



Full wwPDB X-ray Structure Validation Report ⓘ

May 20, 2026 – 08:08 PM EDT

PDB ID : 9YBE / pdb_00009ybe
Title : Rana catesbeiana saxiphilin mutant - F561A:STX (co-crystal)
Authors : Chen, Z.; Zakrzewska, S.; Minor, D.L.
Deposited on : 2025-09-17
Resolution : 2.35 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

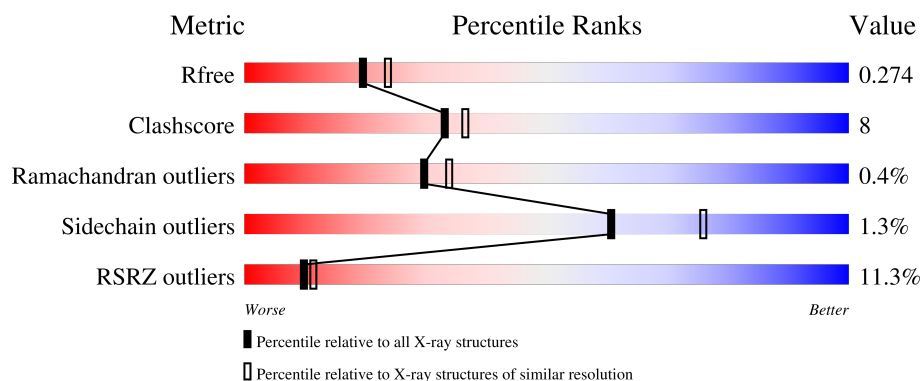
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	<div> <div>14%</div> <div> <div></div> <div>80%</div> <div>17%</div> <div>..</div> </div> </div>
1	B	853	<div> <div>8%</div> <div> <div></div> <div>78%</div> <div>18%</div> <div>.</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13061 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.

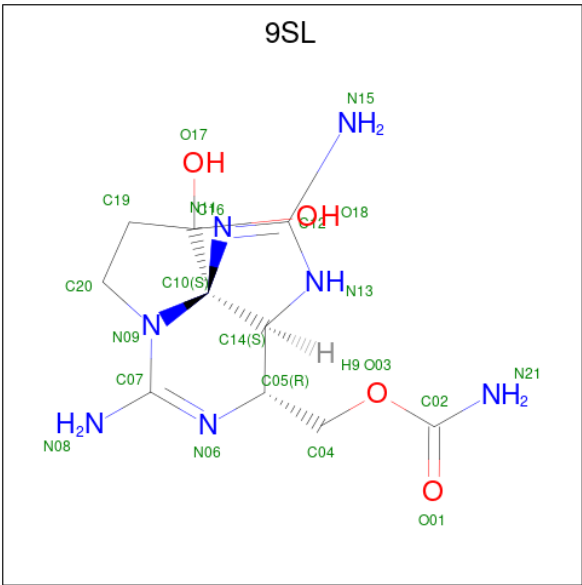
- Molecule 1 is a protein called Saxiphilin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	834	Total	C	N	O	S	0	0	0
			6426	4012	1112	1243	59			
1	B	818	Total	C	N	O	S	0	0	0
			6307	3935	1091	1222	59			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	561	ALA	PHE	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
A	833	PHE	-	expression tag	UNP P31226
A	834	GLN	-	expression tag	UNP P31226
B	561	ALA	PHE	conflict	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) (labeled as "Ligand of Interest" by depositor).



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		

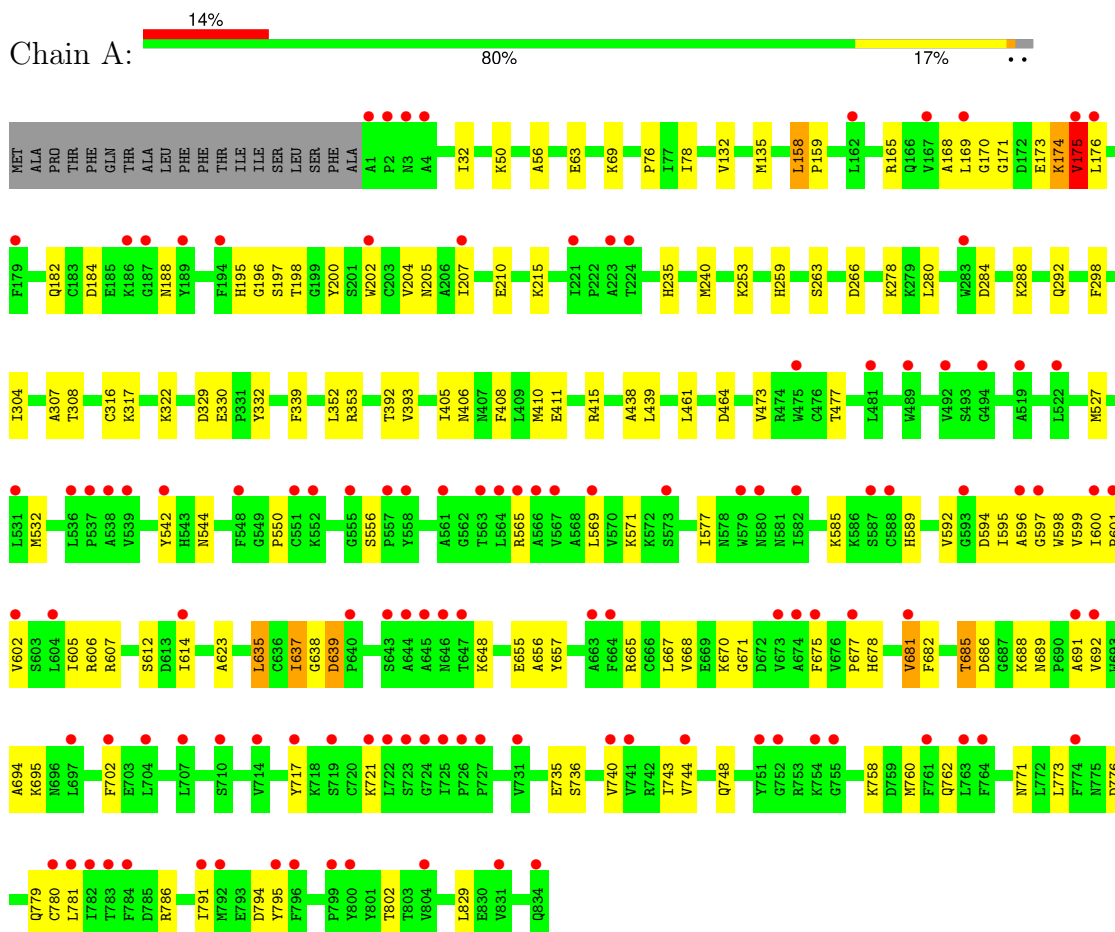
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	158	Total	O	0	0
			158	158		
3	B	128	Total	O	0	0
			128	128		

