



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:12 AM UTC

PDB ID : 8D6S / pdb_00008d6s
Title : Rana catesbeiana saxiphilin mutant - Y558A:STX (co-crystal)
Authors : Chen, Z.; Zakrzewska, S.; Minor, D.L.
Deposited on : 2022-06-06
Resolution : 2.60 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

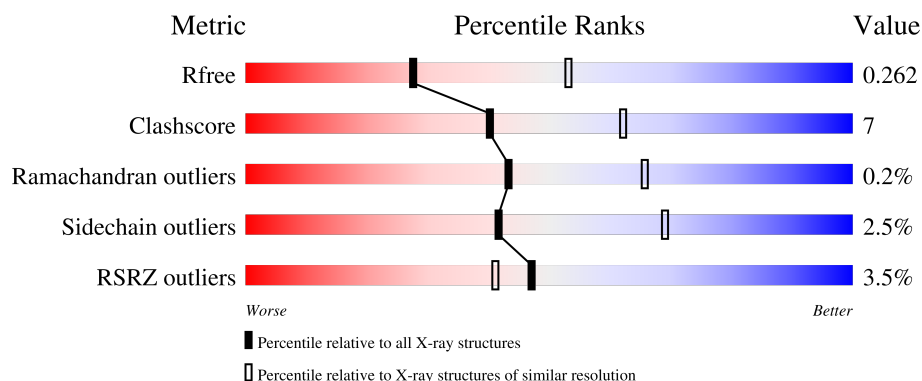
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	851	 4% 80% 15% . .
1	B	851	 3% 76% 19% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12718 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.

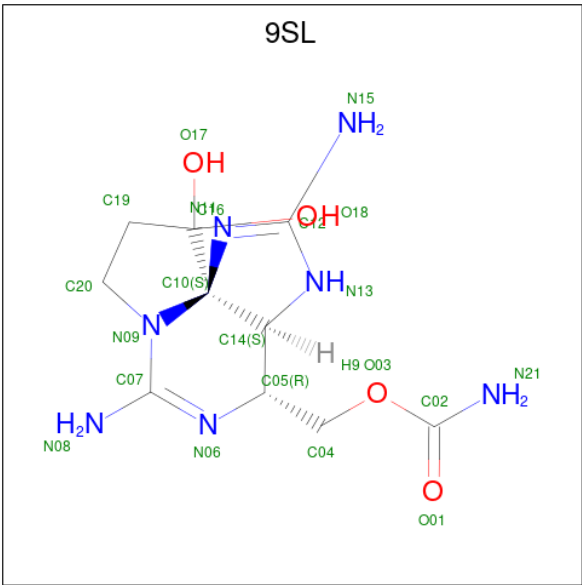
- Molecule 1 is a protein called Saxiphilin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	818	Total	C	N	O	S	0	0	0
			6308	3939	1090	1220	59			
1	B	818	Total	C	N	O	S	0	0	0
			6308	3939	1090	1220	59			

There are 16 discrepancies between the modelled and reference sequences:

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

- 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		

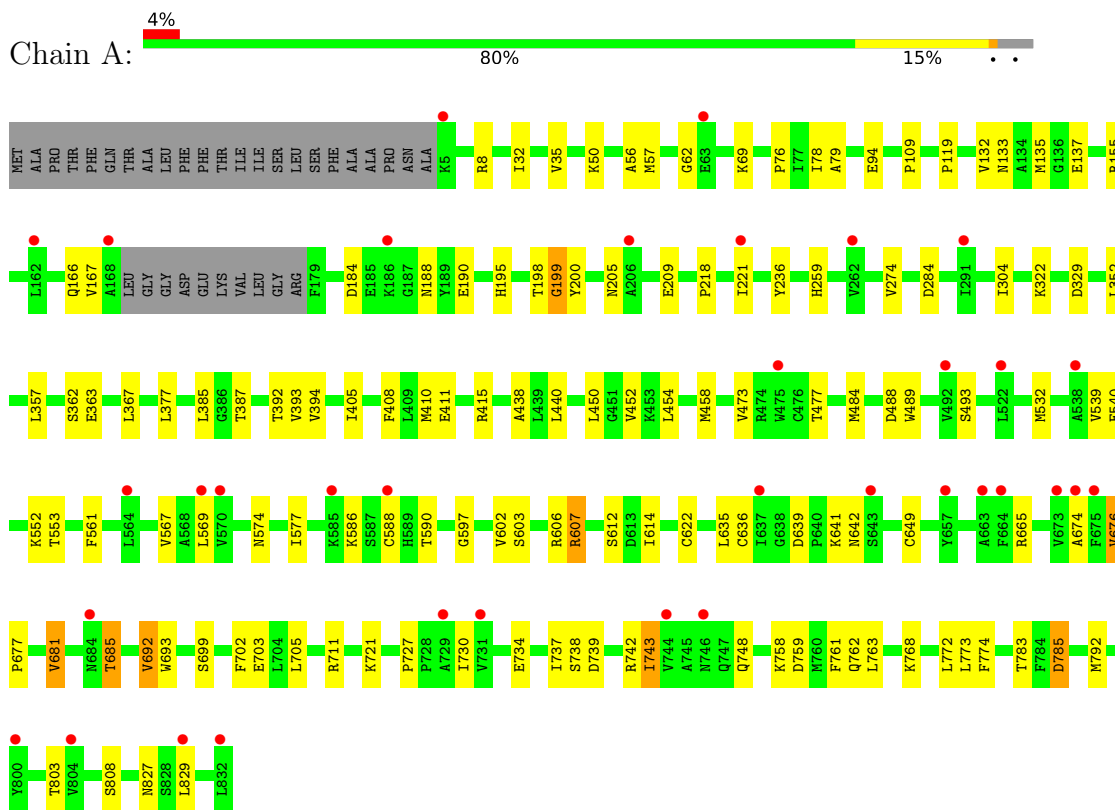
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	36	Total	O	0	0
			36	36		
3	B	24	Total	O	0	0
			24	24		

