



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:31 AM UTC

PDB ID : 6O0F / pdb_00006o0f
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	:	4-5-2 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

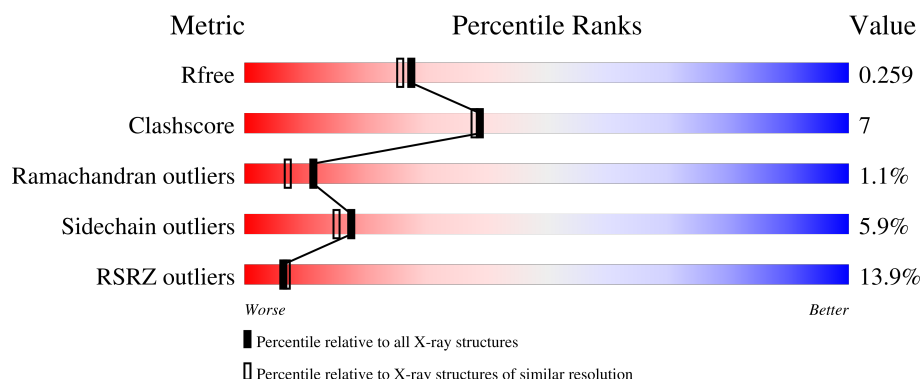
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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}	180053	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (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	15% 75% 18% • 5%
1	B	853	12% 81% 12% • •

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.

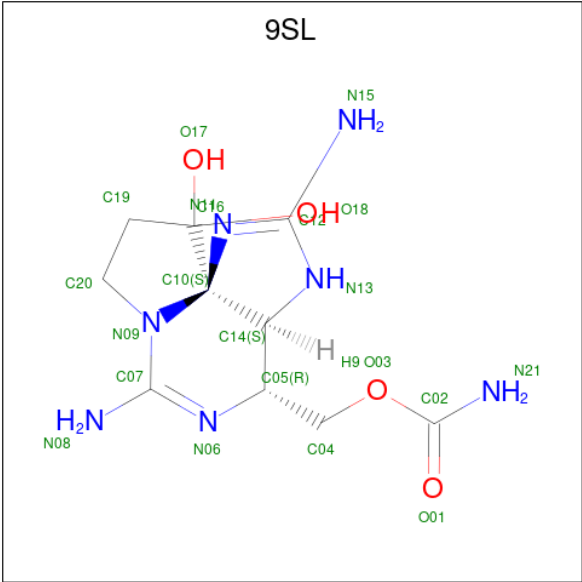
- Molecule 1 is a protein called Saxiphilin.

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 (CCD ID: 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		

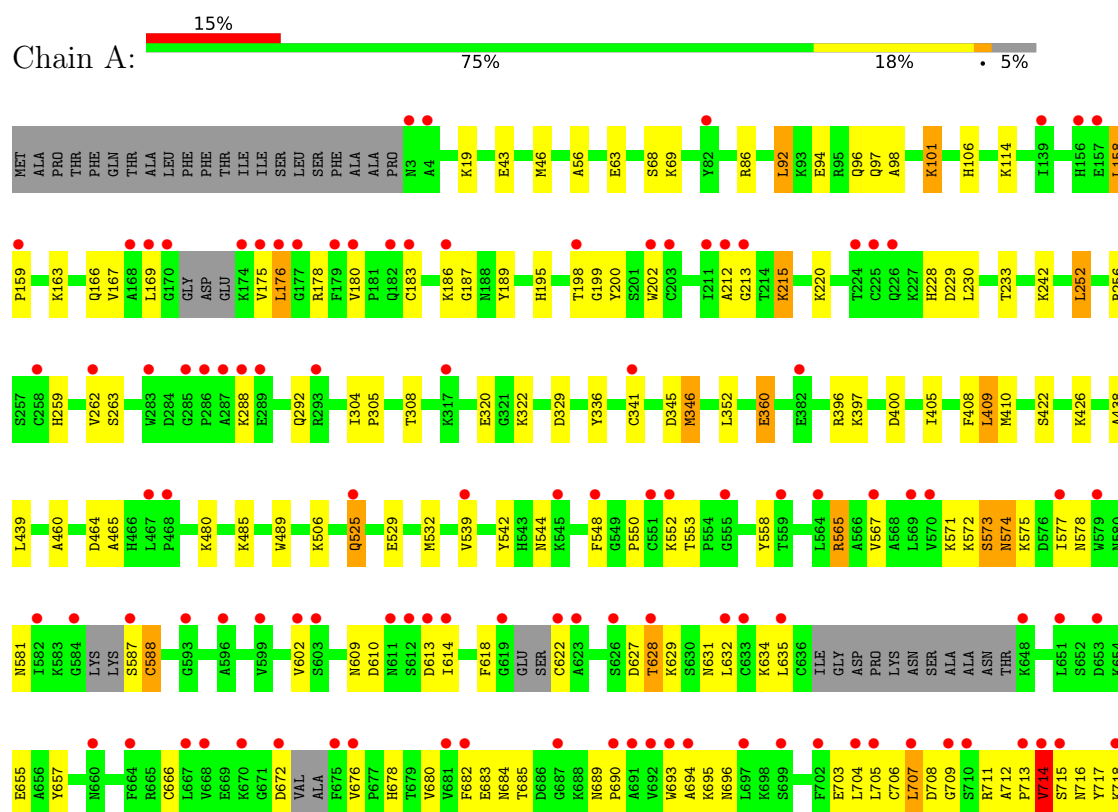
- Molecule 3 is water.