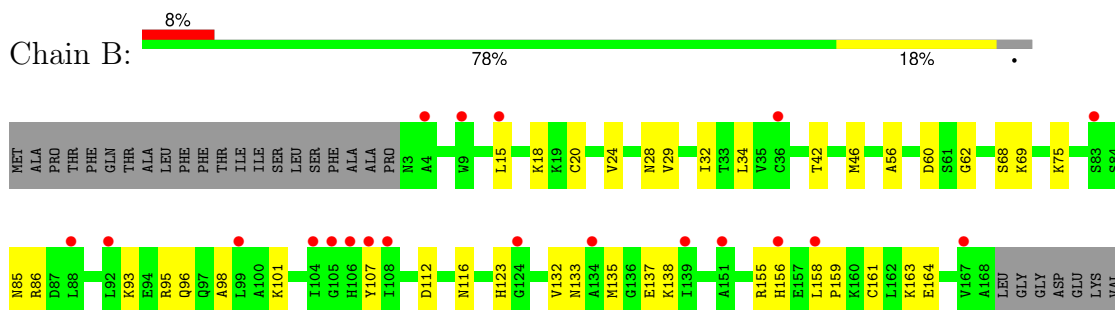
3 Residue-property plots

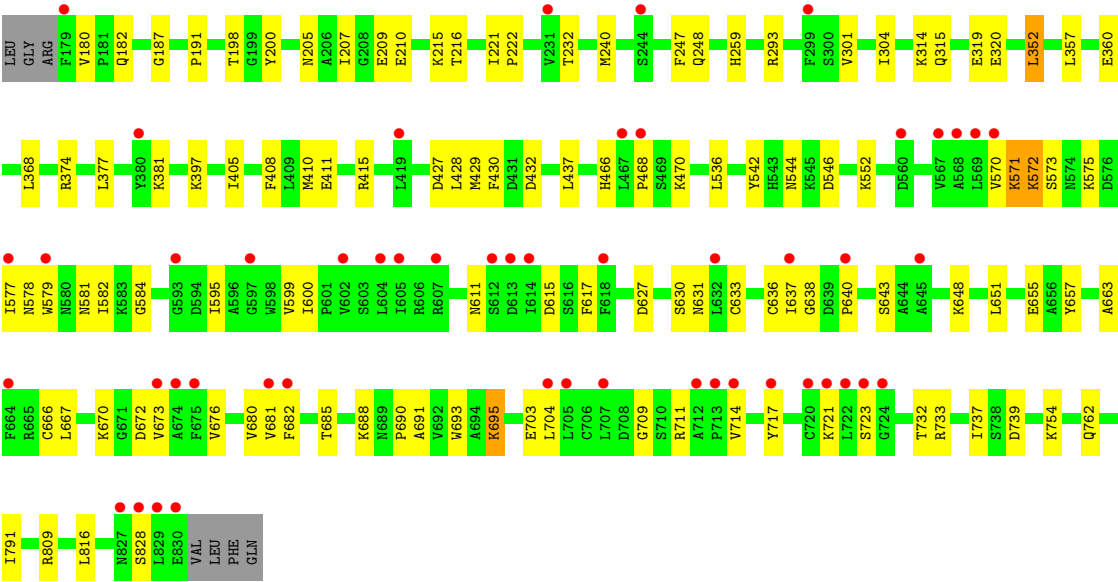
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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	96.06Å 105.11Å 253.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.54 – 2.35 48.54 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.54-2.35) 99.9 (48.54-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.34Å)	Xtriage
Refinement program	PHENIX (1.21.1_5286: ???)	Depositor
R, R_{free}	0.240 , 0.274 0.240 , 0.274	Depositor DCC
R_{free} test set	5411 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	60.0	Xtriage
Anisotropy	0.551	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 54.5	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	0.95	EDS
Total number of atoms	13061	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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	0.15	0/6554	0.31	0/8847
1	B	0.13	0/6432	0.30	0/8681
All	All	0.14	0/12986	0.31	0/17528

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	6426	0	6297	98	0
1	B	6307	0	6168	99	0
2	A	21	0	0	1	0
2	B	21	0	0	0	0
3	A	158	0	0	2	0
3	B	128	0	0	4	0
All	All	13061	0	12465	196	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 8.

