Minor, D.L.
Deposited on : 2019-02-16
Resolution : 2.12 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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

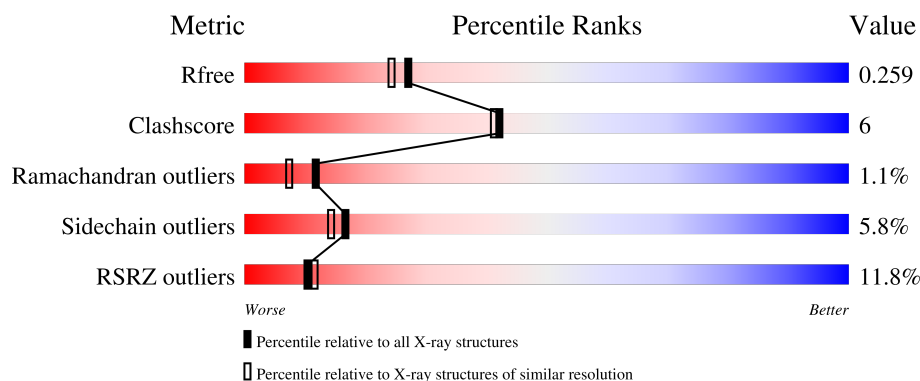
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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}	164625	7689 (2.14-2.10)
Clashscore	180529	8431 (2.14-2.10)
Ramachandran outliers	177936	8366 (2.14-2.10)
Sidechain outliers	177891	8367 (2.14-2.10)
RSRZ outliers	164620	7689 (2.14-2.10)

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	853	
1	B	853	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12816 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.

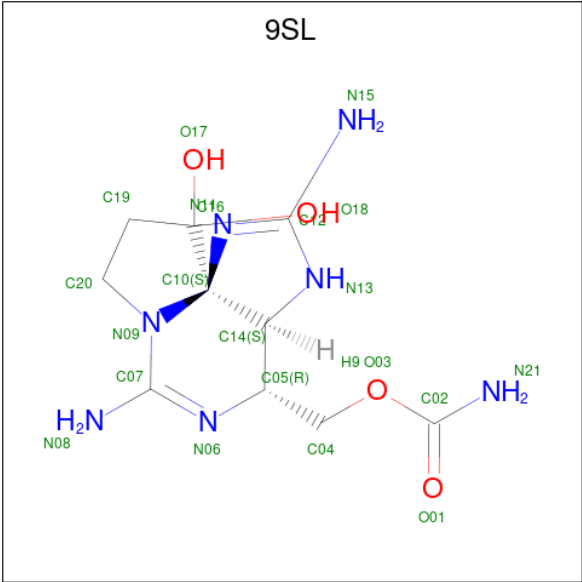
- Molecule 1 is a protein called Saxiphilin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	812	Total	C	N	O	S	0	0	0
			6279	3927	1085	1208	59			
1	B	816	Total	C	N	O	S	0	0	0
			6300	3936	1087	1218	59			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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
A	833	PHE	-	expression tag	UNP P31226
A	834	GLN	-	expression tag	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
B	833	PHE	-	expression tag	UNP P31226
B	834	GLN	-	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 (three-letter code: 9SL) (formula: C₁₀H₁₇N₇O₄).

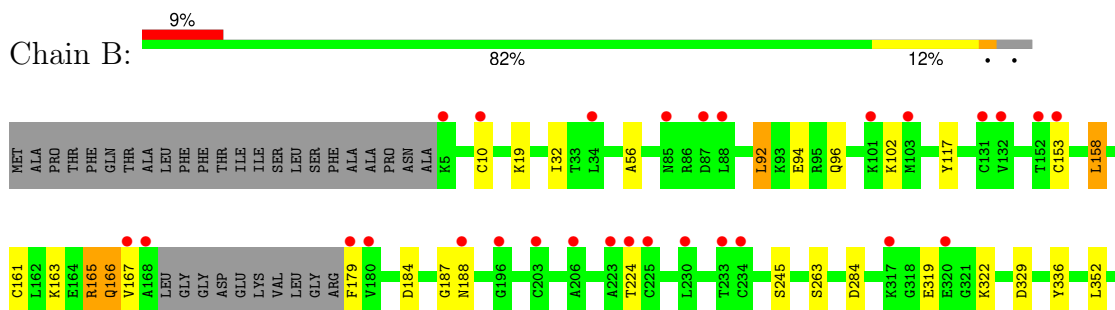
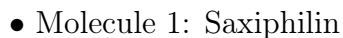


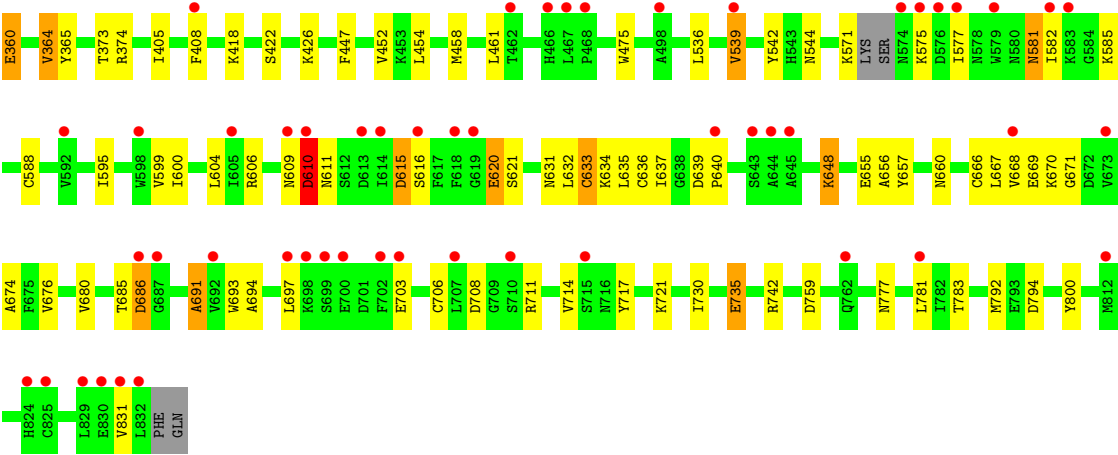
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			21	10	7	4		
2	B	1	Total	C	N	O	0	0
			21	10	7	4		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	102	Total	O	0	0
			102	102		
3	B	93	Total	O	0	0
			93	93		