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

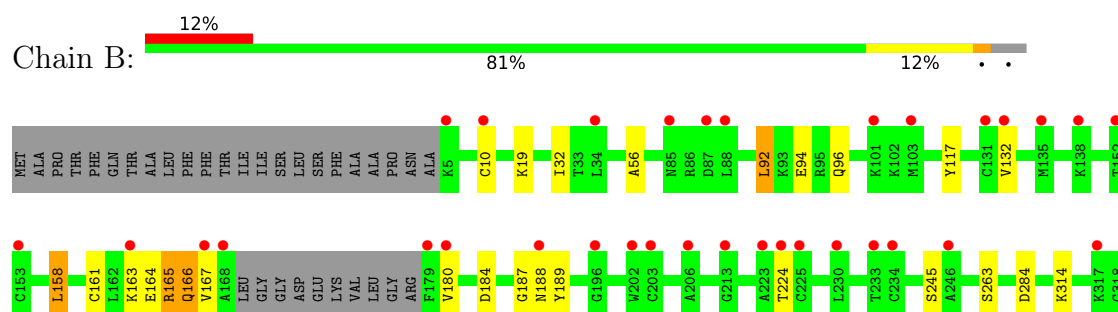
3 Residue-property plots [i](#)

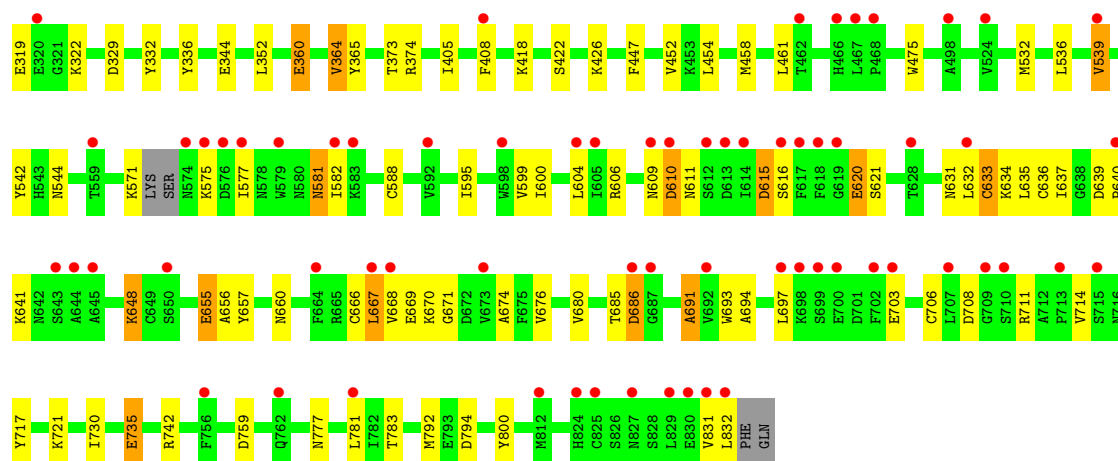
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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	96.56Å 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	7795 reflections (4.98%)	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

5.1 Standard geometry

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	0.12	0/6401	0.39	1/8631 (0.0%)
1	B	0.12	0/6425	0.38	0/8671
All	All	0.12	0/12826	0.38	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	A	574	ASN	N-CA-C	-6.43	104.31	111.71

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

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	96	0
1	B	6300	0	6162	74	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	170	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 7.