All (196) 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:748:GLN:HE22	1:A:781:LEU:H	1.22	0.87
1:A:794:ASP:O	2:A:901:9SL:N11	2.12	0.83
1:A:292:GLN:NE2	1:A:308:THR:H	1.77	0.82
1:A:308:THR:HB	1:B:293:ARG:HD3	1.64	0.77
1:B:135:MET:HE2	1:B:232:THR:HG23	1.66	0.77
1:A:240:MET:HE1	1:A:339:PHE:HD1	1.50	0.77
1:A:760:MET:SD	1:A:760:MET:N	2.59	0.76
1:B:158:LEU:HB2	1:B:163:LYS:HE3	1.69	0.75
1:A:411:GLU:OE1	1:A:415:ARG:NH1	2.21	0.73
1:B:301:VAL:HG22	1:B:315:GLN:HG2	1.71	0.71
1:B:207:ILE:HD11	1:B:209:GLU:HG3	1.75	0.68
1:A:168:ALA:HA	1:A:173:GLU:HB2	1.75	0.67
1:A:691:ALA:HA	1:A:695:LYS:HG3	1.77	0.67
1:A:135:MET:SD	3:A:1136:HOH:O	2.53	0.66
1:A:639:ASP:OD2	1:A:639:ASP:N	2.26	0.66
1:B:247:PHE:O	1:B:374:ARG:NH1	2.27	0.66
1:B:690:PRO:HA	1:B:695:LYS:HE3	1.77	0.66
1:B:158:LEU:O	1:B:163:LYS:NZ	2.26	0.64
1:A:292:GLN:HE22	1:A:308:THR:H	1.42	0.64
1:A:63:GLU:HG2	1:A:263:SER:HB3	1.81	0.63
1:B:301:VAL:HG23	1:B:314:LYS:HB3	1.80	0.63
1:A:735:GLU:OE1	1:A:735:GLU:N	2.22	0.62
1:A:240:MET:HE1	1:A:339:PHE:CD1	2.35	0.62
1:A:410:MET:HE1	1:A:438:ALA:HA	1.82	0.62
1:B:32:ILE:HG21	1:B:408:PHE:HB2	1.83	0.60
1:B:600:ILE:HD12	1:B:723:SER:HB3	1.83	0.60
1:A:740:VAL:O	1:A:744:VAL:HG23	2.02	0.60
1:B:138:LYS:NZ	3:B:1001:HOH:O	2.25	0.60
1:A:681:VAL:O	1:A:685:THR:HG22	2.02	0.60
1:A:602:VAL:HG13	1:A:614:ILE:HG13	1.84	0.59
1:B:60:ASP:OD2	1:B:62:GLY:N	2.31	0.59
1:B:579:TRP:HA	1:B:582:ILE:HD11	1.84	0.58
1:B:410:MET:HE1	1:B:437:LEU:O	2.04	0.58
1:A:477:THR:HG22	1:A:773:LEU:HD11	1.86	0.58
1:A:173:GLU:C	1:A:174:LYS:HD2	2.29	0.58
1:A:569:LEU:HD11	1:A:702:PHE:HB3	1.86	0.57
1:A:56:ALA:HB2	1:A:405:ILE:HD13	1.86	0.57
1:A:76:PRO:HB3	1:A:392:THR:HG21	1.87	0.57
1:B:98:ALA:HA	1:B:101:LYS:HG2	1.86	0.56
1:A:748:GLN:NE2	1:A:781:LEU:H	1.99	0.56
1:B:205:ASN:HD21	1:B:209:GLU:HB2	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:584:GLY:N	1:B:617:PHE:O	2.35	0.56
1:B:571:LYS:O	1:B:573:SER:N	2.38	0.56
1:A:791:ILE:H	1:A:791:ILE:HD12	1.71	0.55
1:A:565:ARG:HG2	1:A:721:LYS:HD2	1.88	0.55
1:A:32:ILE:HG21	1:A:408:PHE:HB2	1.88	0.55
1:A:786:ARG:NH2	1:A:791:ILE:HG13	2.22	0.55
1:A:195:HIS:HB2	1:A:202:TRP:HH2	1.71	0.55
1:B:24:VAL:HG22	1:B:34:LEU:HD12	1.88	0.55
1:B:156:HIS:O	1:B:156:HIS:CG	2.59	0.54
1:B:155:ARG:HD2	1:B:155:ARG:H	1.71	0.54
1:A:174:LYS:C	1:A:176:LEU:H	2.15	0.54
1:B:56:ALA:HB2	1:B:405:ILE:HD13	1.89	0.54
1:A:550:PRO:HA	1:A:556:SER:HB3	1.90	0.54
1:A:758:LYS:O	1:A:762:GLN:NE2	2.41	0.54
1:B:544:ASN:HD22	1:B:546:ASP:H	1.56	0.54
1:B:198:THR:HG23	1:B:200:TYR:H	1.72	0.54
1:B:640:PRO:HA	1:B:643:SER:HB3	1.90	0.54
1:B:216:THR:HG21	1:B:222:PRO:HA	1.90	0.53
1:B:29:VAL:HG22	1:B:411:GLU:HB3	1.90	0.53
1:A:601:PRO:O	1:A:605:ILE:HG13	2.09	0.53
1:B:107:TYR:HB2	1:B:123:HIS:HD2	1.74	0.53
1:B:159:PRO:HG2	1:B:187:GLY:HA3	1.91	0.53
1:B:595:ILE:HA	1:B:599:VAL:HB	1.91	0.52
1:A:284:ASP:HB3	1:A:288:LYS:HD2	1.92	0.52
1:A:577:ILE:HD13	1:A:585:LYS:HG3	1.91	0.52
1:A:569:LEU:HD22	1:A:681:VAL:HG22	1.92	0.52
1:B:205:ASN:ND2	1:B:209:GLU:HB2	2.24	0.52
1:B:240:MET:HE2	1:B:357:LEU:HD23	1.92	0.52
1:B:542:TYR:CZ	1:B:544:ASN:HB3	2.45	0.51
1:B:578:ASN:ND2	1:B:709:GLY:O	2.42	0.51
1:A:638:GLY:HA2	1:A:648:LYS:HA	1.92	0.51
1:B:42:THR:O	1:B:46:MET:HG3	2.10	0.51
1:A:596:ALA:HB3	1:A:677:PRO:HD3	1.93	0.51
1:B:107:TYR:HB2	1:B:123:HIS:CD2	2.46	0.51
1:B:571:LYS:NZ	1:B:667:LEU:O	2.22	0.51
1:A:195:HIS:HB2	1:A:202:TRP:CH2	2.45	0.51
1:B:20:CYS:O	1:B:24:VAL:HG23	2.10	0.50
1:A:667:LEU:HA	1:A:671:GLY:HA3	1.94	0.50
1:B:704:LEU:HD13	1:B:714:VAL:HA	1.93	0.50
1:B:657:TYR:CZ	1:B:666:CYS:HA	2.47	0.50
1:A:595:ILE:O	1:A:600:ILE:HG12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:570:VAL:HG12	1:B:673:VAL:HG12	1.93	0.49
1:B:676:VAL:HG21	1:B:680:VAL:HG11	1.94	0.49
1:A:174:LYS:O	1:A:175:VAL:HG22	2.12	0.49
1:A:205:ASN:HD21	1:A:207:ILE:HG12	1.78	0.49
1:A:69:LYS:NZ	1:A:464:ASP:OD2	2.44	0.49
1:A:235:HIS:HB3	1:A:353:ARG:HD2	1.95	0.49
1:A:598:TRP:HZ3	1:A:623:ALA:HB1	1.77	0.49
1:A:635:LEU:HD21	1:A:670:LYS:HB2	1.93	0.49
1:B:544:ASN:ND2	1:B:546:ASP:H	2.10	0.49
1:A:678:HIS:CG	1:A:717:TYR:CD2	3.00	0.49
1:B:572:LYS:HA	1:B:711:ARG:HH12	1.78	0.48
1:A:607:ARG:HH12	1:A:802:THR:HG22	1.79	0.48
1:B:571:LYS:HE3	1:B:571:LYS:HB2	1.57	0.48
1:B:655:GLU:OE1	1:B:657:TYR:N	2.45	0.48
1:A:135:MET:HG3	1:A:829:LEU:HD12	1.96	0.48