- 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	96.56Å 111.66Å 254.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.33 – 2.12 48.33 – 2.12	Depositor EDS
% Data completeness (in resolution range)	98.7 (48.33-2.12) 99.9 (48.33-2.12)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 2.12Å)	Xtriage
Refinement program	PHENIX (1.12_2829)	Depositor
R, R_{free}	0.238 , 0.259 0.238 , 0.259	Depositor DCC
R_{free} test set	7801 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	50.6	Xtriage
Anisotropy	0.575	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12816	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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: 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	0.25	0/6401	0.47	0/8631
1	B	0.25	0/6425	0.47	1/8671 (0.0%)
All	All	0.25	0/12826	0.47	1/17302 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	153	CYS	CA-CB-SG	-5.40	104.27	114.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	610	ASP	Peptide

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	6279	0	6145	88	0
1	B	6300	0	6162	67	0
2	A	21	0	0	1	0
2	B	21	0	0	1	0
3	A	102	0	0	0	0
3	B	93	0	0	2	0
All	All	12816	0	12307	155	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 (155) 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:572:LYS:HG2	1:A:711:ARG:HH21	1.24	0.99
1:A:573:SER:HB2	1:A:711:ARG:HH22	1.35	0.90
1:A:578:ASN:OD1	1:A:581:ASN:ND2	2.10	0.83
1:A:572:LYS:HG2	1:A:711:ARG:NH2	2.01	0.75
1:A:627:ASP:OD1	1:A:628:THR:N	2.20	0.75
1:B:655:GLU:OE2	1:B:657:TYR:N	2.21	0.73
1:B:657:TYR:HD2	1:B:666:CYS:HB2	1.55	0.72
1:A:567:VAL:HA	1:A:722:LEU:HD13	1.76	0.68
1:A:712:ALA:HB1	1:A:716:ASN:HB2	1.78	0.65
1:B:655:GLU:OE2	1:B:656:ALA:N	2.30	0.64
1:B:158:LEU:HB3	1:B:163:LYS:HG3	1.80	0.64
1:B:575:LYS:HD2	1:B:577:ILE:HD11	1.80	0.62
1:A:785:ASP:OD1	2:A:901:9SL:N13	2.32	0.62
1:A:655:GLU:OE2	1:A:657:TYR:HB2	1.99	0.61
1:B:777:ASN:ND2	3:B:1001:HOH:O	2.31	0.61
1:A:262:VAL:HG22	1:A:304:ILE:HG22	1.82	0.61
1:B:632:LEU:O	1:B:633:CYS:HB2	2.00	0.61
1:A:506:LYS:HE2	1:A:529:GLU:OE2	2.01	0.60
1:B:322:LYS:HD3	1:B:329:ASP:HB3	1.83	0.60
1:A:86:ARG:NH1	1:A:228:HIS:O	2.34	0.60
1:B:635:LEU:H	1:B:635:LEU:HD12	1.65	0.60
1:B:184:ASP:OD1	1:B:188:ASN:N	2.34	0.59
1:A:86:ARG:NH1	1:A:229:ASP:OD1	2.36	0.58
1:B:224:THR:HG21	1:B:536:LEU:HD21	1.84	0.58
1:A:322:LYS:HD3	1:A:329:ASP:HB3	1.84	0.58
1:B:631:ASN:HA	1:B:634:LYS:HD2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:668:VAL:HG21	1:B:697:LEU:HD21	1.86	0.57
1:A:565:ARG:HG2	1:A:678:HIS:ND1	2.19	0.57
1:B:615:ASP:OD1	1:B:616:SER:N	2.38	0.57
1:A:571:LYS:HB2	1:A:574:ASN:HB3	1.87	0.57
1:A:618:PHE:O	1:A:631:ASN:ND2	2.38	0.57
1:A:628:THR:C	1:A:629:LYS:HD3	2.25	0.56
1:B:794:ASP:OD1	2:B:901:9SL:N15	2.39	0.56
1:B:575:LYS:O	1:B:711:ARG:NH1	2.31	0.56
1:A:618:PHE:HD2	1:A:632:LEU:HD11	1.69	0.56
1:B:657:TYR:CD2	1:B:666:CYS:HB2	2.39	0.55
1:A:573:SER:CB	1:A:711:ARG:HH22	2.13	0.55
1:A:712:ALA:O	1:A:714:VAL:N	2.38	0.54
1:A:489:TRP:HE1	1:A:747:GLN:HG2	1.72	0.54
1:A:703:GLU:HB2	1:A:712:ALA:O	2.09	0.53
1:A:587:SER:HA	1:A:672:ASP:HB2	1.91	0.53
1:A:19:LYS:HD2	1:A:422:SER:HB2	1.90	0.52
1:B:742:ARG:NH2	3:B:1005:HOH:O	2.42	0.52
1:A:542:TYR:CZ	1:A:544:ASN:HB3	2.44	0.52
1:B:694:ALA:HA	1:B:697:LEU:HD13	1.91	0.52
1:B:637:ILE:N	1:B:655:GLU:OE1	2.43	0.51
1:A:68:SER:O	1:A:397:LYS:NZ	2.36	0.51
1:A:259:HIS:HB2	1:A:304:ILE:HG23	1.91	0.51
1:B:615:ASP:HB2	1:B:631:ASN:HB2	1.92	0.51
1:A:262:VAL:HG23	1:A:305:PRO:O	2.11	0.51
1:A:690:PRO:HA	1:A:695:LYS:HE2	1.93	0.50
1:A:790:ASP:O	1:A:794:ASP:N	2.40	0.50
1:B:667:LEU:HB2	1:B:674:ALA:HB2	1.94	0.50
1:A:713:PRO:C	1:A:715:SER:H	2.15	0.50
1:A:292:GLN:OE1	1:A:308:THR:N	2.28	0.50
1:B:92:LEU:HD12	1:B:96:GLN:HE21	1.75	0.50
1:B:165:ARG:O	1:B:167:VAL:N	2.46	0.49
1:B:606:ARG:HB2	1:B:611:ASN:HA	1.94	0.49
1:A:56:ALA:HB2	1:A:405:ILE:HD13	1.93	0.49
1:A:485:LYS:HD3	1:A:772:LEU:HB2	1.93	0.49
1:B:336:TYR:CZ	1:B:426:LYS:HD3	2.48	0.49
1:A:634:LYS:HG3	1:A:635:LEU:HD12	1.94	0.49
1:A:682:PHE:O	1:A:685:THR:HG22	2.13	0.48
1:B:635:LEU:HD12	1:B:635:LEU:N	2.28	0.48
1:B:588:CYS:SG	1:B:671:GLY:HA3	2.53	0.48