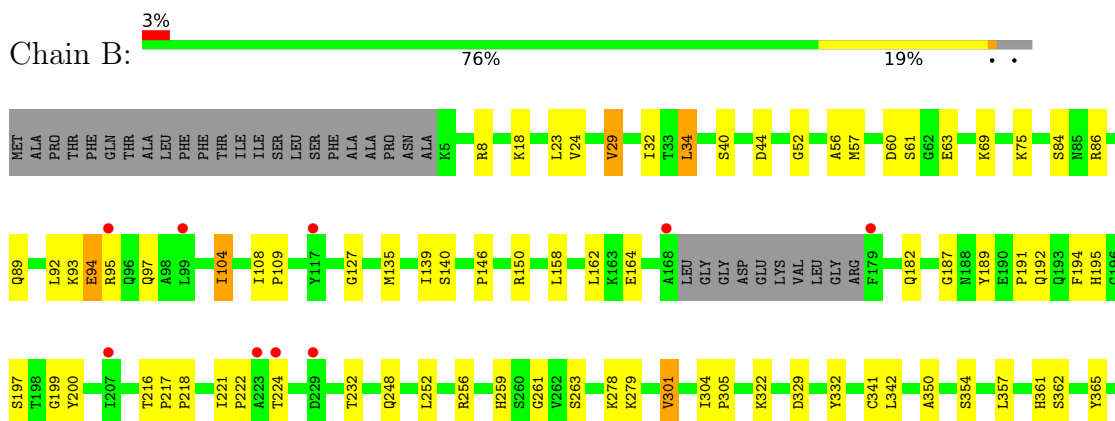
3 Residue-property plots [i](#)

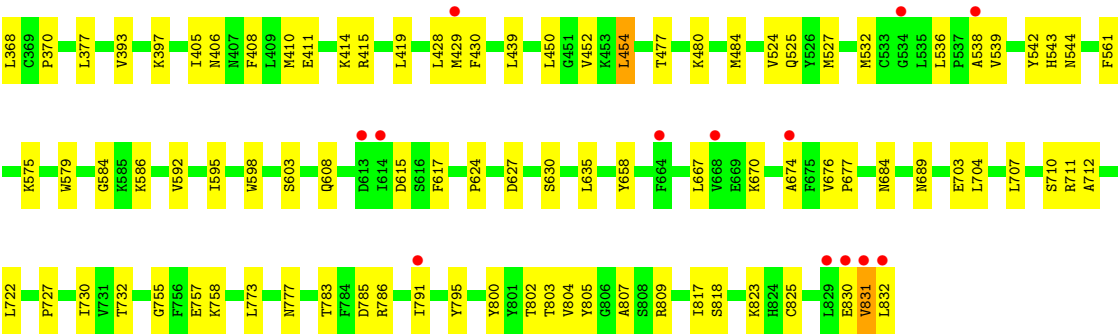
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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	95.98Å 107.14Å 253.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.37 – 2.60 47.37 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.37-2.60) 99.8 (47.37-2.60)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.232 , 0.262 0.232 , 0.262	Depositor DCC
R_{free} test set	3937 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	84.8	Xtriage
Anisotropy	0.528	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 87.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12718	wwPDB-VP
Average B, all atoms (Å ²)	135.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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	0.10	0/6433	0.28	0/8682
1	B	0.09	0/6433	0.27	0/8682
All	All	0.09	0/12866	0.27	0/17364

