Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 06:46 pm BST

PDB ID	:	6O0F
Title	:	Saxiphilin:STX complex, co-crystal
Authors	:	Yen, T.J.; Lolicato, M.; Minor, D.L.
Deposited on	:	2019-02-16
Resolution	:	2.12 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

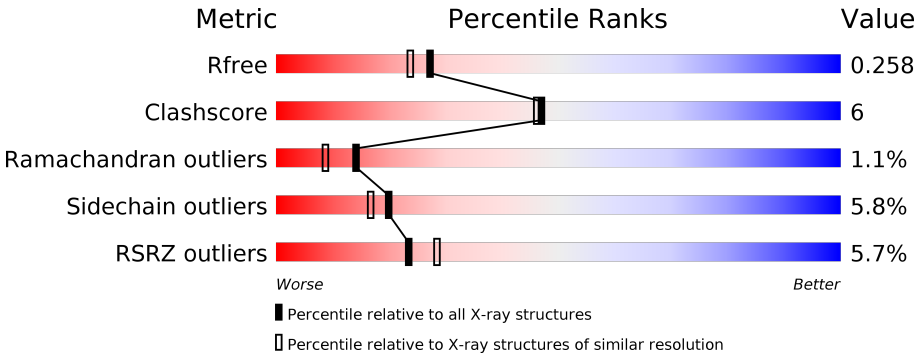
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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}	130704	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (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 on 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 <=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	8% 76% 17% • 5%
1	B	853	3% 82% 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.

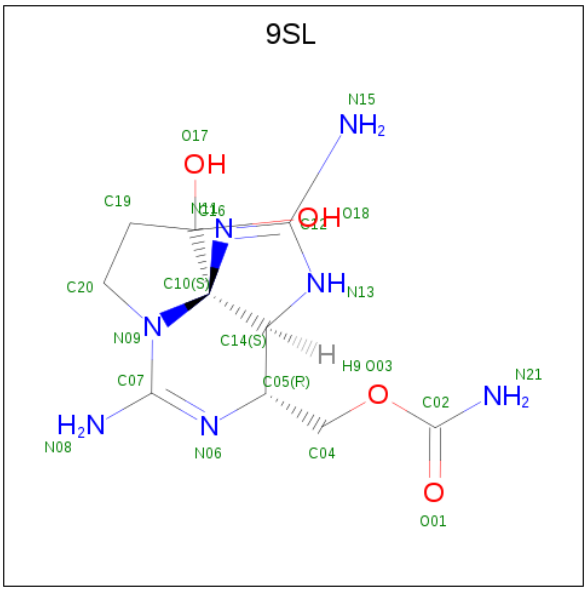
- Molecule 1 is a protein called Saxiphilin.

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 (three-letter code: 9SL) (formula: $C_{10}H_{17}N_7O_4$).



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

- Molecule 3 is water.

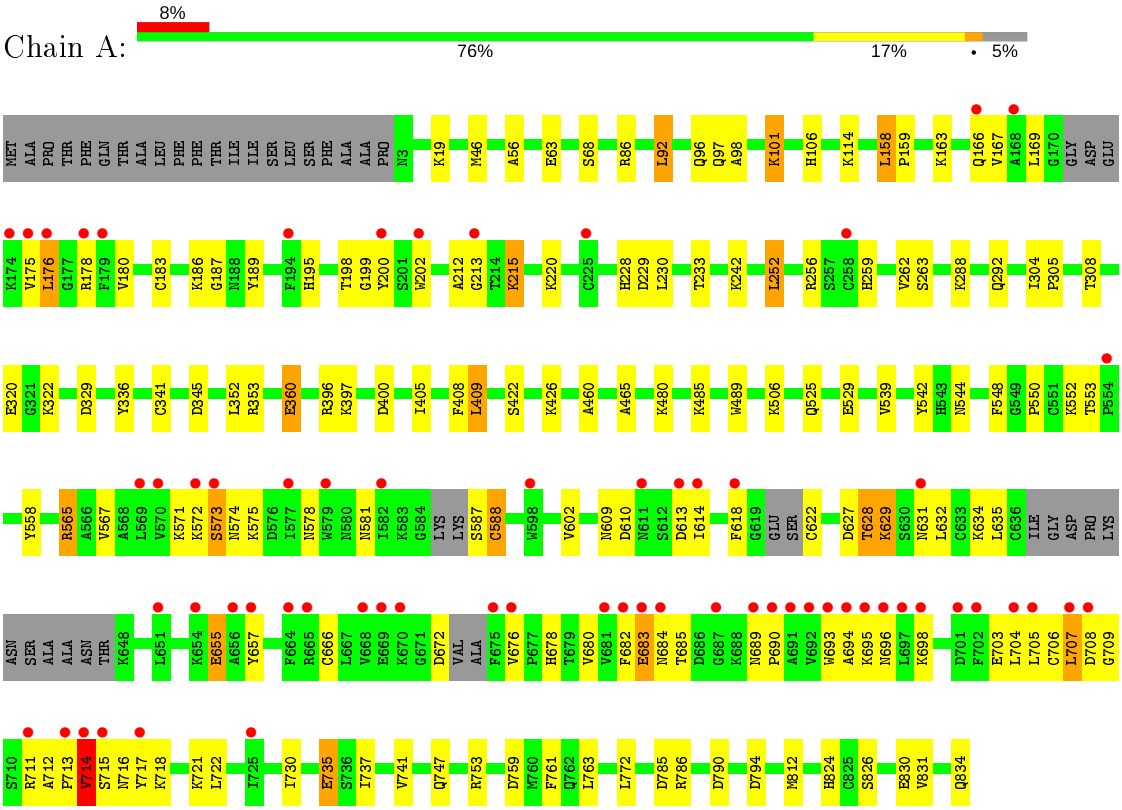
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	102	Total O 102 102	0	0
3	B	93	Total O 93 93	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