1:A:195:HIS:HB2	1:A:202:TRP:HZ3	1.79	0.48
1:A:575:LYS:HE3	1:A:575:LYS:HB2	1.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:609:ASN:N	1:A:609:ASN:OD1	2.46	0.48
1:B:165:ARG:C	1:B:167:VAL:H	2.16	0.48
1:A:460:ALA:HA	1:A:465:ALA:HB2	1.96	0.48
1:A:718:LYS:O	1:A:721:LYS:NZ	2.43	0.48
1:B:759:ASP:OD1	1:B:759:ASP:N	2.46	0.47
1:A:567:VAL:HG11	1:A:704:LEU:HD13	1.96	0.47
1:A:737:ILE:O	1:A:741:VAL:HG12	2.14	0.47
1:A:759:ASP:OD1	1:A:759:ASP:N	2.45	0.47
1:B:542:TYR:CZ	1:B:544:ASN:HB3	2.50	0.47
1:B:32:ILE:HG21	1:B:408:PHE:HB2	1.96	0.47
1:B:56:ALA:HB2	1:B:405:ILE:HD13	1.97	0.47
1:A:183:CYS:SG	1:A:189:TYR:HA	2.55	0.47
1:A:735:GLU:H	1:A:735:GLU:HG3	1.43	0.47
1:A:575:LYS:HZ3	1:A:672:ASP:C	2.19	0.47
1:B:575:LYS:HE3	1:B:575:LYS:HB2	1.73	0.47
1:A:242:LYS:NZ	1:A:345:ASP:OD1	2.39	0.46
1:A:684:ASN:HA	1:A:689:ASN:HB2	1.97	0.46
1:A:408:PHE:HD2	1:A:409:LEU:HD13	1.81	0.46
1:A:693:TRP:CE3	1:A:694:ALA:HB2	2.51	0.46
1:B:685:THR:HG23	1:B:686:ASP:N	2.30	0.46
1:A:98:ALA:O	1:A:106:HIS:NE2	2.37	0.46
1:B:693:TRP:CE3	1:B:694:ALA:HB2	2.51	0.46
1:B:245:SER:HB2	1:B:374:ARG:HH22	1.81	0.46
1:B:571:LYS:HE3	1:B:668:VAL:HA	1.97	0.46
1:B:595:ILE:HA	1:B:599:VAL:HB	1.98	0.46
1:A:159:PRO:HG3	1:A:187:GLY:HA3	1.97	0.46
1:B:19:LYS:HD2	1:B:422:SER:HB2	1.98	0.46
1:B:161:CYS:HB3	1:B:187:GLY:O	2.16	0.46
1:B:717:TYR:O	1:B:721:LYS:HB3	2.16	0.46
1:A:703:GLU:OE2	1:A:711:ARG:HB3	2.16	0.45
1:B:581:ASN:O	1:B:581:ASN:CG	2.54	0.45
1:B:635:LEU:HD23	1:B:670:LYS:CB	2.46	0.45
1:A:396:ARG:NH1	1:A:400:ASP:OD1	2.49	0.45
1:A:588:CYS:HB3	1:A:622:CYS:N	2.31	0.45
1:B:94:GLU:OE1	1:B:117:TYR:OH	2.27	0.45
1:A:176:LEU:HD12	1:A:176:LEU:H	1.81	0.45
1:A:215:LYS:H	1:A:215:LYS:HG2	1.55	0.45
1:B:621:SER:HB2	1:B:632:LEU:HD23	1.99	0.45
1:B:660:ASN:HB3	1:B:680:VAL:HG22	1.99	0.44
1:B:636:CYS:HB3	1:B:655:GLU:OE1	2.17	0.44
1:A:288:LYS:H	1:A:288:LYS:HD2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:TRP:HE1	1:A:747:GLN:CG	2.29	0.44
1:A:539:VAL:HG23	1:A:730:ILE:HD13	1.99	0.44
1:A:602:VAL:HG22	1:A:613:ASP:OD2	2.18	0.44
1:A:761:PHE:HE2	1:A:763:LEU:HD23	1.82	0.44
1:A:97:GLN:O	1:A:101:LYS:HD2	2.18	0.44
1:A:565:ARG:CZ	1:A:718:LYS:HG2	2.48	0.44
1:A:717:TYR:O	1:A:718:LYS:HB2	2.18	0.44
1:A:676:VAL:HB	1:A:680:VAL:HG11	1.99	0.43
1:B:539:VAL:HG12	1:B:730:ILE:HB	1.99	0.43
1:A:550:PRO:CG	1:A:558:TYR:HB3	2.48	0.43
1:A:198:THR:O	1:A:200:TYR:N	2.50	0.43
1:A:572:LYS:C	1:A:574:ASN:H	2.22	0.43
1:B:447:PHE:CZ	1:B:452:VAL:HG12	2.53	0.43
1:B:620:GLU:O	1:B:635:LEU:HD11	2.18	0.43
1:A:46:MET:HB2	1:A:46:MET:HE3	1.88	0.42
1:B:657:TYR:OH	1:B:669:GLU:OE1	2.35	0.42
1:A:92:LEU:HD12	1:A:92:LEU:HA	1.83	0.42
1:B:634:LYS:O	1:B:648:LYS:NZ	2.52	0.42
1:A:786:ARG:NH1	1:A:794:ASP:OD2	2.42	0.42
1:B:454:LEU:O	1:B:458:MET:HG2	2.20	0.42
1:B:539:VAL:HG12	1:B:730:ILE:HG13	2.02	0.42
1:A:92:LEU:O	1:A:96:GLN:HG3	2.20	0.42
1:B:475:TRP:CZ2	1:B:730:ILE:HD12	2.55	0.42
1:B:735:GLU:H	1:B:735:GLU:HG3	1.50	0.42
1:A:602:VAL:HG13	1:A:613:ASP:OD2	2.20	0.41
1:A:613:ASP:O	1:A:613:ASP:OD1	2.38	0.41
1:A:707:LEU:O	1:A:709:GLY:N	2.54	0.41
1:B:635:LEU:HD23	1:B:670:LYS:HB3	2.02	0.41
1:A:572:LYS:HG3	1:A:703:GLU:OE2	2.20	0.41
1:A:158:LEU:HD22	1:A:158:LEU:HA	1.87	0.41
1:A:230:LEU:HD11	1:A:826:SER:HB2	2.02	0.41
1:A:256:ARG:NH2	1:A:345:ASP:O	2.44	0.41
1:A:252:LEU:HD12	1:A:252:LEU:HA	1.88	0.41
1:A:680:VAL:O	1:A:683:GLU:HG2	2.20	0.41
1:B:685:THR:HG23	1:B:686:ASP:H	1.86	0.41
1:B:691:ALA:HB1	1:B:694:ALA:H	1.86	0.41
1:A:360:GLU:H	1:A:360:GLU:HG3	1.55	0.41
1:B:364:VAL:HG13	1:B:365:TYR:CD2	2.55	0.41
1:B:600:ILE:HD11	1:B:800:TYR:CE2	2.56	0.41
1:B:676:VAL:HB	1:B:680:VAL:HG21	2.02	0.41
1:B:686:ASP:HA	1:B:697:LEU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:GLU:HG2	1:A:263:SER:HB2	2.03	0.41
1:A:336:TYR:CZ	1:A:426:LYS:HD3	2.55	0.41
1:A:288:LYS:HD2	1:A:288:LYS:N	2.36	0.41
1:B:632:LEU:O	1:B:633:CYS:CB	2.68	0.40
1:B:360:GLU:H	1:B:360:GLU:HG3	1.57	0.40
1:B:620:GLU:HG2	1:B:634:LYS:HD3	2.03	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	800/853 (94%)	761 (95%)	29 (4%)	10 (1%)	10	6
1	B	810/853 (95%)	774 (96%)	29 (4%)	7 (1%)	14	10
All	All	1610/1706 (94%)	1535 (95%)	58 (4%)	17 (1%)	12	7