1:A:184:ASP:OD1	1:A:188:ASN:N	2.46	0.47
1:B:544:ASN:HD22	1:B:544:ASN:C	2.22	0.47
1:A:170:GLY:O	1:A:174:LYS:NZ	2.47	0.47
1:B:15:LEU:H	1:B:15:LEU:HD12	1.79	0.47
1:B:357:LEU:HD22	1:B:377:LEU:HG	1.96	0.47
1:A:204:VAL:HG12	1:A:210:GLU:HA	1.95	0.47
1:B:112:ASP:OD2	1:B:116:ASN:N	2.47	0.47
1:A:542:TYR:HD2	1:A:779:GLN:HB2	1.80	0.47
1:A:594:ASP:O	1:A:599:VAL:HG23	2.15	0.47
1:A:748:GLN:HE22	1:A:780:CYS:HB2	1.80	0.47
1:B:552:LYS:HG3	1:B:754:LYS:HE3	1.96	0.47
1:B:191:PRO:HD2	1:B:809:ARG:HG3	1.96	0.46
1:B:466:HIS:CE1	1:B:468:PRO:HA	2.50	0.46
1:B:762:GLN:N	1:B:762:GLN:OE1	2.47	0.46
1:A:686:ASP:HB2	1:A:688:LYS:HE2	1.98	0.46
1:A:665:ARG:HA	1:A:668:VAL:HG12	1.96	0.46
1:A:266:ASP:OD1	1:A:353:ARG:NH1	2.49	0.46
1:A:278:LYS:HB3	1:A:280:LEU:HG	1.98	0.46
1:B:636:CYS:HB3	1:B:655:GLU:OE2	2.16	0.46
1:A:317:LYS:HA	1:A:317:LYS:HD3	1.62	0.46
1:B:182:GLN:N	1:B:182:GLN:OE1	2.48	0.46
1:A:748:GLN:NE2	1:A:780:CYS:HB2	2.31	0.46
1:B:248:GLN:HA	1:B:368:LEU:HD11	1.96	0.45
1:A:461:LEU:HD23	1:A:461:LEU:HA	1.84	0.45
1:A:50:LYS:HE3	1:A:50:LYS:HB3	1.84	0.45
1:B:75:LYS:HG2	1:B:397:LYS:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:685:THR:O	1:A:688:LYS:HG2	2.17	0.45
1:A:748:GLN:HE22	1:A:781:LEU:N	2.02	0.45
1:B:615:ASP:CG	1:B:631:ASN:HB2	2.41	0.45
1:B:691:ALA:O	1:B:695:LYS:HG2	2.17	0.45
1:A:78:ILE:HB	1:A:393:VAL:HB	1.99	0.45
1:A:736:SER:O	1:A:740:VAL:HG23	2.17	0.45
1:B:672:ASP:OD1	1:B:673:VAL:HG13	2.17	0.45
1:B:93:LYS:O	1:B:96:GLN:HG3	2.18	0.44
1:B:682:PHE:O	1:B:688:LYS:HD2	2.18	0.44
1:B:381:LYS:HE3	1:B:828:SER:OG	2.17	0.44
1:B:95:ARG:NH1	3:B:1010:HOH:O	2.51	0.44
1:A:771:ASN:H	1:A:776:ASP:CG	2.26	0.44
1:A:532:MET:HA	1:A:532:MET:HE2	2.00	0.43
1:B:133:ASN:HD21	1:B:137:GLU:HB3	1.83	0.43
1:B:240:MET:HE3	1:B:352:LEU:HD11	2.00	0.43
1:A:406:ASN:OD1	1:A:439:LEU:HB2	2.18	0.43
1:B:28:ASN:O	1:B:415:ARG:NH1	2.49	0.43
1:B:85:ASN:ND2	1:B:86:ARG:HG3	2.33	0.43
1:A:165:ARG:NH2	1:A:182:GLN:HA	2.33	0.43
1:B:69:LYS:HB3	1:B:69:LYS:HE2	1.83	0.43
1:B:536:LEU:HB2	1:B:737:ILE:HD11	2.00	0.43
1:B:663:ALA:O	1:B:666:CYS:HB3	2.19	0.43
1:A:527:MET:HG3	1:A:795:TYR:CZ	2.53	0.43
1:A:200:TYR:HD2	1:A:215:LYS:HG2	1.84	0.43
1:A:637:ILE:HD11	1:A:656:ALA:HB3	2.00	0.43
1:B:210:GLU:OE1	1:B:215:LYS:HE3	2.19	0.43
1:B:164:GLU:HB2	3:B:1020:HOH:O	2.19	0.42
1:B:578:ASN:HB3	1:B:581:ASN:ND2	2.33	0.42
1:A:585:LYS:HA	1:A:585:LYS:HD3	1.87	0.42
1:A:589:HIS:CD2	1:A:675:PHE:HD1	2.37	0.42
1:B:638:GLY:H	1:B:648:LYS:NZ	2.18	0.42
1:A:682:PHE:O	1:A:688:LYS:HE3	2.19	0.42
1:A:307:ALA:O	3:A:1001:HOH:O	2.21	0.42
1:A:316:CYS:HB3	1:A:330:GLU:OE2	2.18	0.42
1:A:655:GLU:HG3	1:A:657:TYR:H	1.85	0.42
1:A:171:GLY:O	1:A:174:LYS:NZ	2.49	0.42
1:B:319:GLU:OE2	1:B:320:GLU:N	2.53	0.42
1:B:428:LEU:O	1:B:430:PHE:N	2.48	0.42
1:B:577:ILE:HD11	1:B:672:ASP:HB2	2.01	0.42
1:A:195:HIS:HB3	1:A:198:THR:O	2.20	0.42
1:B:637:ILE:HD11	1:B:670:LYS:NZ	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:597:GLY:HA2	1:A:675:PHE:O	2.21	0.41
1:B:221:ILE:HD12	1:B:221:ILE:H	1.85	0.41
1:B:575:LYS:HE3	1:B:711:ARG:HD3	2.01	0.41
1:B:681:VAL:O	1:B:685:THR:HG23	2.21	0.41
1:B:627:ASP:HB3	1:B:630:SER:HB2	2.03	0.41
1:B:717:TYR:O	1:B:721:LYS:HB3	2.19	0.41
1:B:732:THR:HG23	1:B:733:ARG:O	2.20	0.41
1:A:158:LEU:HD22	1:A:159:PRO:HD2	2.01	0.41
1:A:253:LYS:HG2	1:A:298:PHE:CE1	2.55	0.41
1:A:322:LYS:HD2	1:A:329:ASP:HB3	2.02	0.41
1:B:161:CYS:HA	3:B:1020:HOH:O	2.20	0.41
1:A:195:HIS:HD2	1:A:196:GLY:N	2.18	0.41
1:A:259:HIS:CD2	1:A:304:ILE:HG12	2.56	0.41
1:B:18:LYS:N	1:B:18:LYS:HD3	2.35	0.41
1:A:317:LYS:HG2	1:A:332:TYR:CE1	2.56	0.41
1:A:473:VAL:HG23	1:A:743:ILE:HD12	2.02	0.41
1:A:571:LYS:NZ	1:A:668:VAL:HA	2.36	0.41
1:A:592:VAL:HG22	1:A:598:TRP:CZ3	2.56	0.41
1:A:689:ASN:ND2	1:A:694:ALA:O	2.54	0.41
1:B:68:SER:O	1:B:397:LYS:NZ	2.34	0.41
1:B:791:ILE:HD12	1:B:791:ILE:HA	1.90	0.41
1:A:173:GLU:O	1:A:174:LYS:NZ	2.43	0.40
1:A:542:TYR:CZ	1:A:544:ASN:HB3	2.56	0.40
1:B:259:HIS:CD2	1:B:304:ILE:HG12	2.56	0.40
1:B:429:MET:HE2	1:B:429:MET:HB3	1.86	0.40
1:A:606:ARG:HG2	1:A:612:SER:HB3	2.03	0.40
1:B:427:ASP:H	1:B:432:ASP:CG	2.30	0.40
1:B:703:GLU:OE1	1:B:711:ARG:NH1	2.50	0.40
1:B:582:ILE:H	1:B:582:ILE:HG12	1.68	0.40
1:B:470:LYS:HG2	1:B:739:ASP:OD2	2.21	0.40
1:B:655:GLU:HG3	1:B:657:TYR:H	1.86	0.40
1:B:691:ALA:HB1	1:B:693:TRP:CZ3	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries

of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	832/853 (98%)	794 (95%)	35 (4%)	3 (0%)	30	34
1	B	814/853 (95%)	774 (95%)	37 (4%)	3 (0%)	30	34
All	All	1646/1706 (96%)	1568 (95%)	72 (4%)	6 (0%)	30	34

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	175	VAL
1	B	572	LYS
1	A	197	SER
1	B	611	ASN
1	B	633	CYS
1	A	692	VAL

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	714/730 (98%)	703 (98%)	11 (2%)	57	72
1	B	702/730 (96%)	694 (99%)	8 (1%)	65	79
All	All	1416/1460 (97%)	1397 (99%)	19 (1%)	61	76

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	VAL
1	A	158	LEU
1	A	169	LEU
1	A	174	LYS
1	A	175	VAL
1	A	352	LEU

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Mol	Chain	Res	Type
1	A	635	LEU
1	A	637	ILE
1	A	639	ASP
1	A	681	VAL
1	A	685	THR
1	B	132	VAL
1	B	180	VAL
1	B	352	LEU
1	B	360	GLU
1	B	571	LYS
1	B	651	LEU
1	B	695	LYS
1	B	816	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	192	GLN
1	A	248	GLN
1	A	292	GLN
1	A	416	GLN
1	A	631	ASN
1	A	642	ASN
1	A	748	GLN
1	A	824	HIS
1	A	827	ASN
1	B	118	GLN
1	B	143	ASN
1	B	235	HIS
1	B	326	ASN
1	B	406	ASN
1	B	416	GLN
1	B	544	ASN
1	B	660	ASN
1	B	767	ASN

5.3.3 RNA ⓘ

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	1.76	4 (23%)	14,37,37	3.45	6 (42%)
2	9SL	B	901	-	17,23,23	1.79	5 (29%)	14,37,37	3.26	6 (42%)

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	-	-	4/5/53/53	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	9SL	C07-N09	3.96	1.42	1.35
2	A	901	9SL	C07-N09	3.84	1.42	1.35
2	B	901	9SL	C12-N13	3.03	1.39	1.35
2	A	901	9SL	C12-N13	2.98	1.39	1.35
2	B	901	9SL	O03-C04	-2.95	1.38	1.45
2	A	901	9SL	O03-C04	-2.92	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	9SL	C07-N08	-2.49	1.29	1.34
2	A	901	9SL	C07-N08	-2.42	1.29	1.34
2	B	901	9SL	C12-N15	-2.10	1.29	1.34

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	9SL	N09-C07-N06	-7.18	115.42	125.42
2	A	901	9SL	O03-C02-N21	7.15	120.01	111.11
2	B	901	9SL	O03-C02-N21	6.81	119.58	111.11
2	B	901	9SL	N09-C07-N06	-6.44	116.45	125.42
2	B	901	9SL	C04-O03-C02	5.53	124.04	116.26
2	A	901	9SL	C04-O03-C02	4.91	123.17	116.26
2	A	901	9SL	O01-C02-N21	-3.94	119.36	125.58
2	B	901	9SL	O01-C02-N21	-3.70	119.74	125.58
2	A	901	9SL	O03-C02-O01	-2.67	120.61	123.08
2	B	901	9SL	O03-C02-O01	-2.61	120.67	123.08
2	B	901	9SL	O17-C16-C19	-2.21	106.14	113.09
2	A	901	9SL	N15-C12-N13	2.08	126.10	122.70

There are no chirality outliers.