All (170) 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:43:GLU:HA	1:A:46:MET:HE2	1.75	0.67
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:A:346:MET:HA	1:A:346:MET:HE2	1.79	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:A:628:THR:C	1:A:629:LYS:HD3	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:THR:HG21	1:B:536:LEU:HD21	1.84	0.58
1:A:410:MET:HE1	1:A:438:ALA:HA	1.86	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
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: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:713:PRO:C	1:A:715:SER:H	2.15	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:B:165:ARG:C	1:B:167:VAL:H	2.16	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:A:575:LYS:HZ3	1:A:672:ASP:C	2.19	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:B:581:ASN:O	1:B:581:ASN:CG	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:532:MET:HE1	1:A:809:ARG:HD2	1.95	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
1:A:609:ASN:N	1:A:609:ASN:OD1	2.46	0.48
1:A:460:ALA:HA	1:A:465:ALA:HB2	1.96	0.48
1:B:759:ASP:OD1	1:B:759:ASP:N	2.46	0.47
1:A:572:LYS:C	1:A:574:ASN:H	2.22	0.47
1:A:718:LYS:O	1:A:721:LYS:NZ	2.43	0.47
1:A:69:LYS:NZ	1:A:464:ASP:OD2	2.32	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: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:B:693:TRP:CD1	1:B:693:TRP:H	2.32	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:165:ARG:C	1:B:167:VAL:N	2.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:198:THR:C	1:A:200:TYR:H	2.25	0.44
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
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:164:GLU:OE1	1:B:189:TYR:OH	2.33	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:525:GLN:H	1:A:525:GLN:CD	2.26	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: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:458:MET:HE3	1:B:458:MET:HB3	1.87	0.42
1:B:332:TYR:OH	1:B:344:GLU:OE2	2.27	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:620:GLU:C	1:B:635:LEU:HD11	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:532:MET:HA	1:B:532:MET:HE3	2.03	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:693:TRP:H	1:A:693:TRP:CD1	2.39	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
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:A:628:THR:O	1:A:629:LYS:C	2.64	0.40
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%)	9	5
1	B	810/853 (95%)	774 (96%)	29 (4%)	7 (1%)	14	10
All	All	1610/1706 (94%)	1535 (95%)	58 (4%)	17 (1%)	11	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
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%)	654 (94%)	45 (6%)	16	13
1	B	702/731 (96%)	664 (95%)	38 (5%)	20	18
All	All	1401/1462 (96%)	1318 (94%)	83 (6%)	18	15

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	LEU
1	A	94	GLU
1	A	101	LYS
1	A	114	LYS
1	A	158	LEU
1	A	163	LYS

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Mol	Chain	Res	Type
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	346	MET
1	A	352	LEU
1	A	360	GLU
1	A	409	LEU
1	A	439	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	577	ILE
1	A	588	CYS
1	A	610	ASP
1	A	628	THR
1	A	666	CYS
1	A	696	ASN
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	132	VAL

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Mol	Chain	Res	Type
1	B	158	LEU
1	B	166	GLN
1	B	180	VAL
1	B	263	SER
1	B	284	ASP
1	B	314	LYS
1	B	319	GLU
1	B	352	LEU
1	B	360	GLU
1	B	364	VAL
1	B	373	THR
1	B	418	LYS
1	B	461	LEU
1	B	539	VAL
1	B	581	ASN
1	B	582	ILE
1	B	604	LEU
1	B	609	ASN
1	B	615	ASP
1	B	639	ASP
1	B	641	LYS
1	B	648	LYS
1	B	655	GLU
1	B	667	LEU
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
1	B	832	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	248	GLN
1	A	315	GLN
1	A	323	ASN

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Mol	Chain	Res	Type
1	A	511	GLN
1	A	578	ASN
1	A	581	ASN
1	A	660	ASN
1	A	787	GLN
1	B	6	GLN
1	B	96	GLN
1	B	309	GLN
1	B	315	GLN
1	B	323	ASN
1	B	609	ASN
1	B	787	GLN
1	B	827	ASN