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 [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	6308	0	6177	75	0
1	B	6308	0	6177	90	0
2	A	21	0	0	1	0
2	B	21	0	0	2	0
3	A	36	0	0	3	0
3	B	24	0	0	0	0
All	All	12718	0	12354	165	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 (165) 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:607:ARG:NH2	1:A:803:THR:O	2.14	0.81
1:A:602:VAL:HG23	1:A:614:ILE:HG13	1.63	0.81
1:B:532:MET:HE1	1:B:809:ARG:HD2	1.65	0.79
1:A:703:GLU:HB2	1:A:711:ARG:HH21	1.49	0.76
1:A:590:THR:HG22	1:A:597:GLY:HA3	1.69	0.74
1:B:24:VAL:HG22	1:B:34:LEU:HB3	1.73	0.70
1:A:199:GLY:O	3:A:1001:HOH:O	2.10	0.69
1:A:606:ARG:HG2	1:A:612:SER:HB3	1.75	0.69
1:B:539:VAL:HG12	1:B:783:THR:HA	1.75	0.68
1:B:802:THR:HG22	1:B:807:ALA:HB2	1.76	0.67
1:A:636:CYS:SG	3:A:1003:HOH:O	2.54	0.66
1:B:199:GLY:HA3	1:B:218:PRO:HB3	1.76	0.66
1:A:56:ALA:HB2	1:A:405:ILE:HD13	1.80	0.64
1:A:539:VAL:HG12	1:A:783:THR:HA	1.80	0.64
1:A:135:MET:HG3	1:A:829:LEU:HD22	1.79	0.63
1:B:785:ASP:O	2:B:901:9SL:N15	2.32	0.63
1:B:95:ARG:HA	1:B:109:PRO:HD2	1.80	0.63
1:A:62:GLY:HA2	1:A:458:MET:HE1	1.81	0.63
1:B:278:LYS:NZ	1:B:370:PRO:O	2.33	0.61
1:B:527:MET:HG2	1:B:795:TYR:CE2	2.36	0.61
1:B:635:LEU:HD22	1:B:670:LYS:HE2	1.81	0.61
1:A:685:THR:HG21	1:A:699:SER:HB3	1.83	0.60
1:B:146:PRO:HA	1:B:150:ARG:HH12	1.66	0.60
1:B:703:GLU:OE2	1:B:712:ALA:N	2.34	0.60
1:A:574:ASN:O	1:A:711:ARG:NH1	2.33	0.60
1:A:410:MET:HE1	1:A:438:ALA:HA	1.83	0.59
1:A:94:GLU:HB3	1:A:109:PRO:HG2	1.84	0.59
1:A:411:GLU:OE1	1:A:415:ARG:NH1	2.35	0.59
1:B:354:SER:HA	1:B:357:LEU:HD23	1.84	0.58
1:A:569:LEU:HD22	1:A:681:VAL:HG22	1.86	0.58
1:A:119:PRO:HG3	1:A:155:ARG:HG3	1.87	0.57
1:B:56:ALA:HB2	1:B:405:ILE:HD13	1.85	0.57
1:B:75:LYS:HG2	1:B:397:LYS:HA	1.87	0.56
1:B:139:ILE:HD12	1:B:832:LEU:HB3	1.85	0.56
1:A:569:LEU:HD11	1:A:702:PHE:HB3	1.88	0.56
1:B:192:GLN:HB2	1:B:809:ARG:HH21	1.69	0.55
1:A:184:ASP:OD1	1:A:188:ASN:N	2.40	0.55
1:A:692:VAL:HG13	1:A:693:TRP:H	1.71	0.55
1:A:78:ILE:HB	1:A:393:VAL:HB	1.88	0.55
1:B:195:HIS:NE2	1:B:197:SER:OG	2.39	0.55
1:A:357:LEU:HD22	1:A:377:LEU:HD12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:684:ASN:OD1	1:B:689:ASN:ND2	2.39	0.54
1:A:454:LEU:O	1:A:458:MET:HG2	2.08	0.54
1:B:40:SER:OG	1:B:44:ASP:OD2	2.26	0.54
1:B:191:PRO:HD2	1:B:809:ARG:HG3	1.90	0.54
1:B:575:LYS:HA	1:B:711:ARG:HH12	1.72	0.54
1:A:758:LYS:O	1:A:762:GLN:NE2	2.40	0.54
1:A:665:ARG:HD2	1:A:693:TRP:CE2	2.43	0.53
1:A:32:ILE:HG21	1:A:408:PHE:HB2	1.90	0.53
1:A:362:SER:HA	1:A:377:LEU:HD23	1.90	0.52
1:A:274:VAL:HG21	1:A:385:LEU:HD12	1.90	0.52
1:B:95:ARG:HE	1:B:108:ILE:HG22	1.73	0.52
1:B:23:LEU:HD13	1:B:419:LEU:HD23	1.91	0.52
1:A:473:VAL:HG23	1:A:743:ILE:HD13	1.92	0.52
1:A:539:VAL:HG23	1:A:730:ILE:HB	1.92	0.52
1:A:676:VAL:HG12	1:A:677:PRO:HD2	1.90	0.52
1:B:8:ARG:NH2	1:B:52:GLY:O	2.42	0.51
1:B:818:SER:O	1:B:823:LYS:NZ	2.41	0.51
1:B:525:GLN:HG3	1:B:595:ILE:HD11	1.92	0.51
1:B:755:GLY:O	1:B:758:LYS:NZ	2.44	0.51
1:A:588:CYS:HB2	1:A:674:ALA:HA	1.92	0.51
1:A:133:ASN:HD21	1:A:137:GLU:HB2	1.75	0.50
1:B:75:LYS:HB3	1:B:397:LYS:HD2	1.93	0.50
1:B:248:GLN:HA	1:B:368:LEU:HD11	1.93	0.50
1:A:259:HIS:CD2	1:A:304:ILE:HG12	2.47	0.50
1:B:450:LEU:HD22	1:B:454:LEU:HD12	1.93	0.50
1:B:29:VAL:HG23	1:B:411:GLU:HG2	1.93	0.50
1:B:322:LYS:HD3	1:B:329:ASP:HB3	1.94	0.49
1:B:538:ALA:HB2	1:B:732:THR:HG22	1.93	0.49
1:B:342:LEU:HB2	1:B:350:ALA:HB2	1.94	0.49
1:B:676:VAL:HG12	1:B:677:PRO:O	2.12	0.49
1:B:57:MET:O	1:B:393:VAL:HA	2.12	0.49
1:B:627:ASP:HB3	1:B:630:SER:HB2	1.94	0.49
1:B:603:SER:OG	1:B:803:THR:O	2.31	0.48
1:A:734:GLU:O	1:A:737:ILE:HG12	2.13	0.48
1:B:532:MET:HG2	1:B:817:ILE:HG23	1.95	0.48
1:A:450:LEU:HD23	1:A:454:LEU:HG	1.95	0.48
1:B:361:HIS:HB3	1:B:365:TYR:HD2	1.78	0.48
1:B:579:TRP:HE1	1:B:608:GLN:HE22	1.61	0.48
1:B:624:PRO:HG2	1:B:658:TYR:HA	1.96	0.48
1:A:785:ASP:O	2:A:901:9SL:N15	2.47	0.48