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	714	VAL
1	B	633	CYS
1	B	640	PRO
1	B	691	ALA
1	A	199	GLY
1	A	708	ASP
1	A	830	GLU
1	B	166	GLN
1	B	620	GLU
1	A	175	VAL
1	A	212	ALA
1	A	233	THR

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Mol	Chain	Res	Type
1	B	165	ARG
1	A	213	GLY
1	B	610	ASP
1	A	167	VAL
1	A	614	ILE

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	699/731 (96%)	653 (93%)	46 (7%)	14	11
1	B	702/731 (96%)	667 (95%)	35 (5%)	20	19
All	All	1401/1462 (96%)	1320 (94%)	81 (6%)	17	14

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	LEU
1	A	101	LYS
1	A	114	LYS
1	A	158	LEU
1	A	163	LYS
1	A	166	GLN
1	A	169	LEU
1	A	176	LEU
1	A	178	ARG
1	A	180	VAL
1	A	186	LYS
1	A	215	LYS
1	A	220	LYS
1	A	252	LEU
1	A	320	GLU
1	A	341	CYS
1	A	352	LEU
1	A	353	ARG

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Mol	Chain	Res	Type
1	A	360	GLU
1	A	409	LEU
1	A	480	LYS
1	A	525	GLN
1	A	548	PHE
1	A	552	LYS
1	A	553	THR
1	A	565	ARG
1	A	573	SER
1	A	588	CYS
1	A	610	ASP
1	A	628	THR
1	A	629	LYS
1	A	655	GLU
1	A	666	CYS
1	A	683	GLU
1	A	696	ASN
1	A	698	LYS
1	A	705	LEU
1	A	706	CYS
1	A	707	LEU
1	A	714	VAL
1	A	735	GLU
1	A	753	ARG
1	A	812	MET
1	A	824	HIS
1	A	831	VAL
1	A	834	GLN
1	B	10	CYS
1	B	92	LEU
1	B	102	LYS
1	B	158	LEU
1	B	166	GLN
1	B	179	PHE
1	B	263	SER
1	B	284	ASP
1	B	319	GLU
1	B	352	LEU
1	B	360	GLU
1	B	364	VAL
1	B	373	THR
1	B	418	LYS