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 oligosaccharides 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	6.26	10 (58%)	14,37,37	3.33	8 (57%)

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%)

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
2	9SL	B	901	-	-	3/5/53/53	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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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:

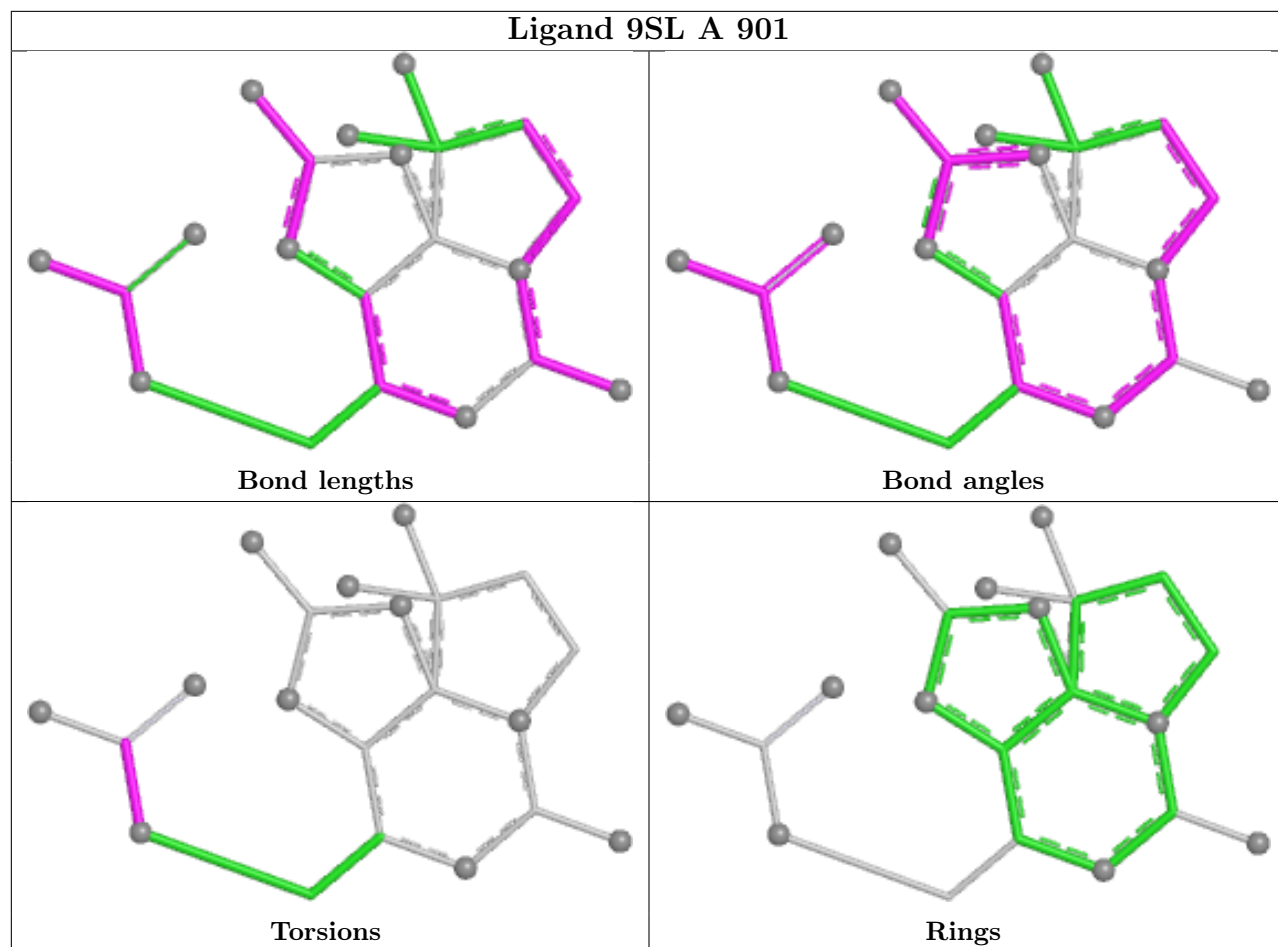
Mol	Chain	Res	Type	Atoms
2	A	901	9SL	O01-C02-O03-C04
2	A	901	9SL	N21-C02-O03-C04
2	B	901	9SL	O01-C02-O03-C04
2	B	901	9SL	N21-C02-O03-C04
2	B	901	9SL	O03-C04-C05-C14