1:B:542:TYR:CZ	1:B:544:ASN:HB3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:641:LYS:O	1:A:642:ASN:ND2	2.47	0.48
1:A:57:MET:O	1:A:393:VAL:HA	2.14	0.48
1:A:195:HIS:HB3	1:A:198:THR:O	2.13	0.47
1:B:140:SER:HB3	1:B:831:VAL:HG13	1.96	0.47
1:B:69:LYS:HE3	1:B:69:LYS:HB2	1.77	0.47
1:A:488:ASP:OD2	1:A:768:LYS:NZ	2.42	0.47
1:A:607:ARG:CZ	1:A:607:ARG:HB2	2.44	0.47
1:A:190:GLU:OE2	1:A:808:SER:HA	2.15	0.47
1:A:603:SER:HB3	1:A:607:ARG:HH22	1.78	0.47
1:B:256:ARG:HG2	1:B:301:VAL:HG23	1.96	0.47
1:B:586:LYS:HB3	1:B:635:LEU:HD11	1.97	0.47
1:B:414:LYS:HB2	1:B:414:LYS:HE3	1.78	0.47
1:B:216:THR:HG21	1:B:222:PRO:HA	1.96	0.46
1:B:94:GLU:HB3	1:B:109:PRO:HG2	1.97	0.46
1:B:93:LYS:O	1:B:97:GLN:HG2	2.15	0.46
1:B:800:TYR:O	1:B:804:VAL:HG22	2.16	0.46
1:A:76:PRO:HA	1:A:394:VAL:HG12	1.97	0.46
1:A:489:TRP:O	1:A:493:SER:HB3	2.16	0.46
1:B:362:SER:HA	1:B:377:LEU:HD13	1.97	0.46
1:A:236:TYR:CE2	1:A:387:THR:HG22	2.51	0.46
1:A:218:PRO:HD3	3:A:1001:HOH:O	2.16	0.46
1:A:477:THR:HG22	1:A:773:LEU:HD21	1.96	0.46
1:B:710:SER:OG	1:B:711:ARG:N	2.49	0.46
1:B:182:GLN:NE2	1:B:194:PHE:H	2.13	0.45
1:B:18:LYS:HA	1:B:18:LYS:HD3	1.79	0.45
1:B:543:HIS:ND1	1:B:777:ASN:OD1	2.49	0.45
1:B:104:ILE:H	1:B:104:ILE:HG13	1.34	0.45
1:B:221:ILE:HD12	1:B:786:ARG:HG3	1.99	0.45
1:B:707:LEU:HD11	1:B:722:LEU:HA	1.99	0.45
1:A:50:LYS:HE3	1:A:50:LYS:HB3	1.82	0.45
1:B:32:ILE:HG21	1:B:408:PHE:HB2	1.99	0.45
1:A:622:CYS:HB2	1:A:635:LEU:HD12	1.99	0.44
1:B:261:GLY:HA2	1:B:305:PRO:HG2	1.99	0.44
1:A:761:PHE:HE2	1:A:763:LEU:HD23	1.82	0.44
1:B:60:ASP:OD1	1:B:61:SER:N	2.51	0.44
1:A:759:ASP:N	1:A:759:ASP:OD1	2.50	0.44
1:B:259:HIS:CD2	1:B:304:ILE:HG12	2.53	0.44
1:B:411:GLU:HG3	1:B:415:ARG:HD2	1.99	0.44
1:B:727:PRO:HD2	2:B:901:9SL:N08	2.33	0.44
1:A:552:LYS:HG3	1:A:553:THR:H	1.81	0.44
1:A:567:VAL:HG12	1:A:721:LYS:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:406:ASN:OD1	1:B:439:LEU:HB2	2.18	0.44
1:B:428:LEU:O	1:B:430:PHE:N	2.51	0.44
1:B:332:TYR:CG	1:B:341:CYS:HB2	2.53	0.43
1:A:8:ARG:HG2	1:A:35:VAL:HB	1.99	0.43
1:B:279:LYS:HE2	1:B:279:LYS:HB3	1.79	0.43
1:A:739:ASP:O	1:A:742:ARG:HB2	2.18	0.43
1:A:540:GLU:HG2	1:A:727:PRO:HG2	2.00	0.43
1:A:377:LEU:HD22	1:A:377:LEU:H	1.83	0.43
1:A:552:LYS:HG3	1:A:553:THR:N	2.34	0.42
1:B:127:GLY:O	1:B:150:ARG:NH2	2.52	0.42
1:B:162:LEU:HD13	1:B:187:GLY:HA2	2.00	0.42
1:A:484:MET:HE3	1:A:768:LYS:HD2	2.00	0.42
1:B:532:MET:HA	1:B:532:MET:HE3	2.00	0.42
1:B:592:VAL:HG23	1:B:598:TRP:CE2	2.54	0.42
1:A:322:LYS:HD2	1:A:329:ASP:HB3	2.02	0.42
1:B:200:TYR:CD1	1:B:217:PRO:HA	2.55	0.42
1:A:76:PRO:HB3	1:A:392:THR:HG21	2.01	0.42
1:A:79:ALA:HB3	1:A:440:LEU:HD21	2.02	0.42
1:B:135:MET:HB3	1:B:232:THR:HG21	2.01	0.42
1:B:538:ALA:N	1:B:730:ILE:O	2.53	0.42
1:B:63:GLU:HG2	1:B:263:SER:HB2	2.02	0.42
1:B:480:LYS:O	1:B:484:MET:HG3	2.19	0.42
1:A:577:ILE:HG22	1:A:705:LEU:HD11	2.01	0.42
1:A:198:THR:O	1:A:200:TYR:N	2.53	0.42
1:A:772:LEU:O	1:A:774:PHE:N	2.47	0.41
1:B:164:GLU:OE1	1:B:189:TYR:OH	2.22	0.41
1:A:205:ASN:N	1:A:209:GLU:O	2.45	0.41
1:B:89:GLN:HB3	1:B:92:LEU:HD12	2.02	0.41
1:B:804:VAL:HG23	1:B:805:TYR:CD2	2.56	0.41
1:A:532:MET:HE2	1:A:792:MET:HE1	2.02	0.41
1:A:692:VAL:HG22	1:A:693:TRP:N	2.35	0.41
1:A:569:LEU:HD12	1:A:703:GLU:O	2.21	0.41
1:B:536:LEU:HD22	1:B:791:ILE:HG12	2.02	0.41
1:A:69:LYS:HB3	1:A:69:LYS:HE3	1.94	0.40
1:B:477:THR:HG22	1:B:773:LEU:HD21	2.03	0.40
1:A:166:GLN:HG2	1:A:167:VAL:H	1.85	0.40
1:A:737:ILE:HG13	1:A:738:SER:N	2.37	0.40
1:B:84:SER:C	1:B:86:ARG:H	2.30	0.40
1:B:224:THR:HG21	1:B:536:LEU:HD21	2.03	0.40
1:B:406:ASN:O	1:B:410:MET:HG2	2.22	0.40
1:B:667:LEU:HB2	1:B:674:ALA:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:584:GLY:N	1:B:617:PHE:O	2.53	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	814/851 (96%)	771 (95%)	40 (5%)	3 (0%)	30	51
1	B	814/851 (96%)	764 (94%)	49 (6%)	1 (0%)	48	70
All	All	1628/1702 (96%)	1535 (94%)	89 (6%)	4 (0%)	43	66