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Mol	Chain	Res	Type
1	B	461	LEU
1	B	539	VAL
1	B	581	ASN
1	B	582	ILE
1	B	585	LYS
1	B	604	LEU
1	B	609	ASN
1	B	610	ASP
1	B	615	ASP
1	B	639	ASP
1	B	648	LYS
1	B	686	ASP
1	B	703	GLU
1	B	706	CYS
1	B	708	ASP
1	B	714	VAL
1	B	735	GLU
1	B	781	LEU
1	B	783	THR
1	B	792	MET
1	B	831	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	578	ASN
1	A	581	ASN
1	B	96	GLN

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
2	9SL	B	901	-	17,23,23	6.19	10 (58%)	14,37,37	3.21	7 (50%)
2	9SL	A	901	-	17,23,23	6.26	10 (58%)	14,37,37	3.33	8 (57%)

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

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	9SL	C12-N13	16.20	1.60	1.35
2	A	901	9SL	C12-N13	16.07	1.60	1.35
2	A	901	9SL	C20-N09	-10.63	1.34	1.47
2	B	901	9SL	C20-N09	-10.16	1.34	1.47
2	B	901	9SL	C19-C20	-8.81	1.37	1.52
2	A	901	9SL	C19-C20	-8.69	1.37	1.52
2	A	901	9SL	C07-N08	7.49	1.47	1.34
2	B	901	9SL	C07-N08	7.45	1.47	1.34
2	B	901	9SL	C02-N21	7.32	1.46	1.33
2	A	901	9SL	C02-N21	7.28	1.46	1.33
2	A	901	9SL	C12-N15	6.14	1.48	1.34
2	B	901	9SL	C12-N15	5.43	1.46	1.34
2	B	901	9SL	C07-N09	5.08	1.45	1.35
2	A	901	9SL	C07-N09	5.02	1.44	1.35
2	A	901	9SL	O03-C02	4.01	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	9SL	O03-C02	3.84	1.41	1.35
2	B	901	9SL	C05-C14	3.60	1.59	1.52
2	A	901	9SL	C05-C14	3.44	1.59	1.52
2	A	901	9SL	C05-N06	-2.80	1.43	1.47
2	B	901	9SL	C05-N06	-2.79	1.43	1.47

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	9SL	O03-C02-N21	7.27	120.16	111.11
2	B	901	9SL	O03-C02-N21	7.23	120.11	111.11
2	A	901	9SL	C19-C20-N09	5.35	109.72	103.81
2	B	901	9SL	C19-C20-N09	5.09	109.44	103.81
2	A	901	9SL	N13-C12-N11	-4.28	104.48	115.62
2	B	901	9SL	O03-C02-O01	-3.94	119.45	123.08
2	B	901	9SL	N13-C12-N11	-3.71	105.97	115.62
2	A	901	9SL	O03-C02-O01	-3.60	119.76	123.08
2	A	901	9SL	O01-C02-N21	-3.49	120.07	125.58
2	A	901	9SL	N15-C12-N11	3.34	130.06	125.42
2	B	901	9SL	O01-C02-N21	-3.27	120.43	125.58
2	A	901	9SL	N09-C07-N06	-2.95	121.31	125.42
2	B	901	9SL	N15-C12-N13	2.84	127.35	122.70
2	B	901	9SL	N09-C07-N06	-2.59	121.82	125.42
2	A	901	9SL	C14-C05-N06	2.12	117.01	111.22

There are no chirality outliers.

All (5) torsion outliers are listed below:

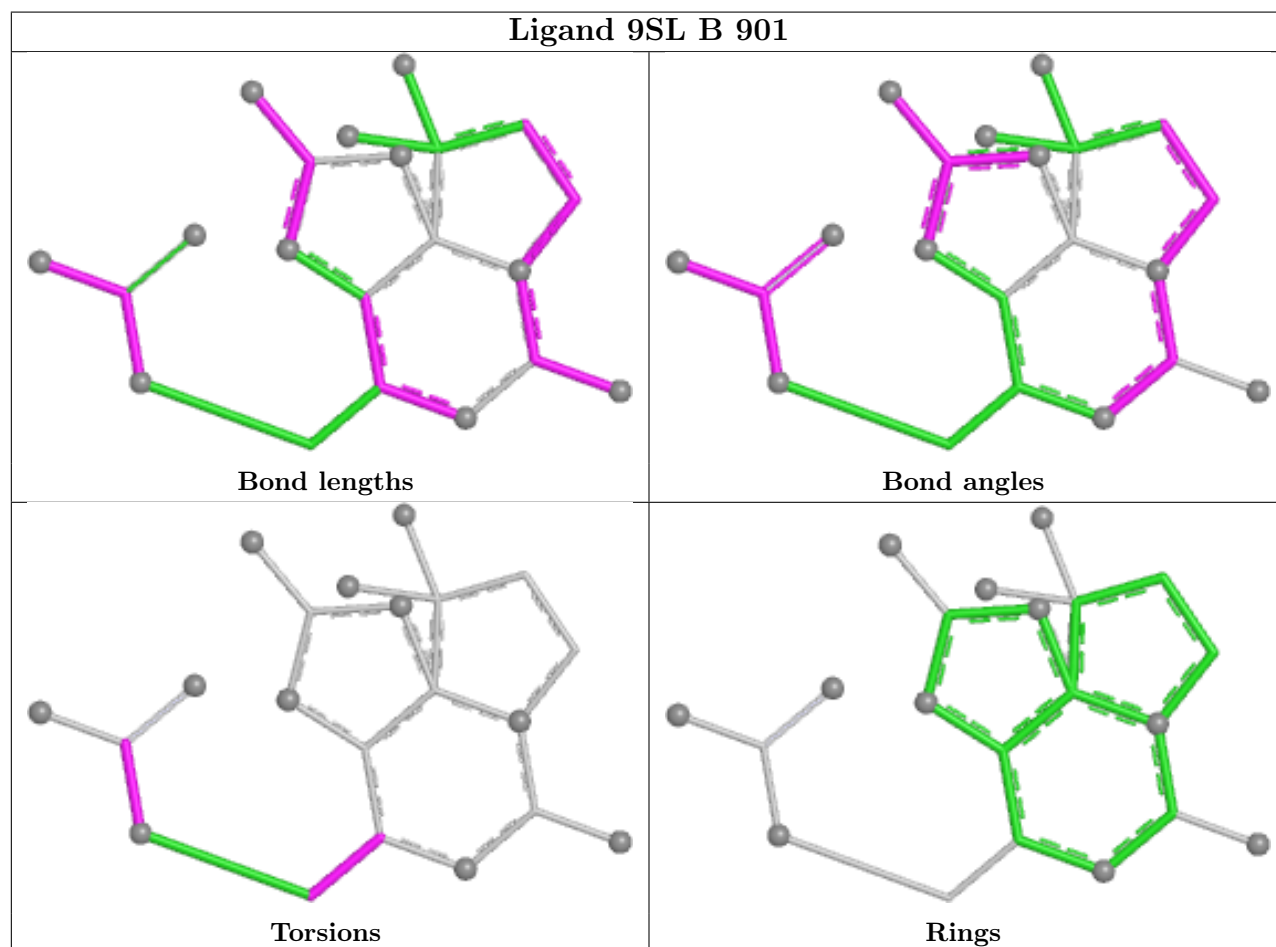
Mol	Chain	Res	Type	Atoms
2	A	901	9SL	O01-C02-O03-C04
2	A	901	9SL	N21-C02-O03-C04
2	B	901	9SL	O01-C02-O03-C04
2	B	901	9SL	N21-C02-O03-C04
2	B	901	9SL	O03-C04-C05-C14