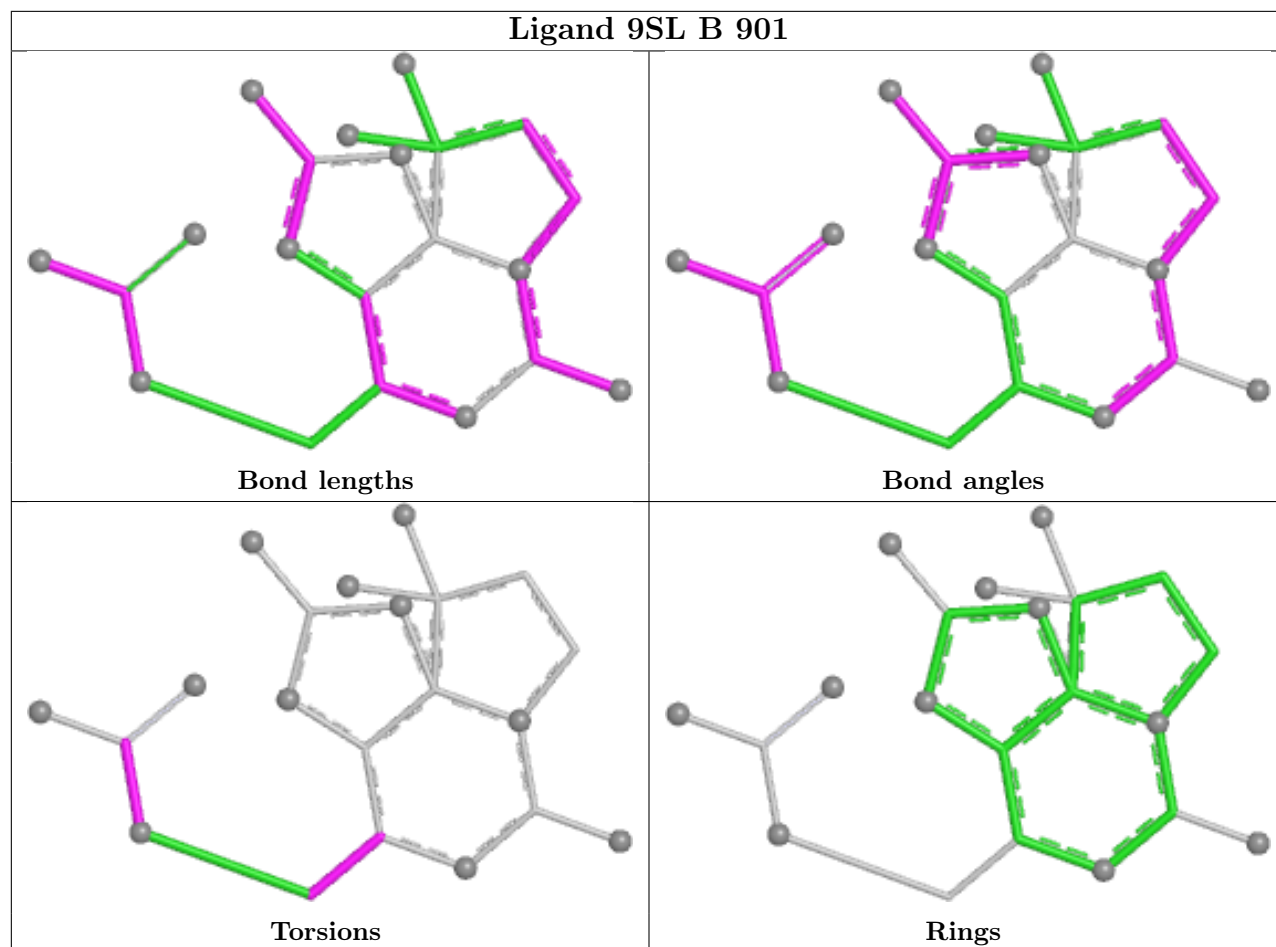
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	9SL	1	0
2	B	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%)	1.02	127 (15%) 5 5	48, 81, 173, 227	0
1	B	816/853 (95%)	0.97	99 (12%) 8 9	51, 83, 153, 244	0
All	All	1628/1706 (95%)	0.99	226 (13%) 6 7	48, 82, 168, 244	0