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	692	VAL
1	A	199	GLY
1	B	429	MET
1	A	639	ASP

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	703/728 (97%)	685 (97%)	18 (3%)	40	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	703/728 (97%)	686 (98%)	17 (2%)	43 70
All	All	1406/1456 (97%)	1371 (98%)	35 (2%)	42 69

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	VAL
1	A	221	ILE
1	A	284	ASP
1	A	352	LEU
1	A	363	GLU
1	A	367	LEU
1	A	452	VAL
1	A	561	PHE
1	A	586	LYS
1	A	607	ARG
1	A	649	CYS
1	A	676	VAL
1	A	681	VAL
1	A	685	THR
1	A	743	ILE
1	A	748	GLN
1	A	785	ASP
1	A	827	ASN
1	B	29	VAL
1	B	34	LEU
1	B	94	GLU
1	B	104	ILE
1	B	158	LEU
1	B	252	LEU
1	B	301	VAL
1	B	452	VAL
1	B	454	LEU
1	B	524	VAL
1	B	561	PHE
1	B	615	ASP
1	B	704	LEU
1	B	757	GLU
1	B	825	CYS
1	B	830	GLU
1	B	831	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	HIS
1	A	148	GLN
1	A	192	GLN
1	A	235	HIS
1	A	315	GLN
1	A	335	ASN
1	A	378	ASN
1	A	580	ASN
1	A	642	ASN
1	B	21	ASN
1	B	89	GLN
1	B	128	HIS
1	B	188	ASN
1	B	248	GLN
1	B	309	GLN
1	B	608	GLN
1	B	696	ASN
1	B	787	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no 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	B	901	-	17,23,23	3.46	8 (47%)	14,37,37	2.92	7 (50%)
2	9SL	A	901	1	17,23,23	3.50	8 (47%)	14,37,37	2.92	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	B	901	-	-	2/5/53/53	0/3/3/3
2	9SL	A	901	1	-	4/5/53/53	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	9SL	C12-N13	6.98	1.46	1.35
2	A	901	9SL	C12-N13	6.97	1.46	1.35
2	B	901	9SL	C02-N21	6.75	1.45	1.33
2	A	901	9SL	C07-N08	6.67	1.45	1.34
2	A	901	9SL	C02-N21	6.66	1.45	1.33
2	B	901	9SL	C07-N08	6.43	1.45	1.34
2	A	901	9SL	C12-N15	4.83	1.45	1.34
2	B	901	9SL	C12-N15	4.77	1.45	1.34
2	A	901	9SL	C05-C14	3.47	1.59	1.52
2	B	901	9SL	C05-C14	3.37	1.59	1.52
2	B	901	9SL	O03-C02	3.37	1.40	1.35
2	A	901	9SL	O03-C02	3.26	1.40	1.35
2	A	901	9SL	C07-N09	2.55	1.40	1.35
2	B	901	9SL	C07-N09	2.11	1.39	1.35
2	A	901	9SL	O03-C04	-2.06	1.40	1.45
2	B	901	9SL	O03-C04	-2.05	1.40	1.45

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	9SL	O03-C02-N21	7.32	120.21	111.11
2	B	901	9SL	O03-C02-N21	7.28	120.17	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	9SL	N09-C07-N06	-4.21	119.56	125.42
2	B	901	9SL	N09-C07-N06	-4.14	119.66	125.42
2	A	901	9SL	O03-C02-O01	-3.59	119.77	123.08
2	B	901	9SL	O01-C02-N21	-3.53	120.00	125.58
2	B	901	9SL	O03-C02-O01	-3.53	119.83	123.08
2	A	901	9SL	O01-C02-N21	-3.52	120.02	125.58
2	A	901	9SL	C14-C05-N06	2.89	119.09	111.22
2	B	901	9SL	C14-C05-N06	2.87	119.04	111.22
2	A	901	9SL	C19-C20-N09	-2.38	101.19	103.81
2	B	901	9SL	C19-C20-N09	-2.30	101.28	103.81
2	B	901	9SL	C14-N13-C12	-2.05	105.42	109.36

There are no chirality outliers.