All (6) 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-N06
2	B	901	9SL	O03-C04-C05-C14

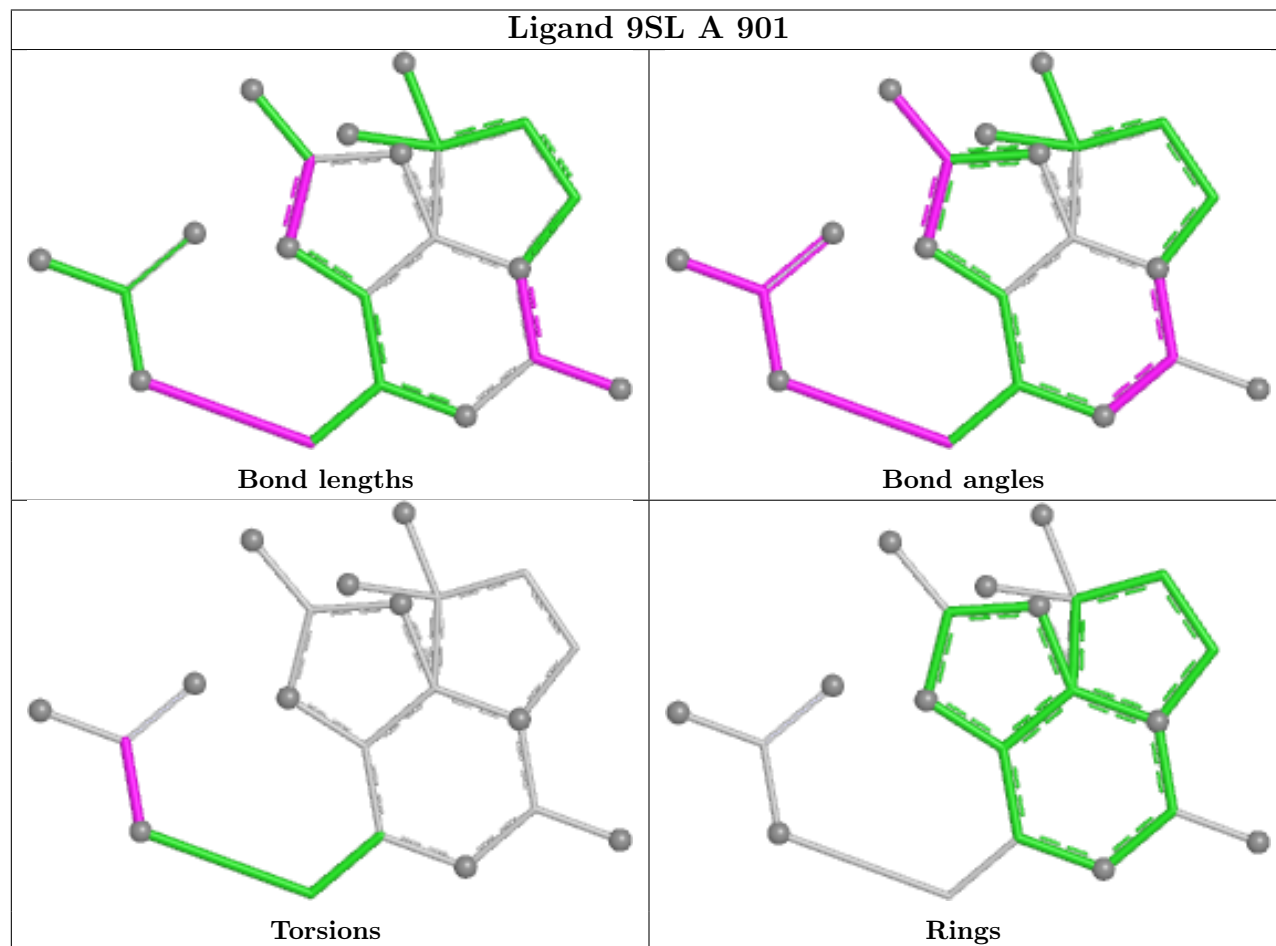
There are no ring outliers.

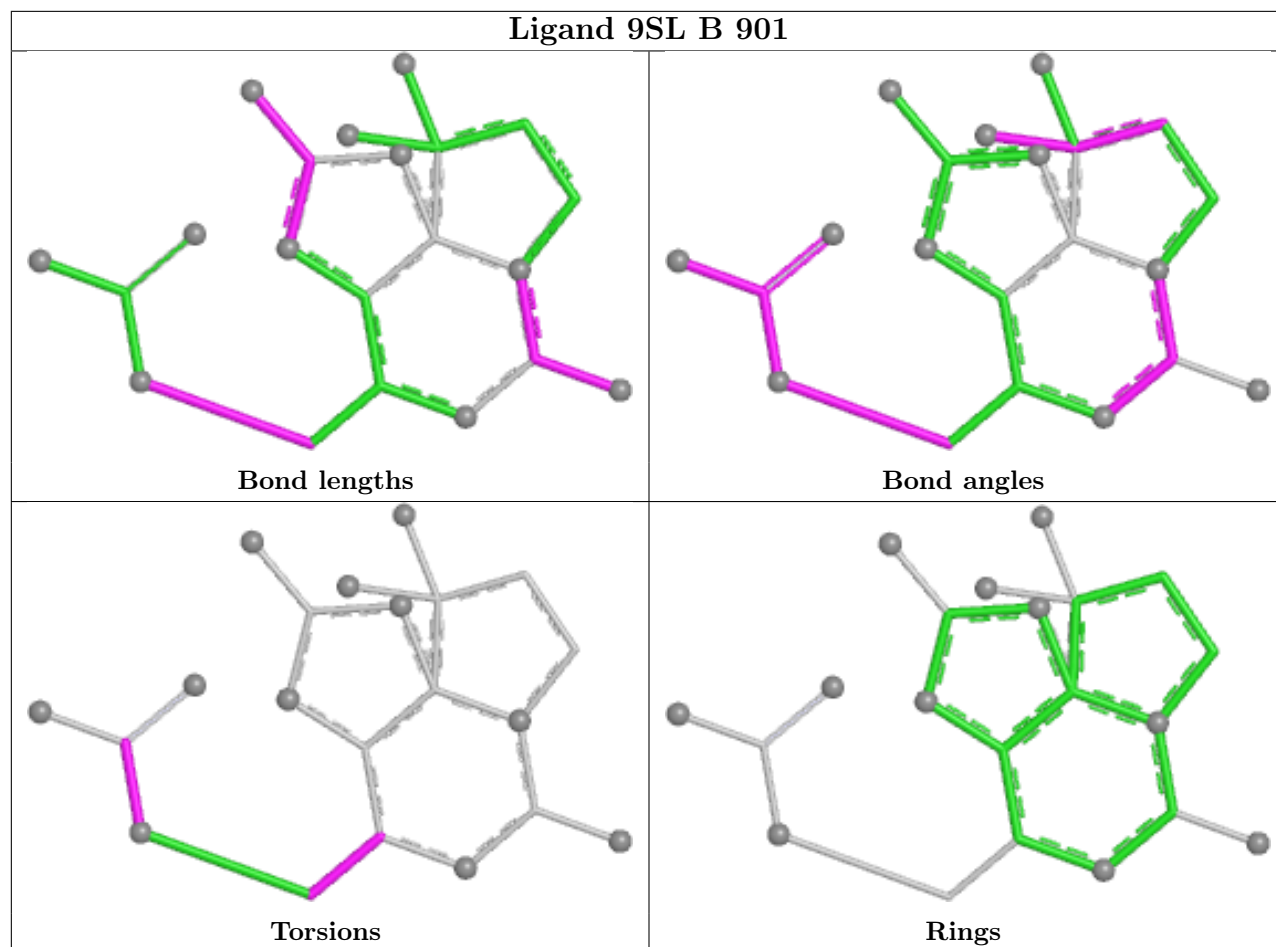
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
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	834/853 (97%)	0.84	116 (13%) 6 7	47, 86, 172, 212	0
1	B	818/853 (95%)	0.81	71 (8%) 16 18	52, 87, 159, 209	0
All	All	1652/1706 (96%)	0.83	187 (11%) 10 11	47, 86, 168, 212	0