All (226) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	829	LEU	6.8
1	B	168	ALA	6.7
1	A	614	ILE	6.3
1	B	10	CYS	6.1
1	B	614	ILE	6.0
1	A	4	ALA	5.9
1	A	212	ALA	5.8
1	B	85	ASN	5.7
1	B	179	PHE	5.5
1	A	692	VAL	5.4
1	A	834	GLN	5.4
1	B	832	LEU	5.3
1	B	88	LEU	5.3
1	A	632	LEU	5.2
1	A	705	LEU	5.0
1	B	153	CYS	5.0
1	A	176	LEU	4.9
1	B	5	LYS	4.9
1	A	613	ASP	4.8
1	A	175	VAL	4.8
1	B	831	VAL	4.8
1	A	648	LYS	4.8
1	A	664	PHE	4.7
1	A	587	SER	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	619	GLY	4.6
1	B	467	LEU	4.6
1	B	224	THR	4.5
1	B	180	VAL	4.5
1	B	825	CYS	4.5
1	A	707	LEU	4.4
1	A	569	LEU	4.4
1	A	467	LEU	4.3
1	A	183	CYS	4.2
1	B	577	ILE	4.2
1	B	830	GLU	4.2
1	A	225	CYS	4.2
1	A	258	CYS	4.1
1	B	619	GLY	4.0
1	A	635	LEU	3.9
1	A	3	ASN	3.9
1	A	213	GLY	3.8
1	A	704	LEU	3.8
1	B	579	TRP	3.8
1	A	170	GLY	3.7
1	A	833	PHE	3.7
1	A	582	ILE	3.7
1	A	672	ASP	3.7
1	B	167	VAL	3.7
1	B	703	GLU	3.7
1	A	180	VAL	3.6
1	A	82	TYR	3.6
1	A	579	TRP	3.6
1	A	724	GLY	3.6
1	A	283	TRP	3.6
1	A	722	LEU	3.6
1	A	702	PHE	3.5
1	B	644	ALA	3.5
1	B	583	LYS	3.5
1	A	697	LEU	3.4
1	B	225	CYS	3.4
1	A	224	THR	3.4
1	A	468	PRO	3.4
1	A	211	ILE	3.4
1	B	87	ASP	3.4
1	A	177	GLY	3.4
1	A	675	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	576	ASP	3.3
1	A	287	ALA	3.3
1	B	824	HIS	3.3
1	B	610	ASP	3.3
1	A	341	CYS	3.2
1	B	702	PHE	3.2
1	A	593	GLY	3.2
1	B	574	ASN	3.2
1	A	198	THR	3.1
1	A	293	ARG	3.1
1	B	645	ALA	3.1
1	B	692	VAL	3.1
1	A	548	PHE	3.0
1	A	179	PHE	3.0
1	A	824	HIS	3.0
1	B	466	HIS	3.0
1	A	169	LEU	3.0
1	B	131	CYS	3.0
1	A	714	VAL	3.0
1	B	468	PRO	3.0
1	B	230	LEU	2.9
1	A	721	LYS	2.9
1	B	686	ASP	2.9
1	A	681	VAL	2.9
1	B	812	MET	2.9
1	A	612	SER	2.9
1	B	613	ASP	2.8
1	A	804	VAL	2.8
1	B	233	THR	2.8
1	B	609	ASN	2.8
1	A	584	GLY	2.8
1	A	800	TYR	2.8
1	B	582	ILE	2.8
1	A	660	ASN	2.7
1	A	830	GLU	2.7
1	B	196	GLY	2.7
1	A	202	TRP	2.7
1	B	320	GLU	2.7
1	A	157	GLU	2.7
1	A	827	ASN	2.7
1	A	577	ILE	2.7
1	A	725	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	707	LEU	2.6
1	A	713	PRO	2.6