All (6) torsion outliers are listed below:

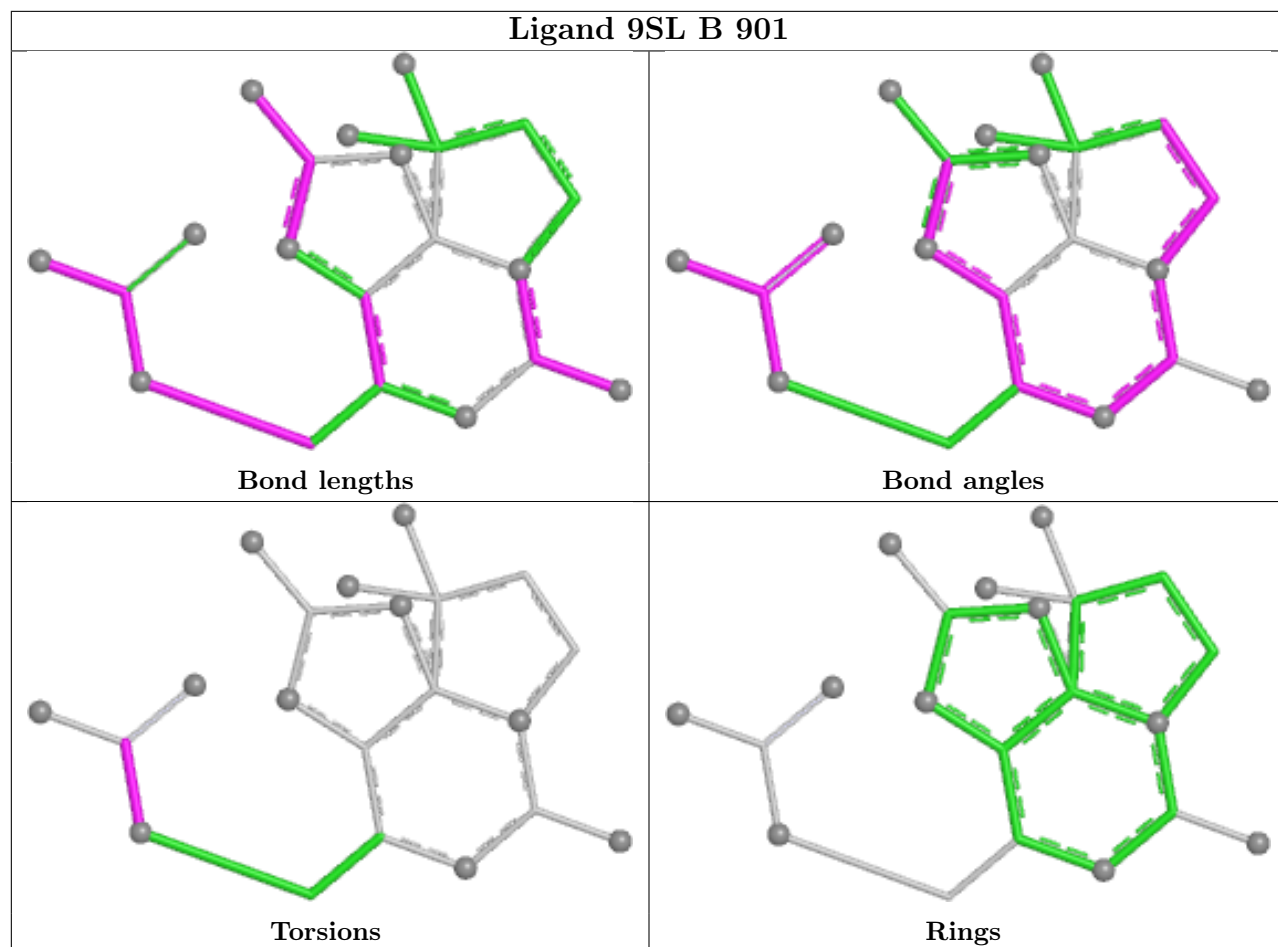
Mol	Chain	Res	Type	Atoms
2	A	901	9SL	O01-C02-O03-C04
2	A	901	9SL	N21-C02-O03-C04
2	A	901	9SL	O03-C04-C05-N06
2	A	901	9SL	O03-C04-C05-C14
2	B	901	9SL	O01-C02-O03-C04
2	B	901	9SL	N21-C02-O03-C04