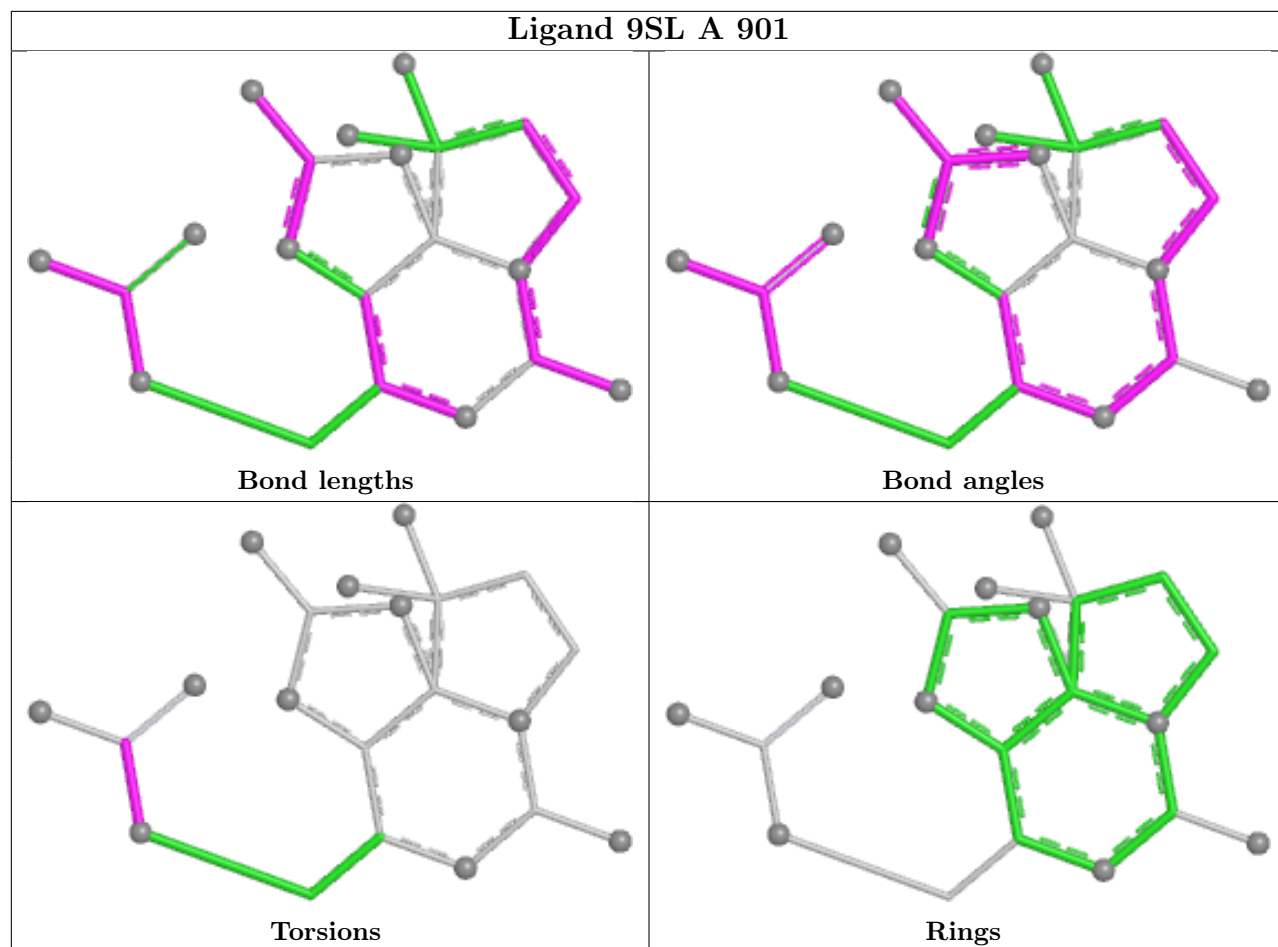
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	901	9SL	1	0
2	A	901	9SL	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	812/853 (95%)	0.90	113 (13%) 7 8	48, 81, 173, 227	0
1	B	816/853 (95%)	0.86	79 (9%) 15 16	51, 83, 153, 244	0
All	All	1628/1706 (95%)	0.88	192 (11%) 10 11	48, 82, 168, 244	0