1	A	670	LYS	2.6
1	A	676	VAL	2.6
1	A	551	CYS	2.6
1	A	628	THR	2.6
1	A	801	TYR	2.6
1	B	700	GLU	2.6
1	A	651	LEU	2.6
1	A	832	LEU	2.6
1	A	715	SER	2.6
1	B	223	ALA	2.6
1	B	34	LEU	2.6
1	A	682	PHE	2.5
1	B	668	VAL	2.5
1	B	103	MET	2.5
1	A	754	LYS	2.5
1	B	188	ASN	2.5
1	B	498	ALA	2.5
1	A	626	SER	2.5
1	B	673	VAL	2.5
1	A	795	TYR	2.5
1	B	575	LYS	2.5
1	A	611	ASN	2.5
1	A	168	ALA	2.5
1	B	640	PRO	2.5
1	B	699	SER	2.5
1	A	693	TRP	2.5
1	A	570	VAL	2.5
1	A	668	VAL	2.5
1	B	605	ILE	2.5
1	B	234	CYS	2.5
1	B	462	THR	2.5
1	A	288	LYS	2.5
1	B	408	PHE	2.5
1	A	831	VAL	2.4
1	B	539	VAL	2.4
1	B	152	THR	2.4
1	A	285	GLY	2.4
1	B	132	VAL	2.4
1	A	382	GLU	2.4
1	B	592	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	317	LYS	2.4
1	A	596	ALA	2.4
1	A	623	ALA	2.4
1	B	781	LEU	2.4
1	B	101	LYS	2.4
1	B	598	TRP	2.4
1	A	691	ALA	2.3
1	A	752	GLY	2.3
1	A	186	LYS	2.3
1	A	545	LYS	2.3
1	B	618	PHE	2.3
1	A	710	SER	2.3
1	A	564	LEU	2.3
1	A	667	LEU	2.3
1	B	687	GLY	2.3
1	A	653	ASP	2.3
1	A	226	GLN	2.3
1	A	690	PRO	2.3
1	A	694	ALA	2.3
1	A	805	TYR	2.3
1	B	697	LEU	2.3
1	A	174	LYS	2.3
1	A	289	GLU	2.2
1	B	616	SER	2.2
1	A	139	ILE	2.2
1	B	206	ALA	2.2
1	B	643	SER	2.2
1	A	286	PRO	2.2
1	A	552	LYS	2.2
1	A	559	THR	2.2
1	A	746	ASN	2.2
1	A	709	GLY	2.2
1	B	203	CYS	2.2
1	B	715	SER	2.2
1	A	159	PRO	2.2
1	B	762	GLN	2.2
1	A	203	CYS	2.2
1	A	633	CYS	2.2
1	B	698	LYS	2.2
1	A	599	VAL	2.1
1	B	246	ALA	2.1
1	B	710	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	628	THR	2.1
1	A	317	LYS	2.1
1	B	667	LEU	2.1
1	A	182	GLN	2.1
1	B	713	PRO	2.1
1	B	617	PHE	2.1
1	A	262	VAL	2.1
1	A	539	VAL	2.1
1	A	603	SER	2.1
1	A	699	SER	2.1
1	B	632	LEU	2.1
1	B	650	SER	2.1
1	B	135	MET	2.1
1	B	827	ASN	2.1
1	B	559	THR	2.1
1	B	213	GLY	2.1
1	B	138	LYS	2.1
1	A	567	VAL	2.1
1	A	602	VAL	2.1
1	B	524	VAL	2.1
1	B	202	TRP	2.1
1	A	812	MET	2.0
1	A	525	GLN	2.0
1	B	163	LYS	2.0
1	B	709	GLY	2.0
1	B	664	PHE	2.0
1	B	756	PHE	2.0
1	B	612	SER	2.0
1	B	604	LEU	2.0
1	A	622	CYS	2.0
1	A	156	HIS	2.0
1	A	718	LYS	2.0
1	A	555	GLY	2.0
1	A	687	GLY	2.0