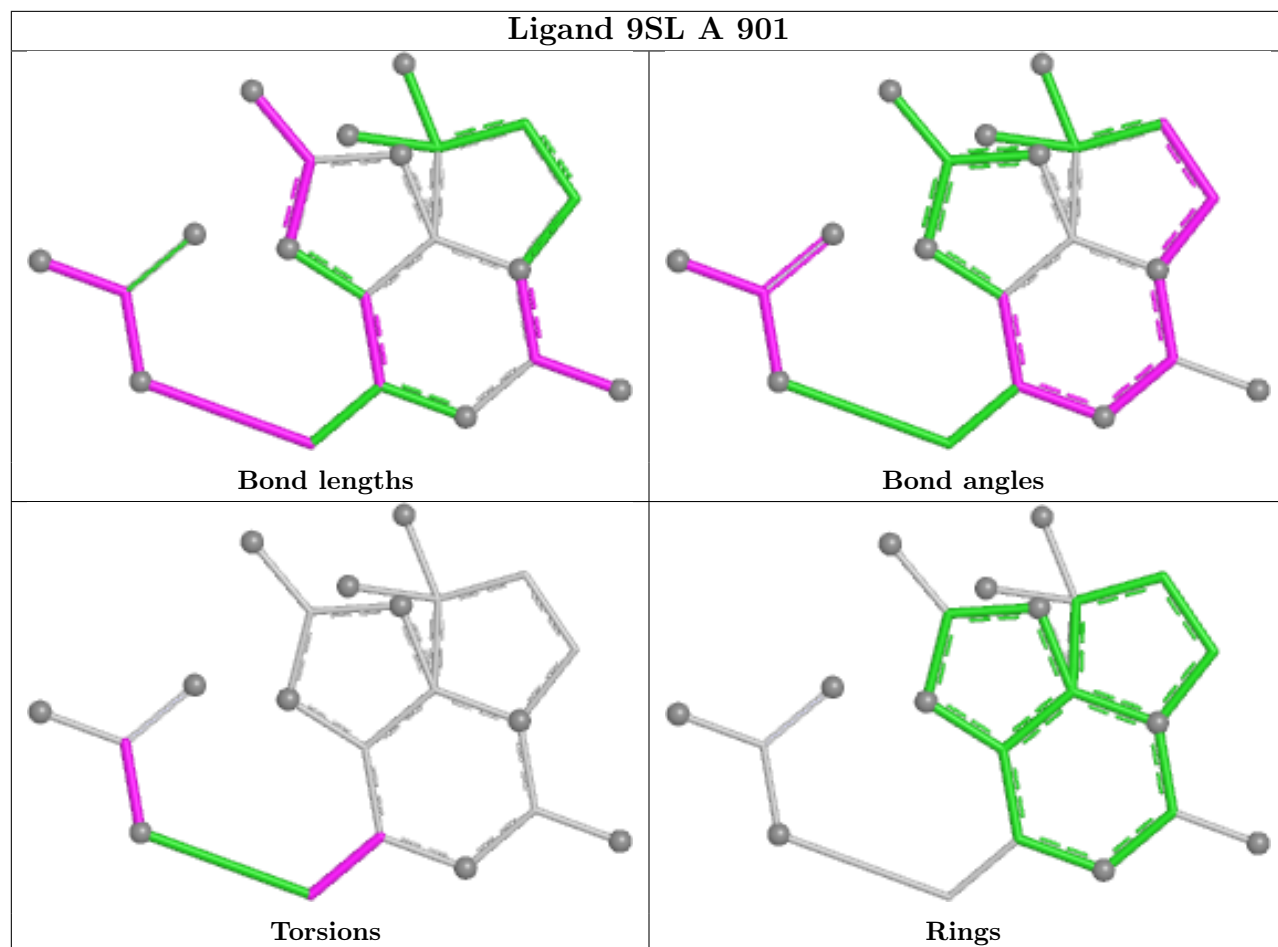
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	901	9SL	2	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	818/851 (96%)	0.37	35 (4%) 40 34	80, 120, 202, 248	0
1	B	818/851 (96%)	0.38	22 (2%) 56 50	84, 129, 208, 256	0
All	All	1636/1702 (96%)	0.37	57 (3%) 47 41	80, 126, 206, 256	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	832	LEU	5.4
1	A	674	ALA	5.0
1	B	664	PHE	4.7
1	B	831	VAL	4.6
1	B	832	LEU	4.4
1	B	613	ASP	4.2
1	A	162	LEU	4.1
1	B	168	ALA	4.1
1	B	207	ILE	4.1
1	B	674	ALA	4.0
1	B	614	ILE	3.8
1	A	569	LEU	3.8
1	A	664	PHE	3.7
1	A	570	VAL	3.4
1	A	5	LYS	3.3
1	A	684	ASN	3.0
1	B	179	PHE	2.9
1	A	588	CYS	2.9
1	A	637	ILE	2.9
1	A	206	ALA	2.9
1	A	291	ILE	2.9
1	A	663	ALA	2.8
1	B	830	GLU	2.8
1	A	221	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	224	THR	2.7
1	A	746	ASN	2.6
1	B	668	VAL	2.6
1	A	829	LEU	2.5
1	A	262	VAL	2.5
1	A	729	ALA	2.5
1	A	643	SER	2.5
1	B	95	ARG	2.5
1	A	186	LYS	2.5
1	A	585	LYS	2.5
1	B	99	LEU	2.5
1	A	168	ALA	2.5
1	A	564	LEU	2.4
1	A	673	VAL	2.4
1	A	804	VAL	2.4
1	A	731	VAL	2.4
1	A	63	GLU	2.3
1	B	117	TYR	2.3
1	A	475	TRP	2.3
1	A	657	TYR	2.2
1	A	800	TYR	2.2
1	B	223	ALA	2.2
1	A	538	ALA	2.2
1	A	744	VAL	2.2
1	A	522	LEU	2.1
1	B	429	MET	2.1
1	A	675	PHE	2.1
1	B	829	LEU	2.1
1	B	229	ASP	2.1
1	A	492	VAL	2.0
1	B	538	ALA	2.0
1	B	534	GLY	2.0
1	B	791	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