All (187) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	ALA	4.8
1	A	724	GLY	4.6
1	A	564	LEU	4.4
1	B	104	ILE	4.2
1	B	4	ALA	4.2
1	A	604	LEU	4.0
1	A	675	PHE	4.0
1	A	579	TRP	3.9
1	B	568	ALA	3.9
1	B	569	LEU	3.9
1	B	829	LEU	3.9
1	B	579	TRP	3.8
1	B	614	ILE	3.8
1	B	674	ALA	3.8
1	A	640	PRO	3.8
1	A	283	TRP	3.8
1	A	569	LEU	3.8
1	A	176	LEU	3.7
1	A	725	ILE	3.6
1	B	179	PHE	3.6
1	A	722	LEU	3.6
1	B	664	PHE	3.5
1	A	664	PHE	3.5
1	B	88	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	99	LEU	3.4
1	B	467	LEU	3.4
1	B	705	LEU	3.3
1	A	175	VAL	3.3
1	B	158	LEU	3.3
1	B	567	VAL	3.3
1	B	828	SER	3.3
1	B	830	GLU	3.3
1	A	645	ALA	3.2
1	B	613	ASP	3.2
1	B	577	ILE	3.2
1	A	221	ILE	3.2
1	A	796	PHE	3.1
1	A	162	LEU	3.1
1	A	723	SER	3.1
1	B	299	PHE	3.1
1	A	597	GLY	3.1
1	A	561	ALA	3.1
1	A	744	VAL	3.1
1	B	707	LEU	3.1
1	A	596	ALA	3.0
1	A	644	ALA	3.0
1	A	800	TYR	3.0
1	A	726	PRO	3.0
1	A	567	VAL	3.0
1	A	602	VAL	2.9
1	A	834	GLN	2.9
1	B	605	ILE	2.9
1	A	795	TYR	2.9
1	A	169	LEU	2.9
1	A	763	LEU	2.9
1	A	551	CYS	2.9
1	A	799	PRO	2.9
1	A	179	PHE	2.9
1	A	707	LEU	2.9
1	A	731	VAL	2.9
1	A	563	THR	2.9
1	A	2	PRO	2.9
1	A	522	LEU	2.9
1	B	645	ALA	2.9
1	B	720	CYS	2.9
1	B	156	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	558	TYR	2.8
1	A	804	VAL	2.8
1	A	539	VAL	2.8
1	B	618	PHE	2.8
1	A	647	THR	2.7
1	A	782	ILE	2.7
1	A	752	GLY	2.7
1	A	537	PRO	2.7
1	B	721	LYS	2.7
1	B	722	LEU	2.7
1	A	566	ALA	2.7
1	B	602	VAL	2.7
1	A	791	ILE	2.7
1	A	784	PHE	2.7
1	A	719	SER	2.7
1	B	704	LEU	2.7
1	A	831	VAL	2.6
1	A	600	ILE	2.6
1	B	108	ILE	2.6
1	A	4	ALA	2.6
1	A	674	ALA	2.6
1	A	167	VAL	2.6
1	B	124	GLY	2.6
1	A	601	PRO	2.6
1	A	582	ILE	2.6
1	B	597	GLY	2.5
1	A	673	VAL	2.5
1	A	721	LYS	2.5
1	A	189	TYR	2.5
1	A	663	ALA	2.5
1	A	691	ALA	2.5
1	B	83	SER	2.5
1	A	223	ALA	2.5
1	B	712	ALA	2.5
1	B	36	CYS	2.4
1	B	723	SER	2.4
1	A	681	VAL	2.4
1	B	92	LEU	2.4
1	A	187	GLY	2.4
1	B	468	PRO	2.4
1	A	207	ILE	2.4
1	A	774	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	519	ALA	2.4
1	A	224	THR	2.4
1	B	244	SER	2.4
1	A	475	TRP	2.4
1	A	751	TYR	2.4
1	B	560	ASP	2.4
1	A	643	SER	2.4
1	A	714	VAL	2.4
1	A	761	PHE	2.4
1	B	717	TYR	2.3
1	A	740	VAL	2.3
1	A	781	LEU	2.3
1	A	717	TYR	2.3
1	B	612	SER	2.3
1	A	702	PHE	2.3
1	B	681	VAL	2.3
1	A	780	CYS	2.3
1	B	107	TYR	2.3
1	B	637	ILE	2.3
1	A	692	VAL	2.3
1	B	675	PHE	2.3
1	B	604	LEU	2.3
1	B	231	VAL	2.3
1	A	580	ASN	2.2
1	A	646	ASN	2.2
1	B	827	ASN	2.2
1	A	494	GLY	2.2
1	A	593	GLY	2.2
1	A	194	PHE	2.2
1	A	764	PHE	2.2
1	B	607	ARG	2.2
1	B	593	GLY	2.2
1	A	538	ALA	2.2
1	A	542	TYR	2.2
1	A	704	LEU	2.2
1	B	632	LEU	2.2
1	A	588	CYS	2.2
1	B	105	GLY	2.2
1	A	614	ILE	2.2
1	A	3	ASN	2.2
1	A	548	PHE	2.2
1	A	792	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	727	PRO	2.2
1	A	555	GLY	2.2
1	A	489	TRP	2.1
1	A	536	LEU	2.1
1	B	9	TRP	2.1
1	B	15	LEU	2.1
1	B	570	VAL	2.1
1	B	724	GLY	2.1
1	B	134	ALA	2.1
1	A	697	LEU	2.1
1	A	754	LYS	2.1
1	A	492	VAL	2.1
1	A	557	PRO	2.1
1	A	783	THR	2.1
1	A	531	LEU	2.1
1	B	640	PRO	2.1
1	B	673	VAL	2.1
1	B	714	VAL	2.1
1	A	202	TRP	2.1
1	A	710	SER	2.1
1	A	552	LYS	2.1
1	B	106	HIS	2.1
1	B	419	LEU	2.1
1	A	677	PRO	2.1
1	A	741	VAL	2.1
1	A	755	GLY	2.1
1	A	565	ARG	2.1
1	A	573	SER	2.0
1	A	587	SER	2.0
1	B	139	ILE	2.0
1	B	713	PRO	2.0
1	B	380	TYR	2.0
1	B	167	VAL	2.0
1	B	682	PHE	2.0
1	A	186	LYS	2.0
1	B	151	ALA	2.0
1	A	481	LEU	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](#)