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

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](#)

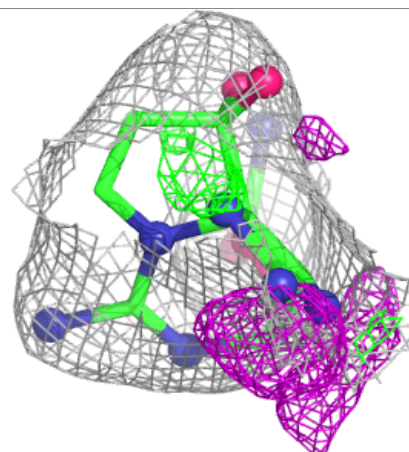
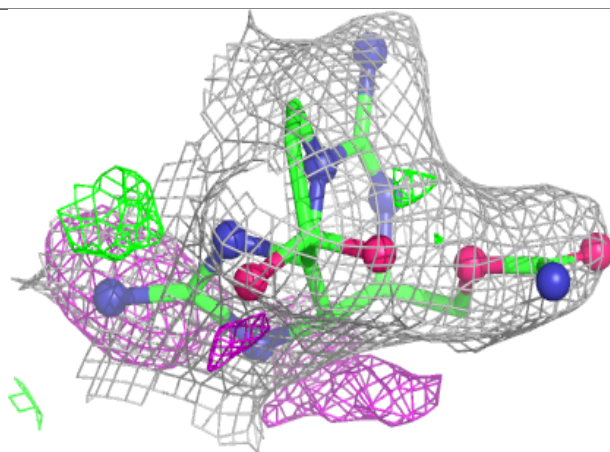
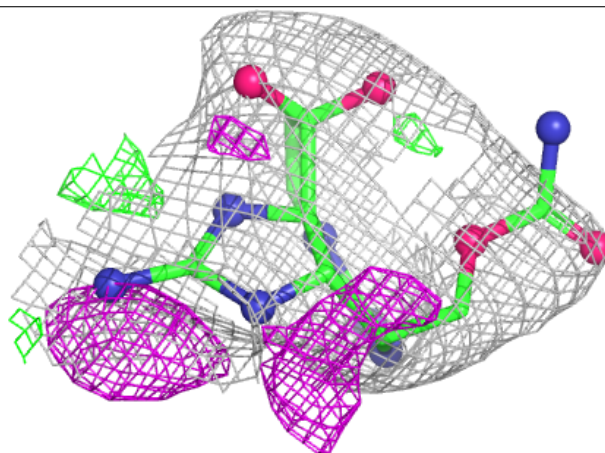
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	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.

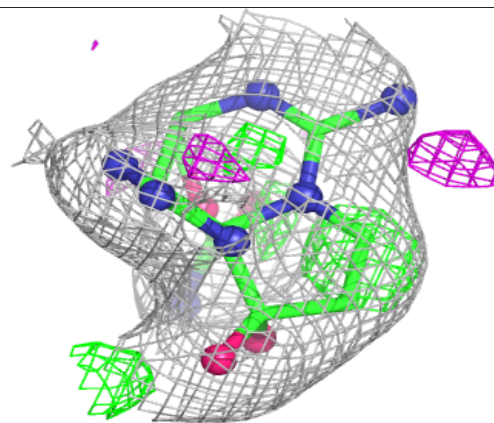
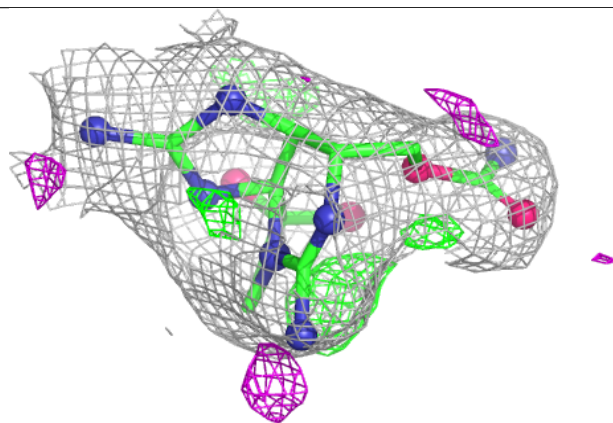
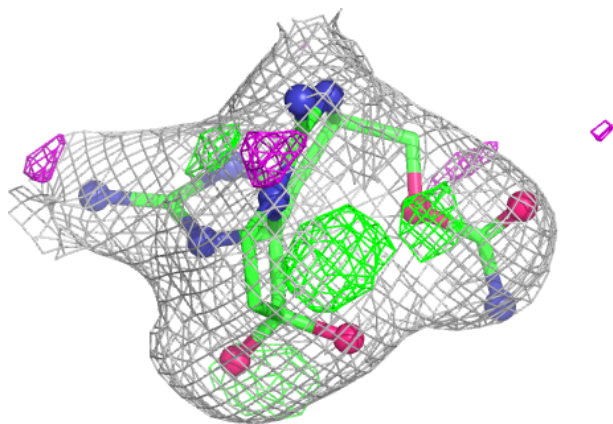
Electron density around 9SL A 901:

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.