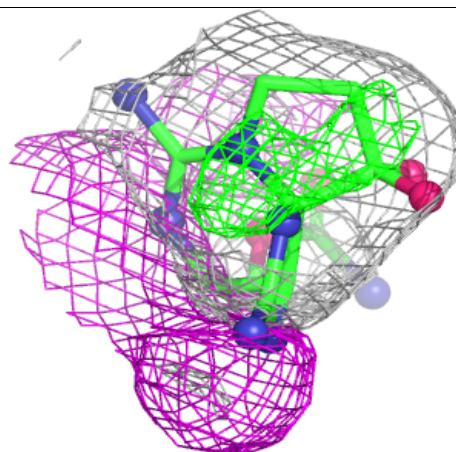
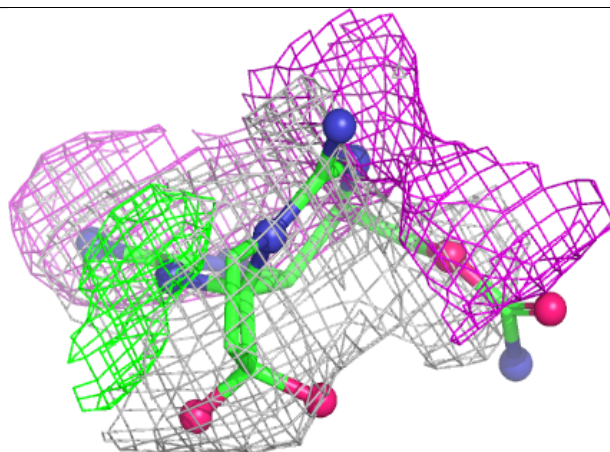
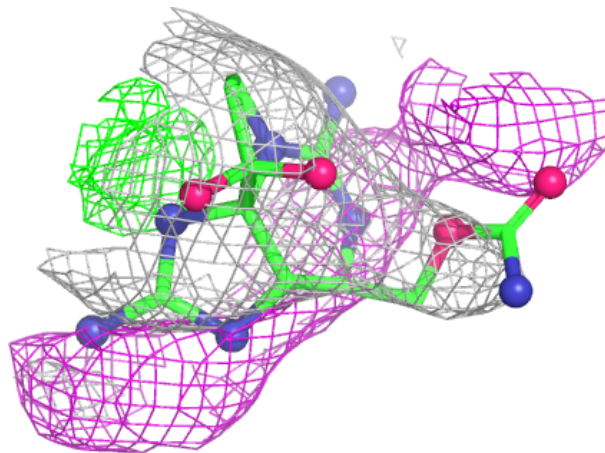
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	0.61	0.15	177,196,207,215	0
2	9SL	B	901	21/21	0.91	0.10	116,147,157,158	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

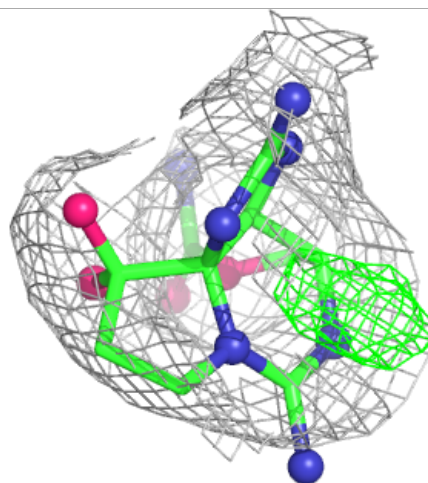
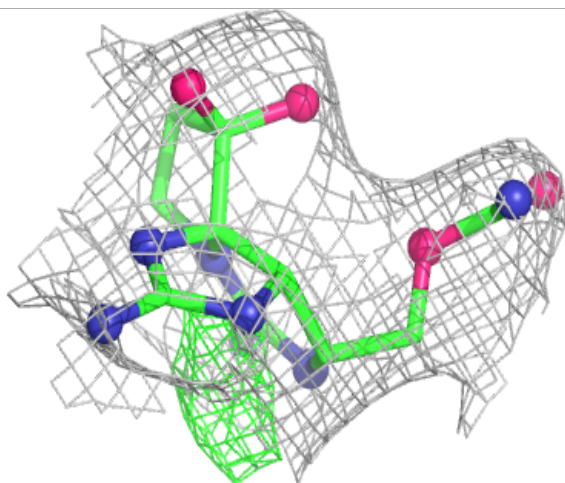
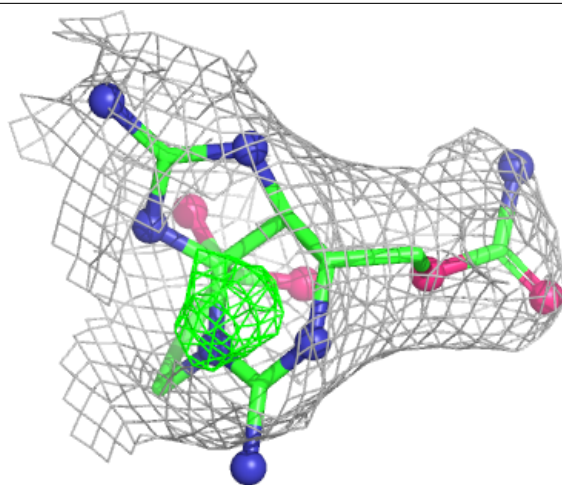
Electron density around 9SL A 901:

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



Electron density around 9SL B 901:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.