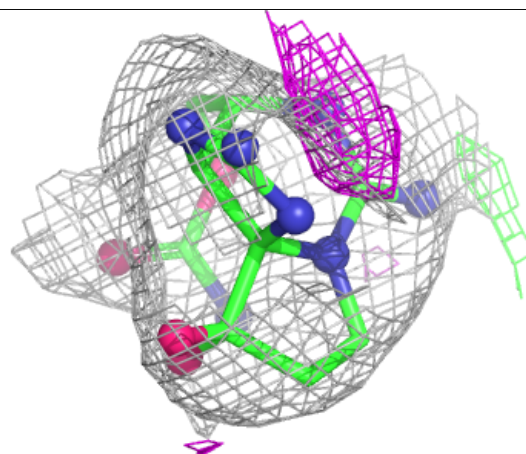
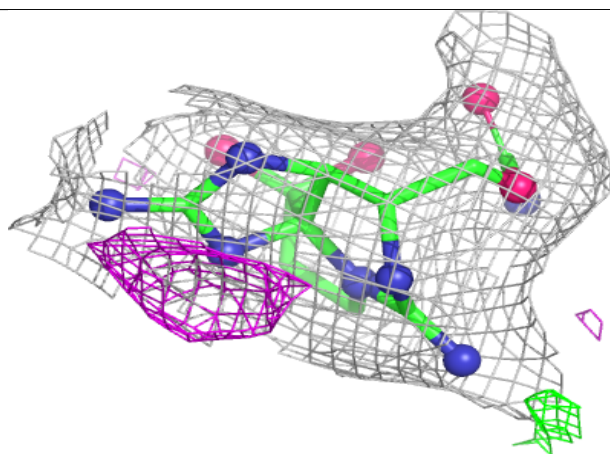
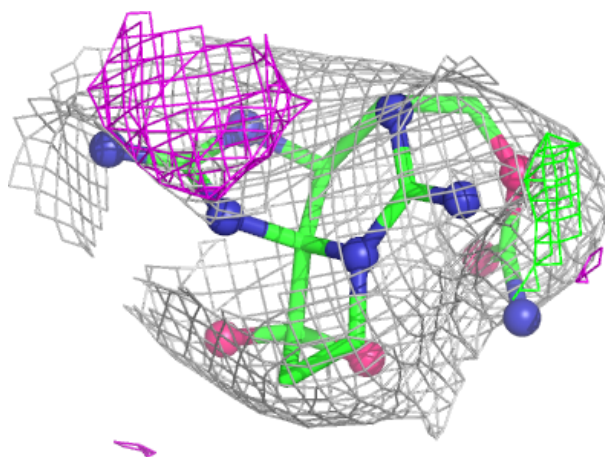
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	9SL	A	901	21/21	0.81	0.12	118,125,132,150	0
2	9SL	B	901	21/21	0.91	0.12	72,87,102,103	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.

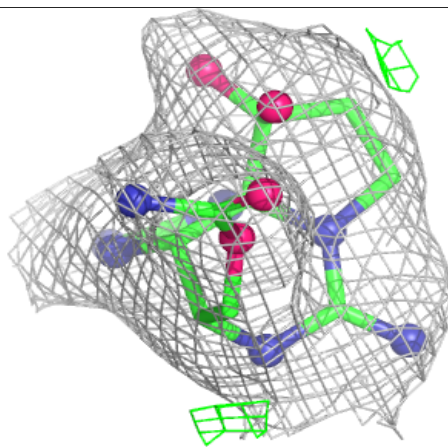
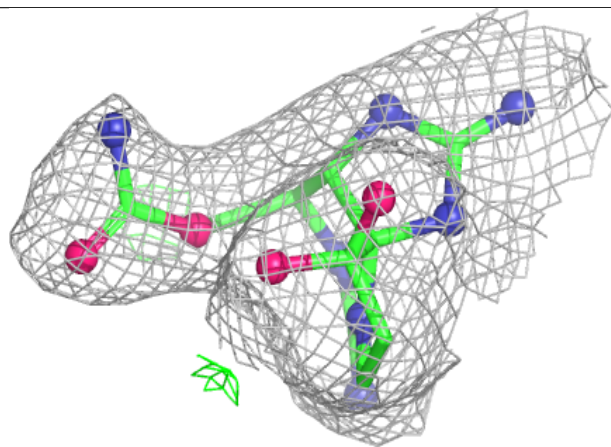
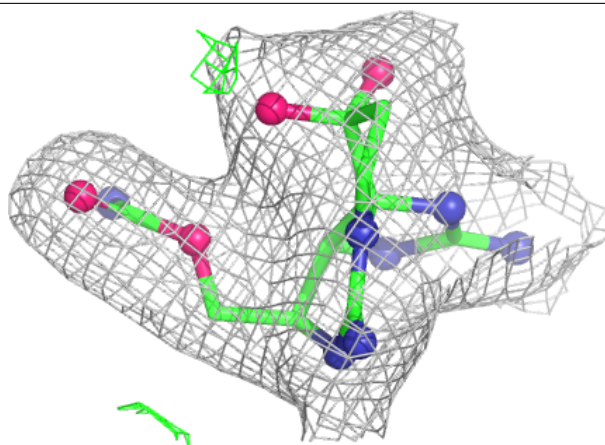
Electron density around 9SL A 901:

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.