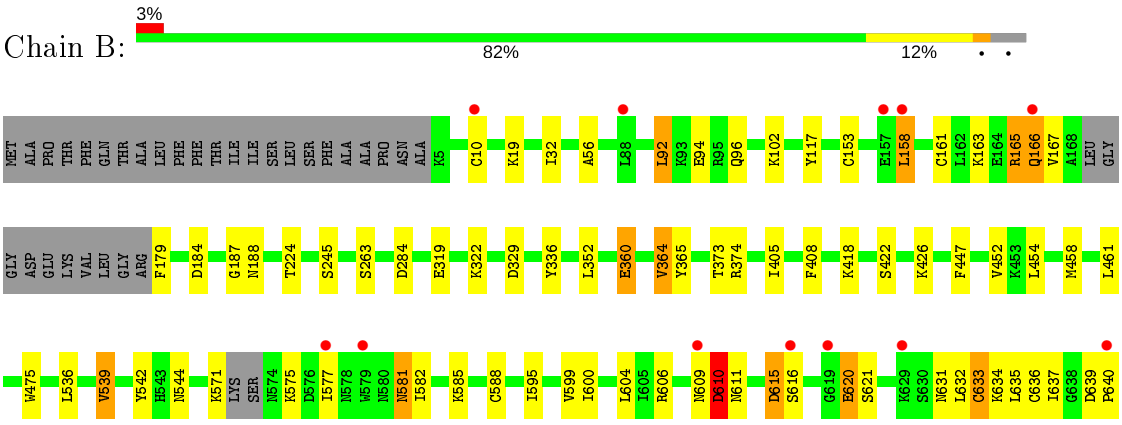
- Molecule 1: Saxiphilin

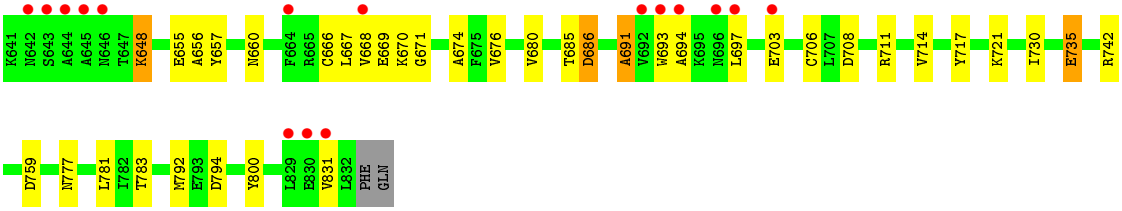
Chain A:



- Molecule 1: Saxiphilin

Chain B:




K641
N642
S643
A644
A645
N646
T647
K648
E655
A656
Y657
N660
F664
R665
C666
L667
V668
E669
K670
G671
A674
F675
V676
V680
T685
D686
A691
V692
W693
A694
K695
N696
L697
E703
C706
L707
D708
R711
V714
Y717
K721
I730
E735
R742
D759
N777
L781
I782
T783
M792
E793
D794
V800
L829
E830
V831
L832
PHE
GLN