All (192) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	829	LEU	6.6
1	B	168	ALA	6.5
1	A	614	ILE	6.2
1	B	614	ILE	5.9
1	B	10	CYS	5.9
1	A	4	ALA	5.7
1	A	212	ALA	5.6
1	B	85	ASN	5.6
1	A	834	GLN	5.3
1	B	179	PHE	5.2
1	A	692	VAL	5.2
1	B	832	LEU	5.1
1	B	88	LEU	5.1
1	A	632	LEU	5.0
1	B	5	LYS	4.9
1	A	705	LEU	4.8
1	B	153	CYS	4.8
1	A	613	ASP	4.8
1	A	176	LEU	4.7
1	A	648	LYS	4.7
1	A	175	VAL	4.6
1	B	831	VAL	4.6
1	A	587	SER	4.6
1	A	664	PHE	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	619	GLY	4.4
1	B	224	THR	4.4
1	B	467	LEU	4.4
1	B	825	CYS	4.3
1	B	180	VAL	4.3
1	A	707	LEU	4.2
1	A	569	LEU	4.2
1	B	830	GLU	4.1
1	A	467	LEU	4.1
1	A	183	CYS	4.1
1	B	577	ILE	4.1
1	A	225	CYS	4.0
1	A	258	CYS	3.9
1	A	3	ASN	3.8
1	B	619	GLY	3.8
1	A	635	LEU	3.7
1	A	213	GLY	3.7
1	A	704	LEU	3.6
1	A	672	ASP	3.6
1	B	703	GLU	3.6
1	A	582	ILE	3.6
1	B	579	TRP	3.6
1	A	170	GLY	3.5
1	A	833	PHE	3.5
1	B	167	VAL	3.5
1	A	180	VAL	3.5
1	A	82	TYR	3.4
1	B	583	LYS	3.4
1	A	724	GLY	3.4
1	A	579	TRP	3.4
1	A	722	LEU	3.4
1	A	283	TRP	3.4
1	B	644	ALA	3.4
1	A	702	PHE	3.3
1	B	87	ASP	3.3
1	A	224	THR	3.3
1	A	697	LEU	3.3
1	A	211	ILE	3.2
1	A	468	PRO	3.2
1	B	225	CYS	3.2
1	B	576	ASP	3.2
1	A	177	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	824	HIS	3.2
1	A	675	PHE	3.2
1	B	610	ASP	3.2
1	A	287	ALA	3.1
1	A	341	CYS	3.1
1	B	702	PHE	3.0
1	B	574	ASN	3.0
1	A	593	GLY	3.0
1	A	293	ARG	3.0
1	A	198	THR	3.0
1	B	692	VAL	2.9
1	B	645	ALA	2.9
1	A	824	HIS	2.9
1	B	466	HIS	2.9
1	A	721	LYS	2.9
1	A	548	PHE	2.9
1	A	169	LEU	2.8
1	B	686	ASP	2.8
1	A	179	PHE	2.8
1	B	131	CYS	2.8
1	B	468	PRO	2.8
1	A	714	VAL	2.8
1	B	230	LEU	2.8
1	B	812	MET	2.8
1	B	613	ASP	2.8
1	A	612	SER	2.8
1	A	681	VAL	2.7
1	B	609	ASN	2.7
1	B	233	THR	2.7
1	A	804	VAL	2.7
1	A	830	GLU	2.7
1	A	584	GLY	2.7
1	B	320	GLU	2.7
1	A	660	ASN	2.6
1	A	800	TYR	2.6
1	A	157	GLU	2.6
1	B	582	ILE	2.6
1	B	196	GLY	2.6
1	A	670	LYS	2.6
1	A	827	ASN	2.6
1	A	577	ILE	2.5
1	A	725	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	202	TRP	2.5
1	B	700	GLU	2.5
1	A	713	PRO	2.5
1	B	707	LEU	2.5
1	A	551	CYS	2.5
1	A	628	THR	2.5
1	A	676	VAL	2.5
1	A	715	SER	2.5
1	A	754	LYS	2.5
1	A	801	TYR	2.4
1	B	575	LYS	2.4
1	B	103	MET	2.4
1	A	651	LEU	2.4
1	A	832	LEU	2.4
1	B	188	ASN	2.4
1	A	626	SER	2.4
1	B	34	LEU	2.4
1	A	611	ASN	2.4
1	B	223	ALA	2.4
1	A	288	LYS	2.4
1	B	668	VAL	2.4
1	B	699	SER	2.4
1	A	682	PHE	2.4
1	B	498	ALA	2.4
1	B	673	VAL	2.4
1	B	640	PRO	2.4
1	A	795	TYR	2.4
1	B	605	ILE	2.4
1	A	168	ALA	2.3
1	B	234	CYS	2.3
1	B	462	THR	2.3
1	A	570	VAL	2.3
1	A	668	VAL	2.3
1	A	382	GLU	2.3
1	B	317	LYS	2.3
1	B	152	THR	2.3
1	A	831	VAL	2.3
1	B	539	VAL	2.3
1	A	693	TRP	2.3
1	B	408	PHE	2.3
1	B	101	LYS	2.3
1	B	132	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	285	GLY	2.3
1	A	186	LYS	2.3
1	A	545	LYS	2.3
1	B	592	VAL	2.2
1	B	781	LEU	2.2
1	A	596	ALA	2.2
1	A	623	ALA	2.2
1	A	710	SER	2.2
1	A	653	ASP	2.2
1	A	174	LYS	2.2
1	A	226	GLN	2.2
1	A	691	ALA	2.2
1	A	752	GLY	2.2
1	B	618	PHE	2.2
1	A	289	GLU	2.2
1	A	564	LEU	2.2
1	A	667	LEU	2.2
1	B	598	TRP	2.2
1	A	690	PRO	2.2
1	B	687	GLY	2.2
1	B	697	LEU	2.1
1	A	552	LYS	2.1
1	B	616	SER	2.1
1	A	694	ALA	2.1
1	A	805	TYR	2.1
1	A	139	ILE	2.1
1	B	643	SER	2.1
1	A	746	ASN	2.1
1	B	698	LYS	2.1
1	A	559	THR	2.1
1	B	715	SER	2.1
1	B	206	ALA	2.1
1	A	286	PRO	2.1
1	B	762	GLN	2.1
1	B	203	CYS	2.1
1	A	709	GLY	2.0
1	A	159	PRO	2.0
1	A	317	LYS	2.0
1	A	203	CYS	2.0
1	A	633	CYS	2.0
1	B	710	SER	2.0
1	A	599	VAL	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](#)