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.17 (at 2.12Å)	Xtriage
Refinement program	PHENIX (1.12_2829)	Depositor
R, R_{free}	0.238 , 0.259 0.237 , 0.258	Depositor DCC
R_{free} test set	7795 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	50.6	Xtriage
Anisotropy	0.575	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 54.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.25	0/6401	0.47	0/8631
1	B	0.25	0/6425	0.47	1/8671 (0.0%)
All	All	0.25	0/12826	0.47	1/17302 (0.0%)

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

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

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

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	610	ASP	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6279	0	6145	88	0
1	B	6300	0	6162	67	0
2	A	21	0	0	1	0
2	B	21	0	0	1	0
3	A	102	0	0	0	0
3	B	93	0	0	2	0
All	All	12816	0	12307	155	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (155) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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

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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:TYR:CZ	1:A:426:LYS:HD3	2.55	0.41
1:A:63:GLU:HG2	1:A:263:SER:HB2	2.03	0.41
1:A:288:LYS:HD2	1:A:288:LYS:N	2.36	0.41
1:B:632:LEU:O	1:B:633:CYS:CB	2.68	0.40
1:B:360:GLU:HG3	1:B:360:GLU:H	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

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	800/853 (94%)	761 (95%)	29 (4%)	10 (1%)	12 7
1	B	810/853 (95%)	774 (96%)	29 (4%)	7 (1%)	17 12
All	All	1610/1706 (94%)	1535 (95%)	58 (4%)	17 (1%)	14 9

All (17) Ramachandran outliers are listed below:

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

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

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	699/731 (96%)	653 (93%)	46 (7%)	16	13
1	B	702/731 (96%)	667 (95%)	35 (5%)	24	22
All	All	1401/1462 (96%)	1320 (94%)	81 (6%)	20	17

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

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

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

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

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

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

5.3.3 RNA (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 carbohydrates 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	6.11	11 (64%)	13,37,37	3.40	8 (61%)
2	9SL	A	901	1	17,23,23	6.17	11 (64%)	13,37,37	3.47	8 (61%)

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	-	2/5/53/53	0/3/3/3

All (22) 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	-10.72	1.34	1.47
2	B	901	9SL	C20-N09	-10.24	1.34	1.47
2	B	901	9SL	C19-C20	-8.20	1.37	1.52
2	A	901	9SL	C19-C20	-8.10	1.37	1.52
2	A	901	9SL	C07-N08	7.25	1.47	1.34
2	B	901	9SL	C07-N08	7.22	1.47	1.34
2	B	901	9SL	C02-N21	7.07	1.46	1.33
2	A	901	9SL	C02-N21	7.04	1.46	1.33
2	A	901	9SL	C12-N15	6.04	1.48	1.34
2	B	901	9SL	C12-N15	5.35	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	4.15	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	9SL	O03-C02	3.98	1.41	1.35
2	B	901	9SL	C05-C14	3.20	1.59	1.52
2	A	901	9SL	C05-C14	3.06	1.59	1.52
2	A	901	9SL	C05-N06	-2.62	1.43	1.47
2	B	901	9SL	C05-N06	-2.60	1.43	1.47
2	A	901	9SL	O01-C02	-2.22	1.18	1.21
2	B	901	9SL	O01-C02	-2.12	1.19	1.21

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	901	9SL	O03-C02-N21	7.31	120.16	111.08
2	B	901	9SL	O03-C02-N21	7.27	120.11	111.08
2	A	901	9SL	C19-C20-N09	5.21	109.72	103.83
2	B	901	9SL	C19-C20-N09	4.96	109.44	103.83
2	A	901	9SL	N13-C12-N11	-4.33	104.48	115.45
2	B	901	9SL	C04-C05-N06	-3.83	102.72	108.57
2	B	901	9SL	O03-C02-O01	-3.83	119.45	123.07
2	B	901	9SL	N13-C12-N11	-3.74	105.97	115.45
2	A	901	9SL	O03-C02-O01	-3.50	119.76	123.07
2	A	901	9SL	O01-C02-N21	-3.30	120.07	125.51
2	A	901	9SL	C04-C05-N06	-3.23	103.63	108.57
2	B	901	9SL	O01-C02-N21	-3.08	120.43	125.51
2	A	901	9SL	N15-C12-N11	3.02	130.06	125.35
2	B	901	9SL	N15-C12-N13	3.01	127.35	122.64
2	A	901	9SL	N09-C07-N06	-2.95	121.31	125.42
2	B	901	9SL	N09-C07-N06	-2.59	121.82	125.42

There are no chirality outliers.