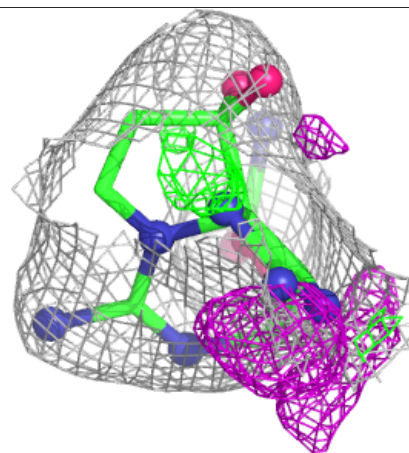
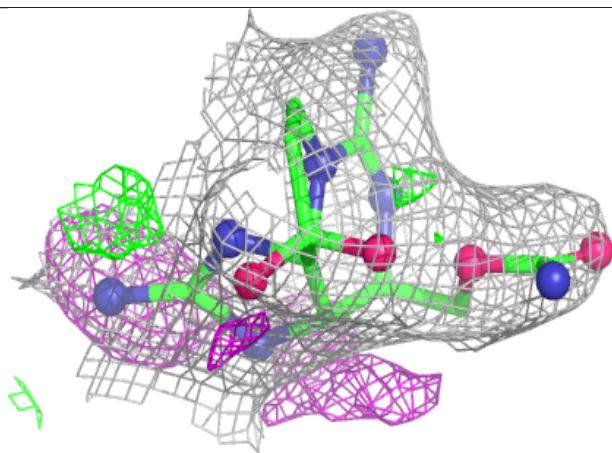
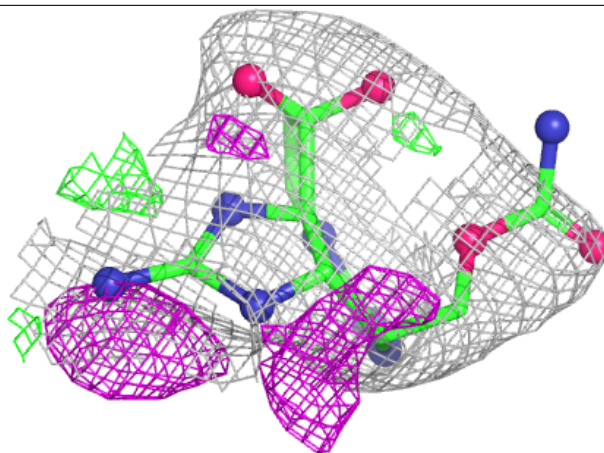
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	9SL	A	901	21/21	0.81	0.15	90,110,127,130	0
2	9SL	B	901	21/21	0.91	0.12	66,72,98,100	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.

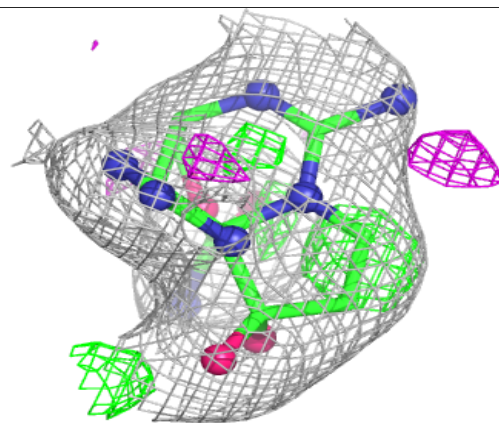
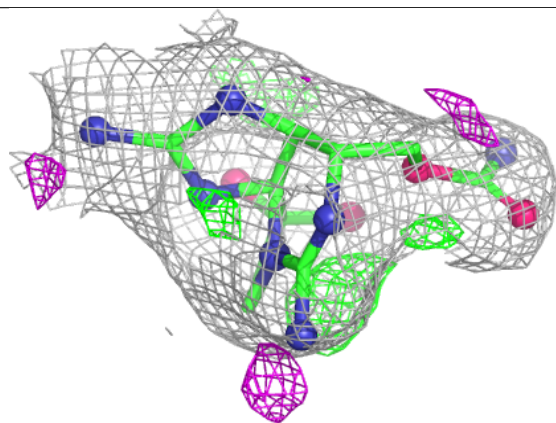
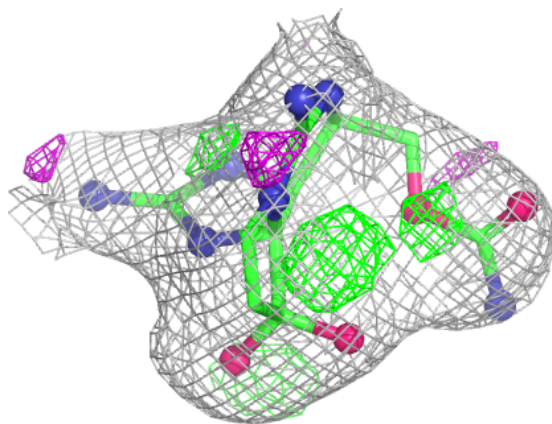
Electron density around 9SL A 901:

$2mF_o-DF_c$ (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 ⓘ

There are no such residues in this entry.