All (4) torsion outliers are listed below:

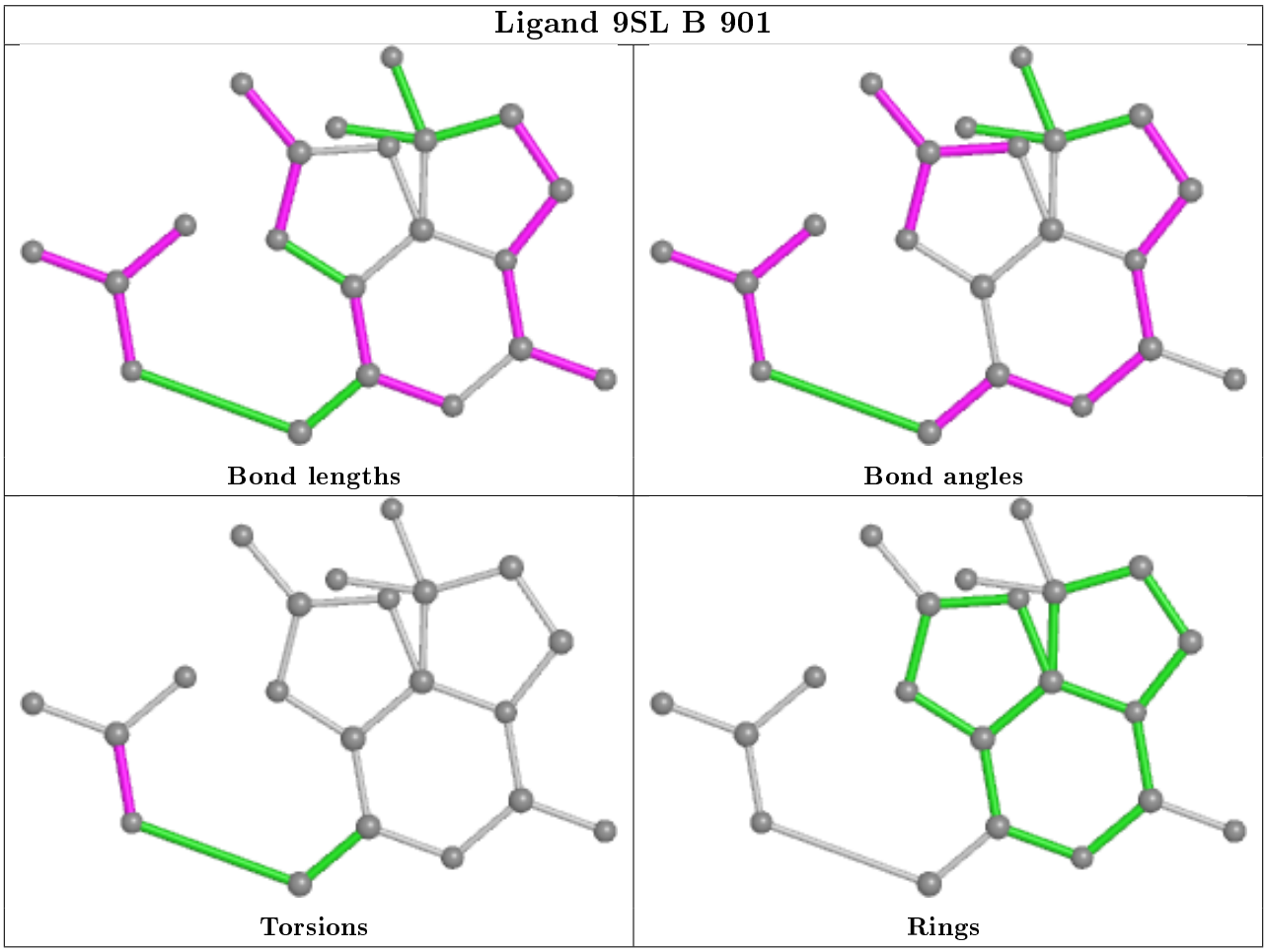
Mol	Chain	Res	Type	Atoms
2	B	901	9SL	O01-C02-O03-C04
2	B	901	9SL	N21-C02-O03-C04
2	A	901	9SL	O01-C02-O03-C04
2	A	901	9SL	N21-C02-O03-C04

There are no ring outliers.

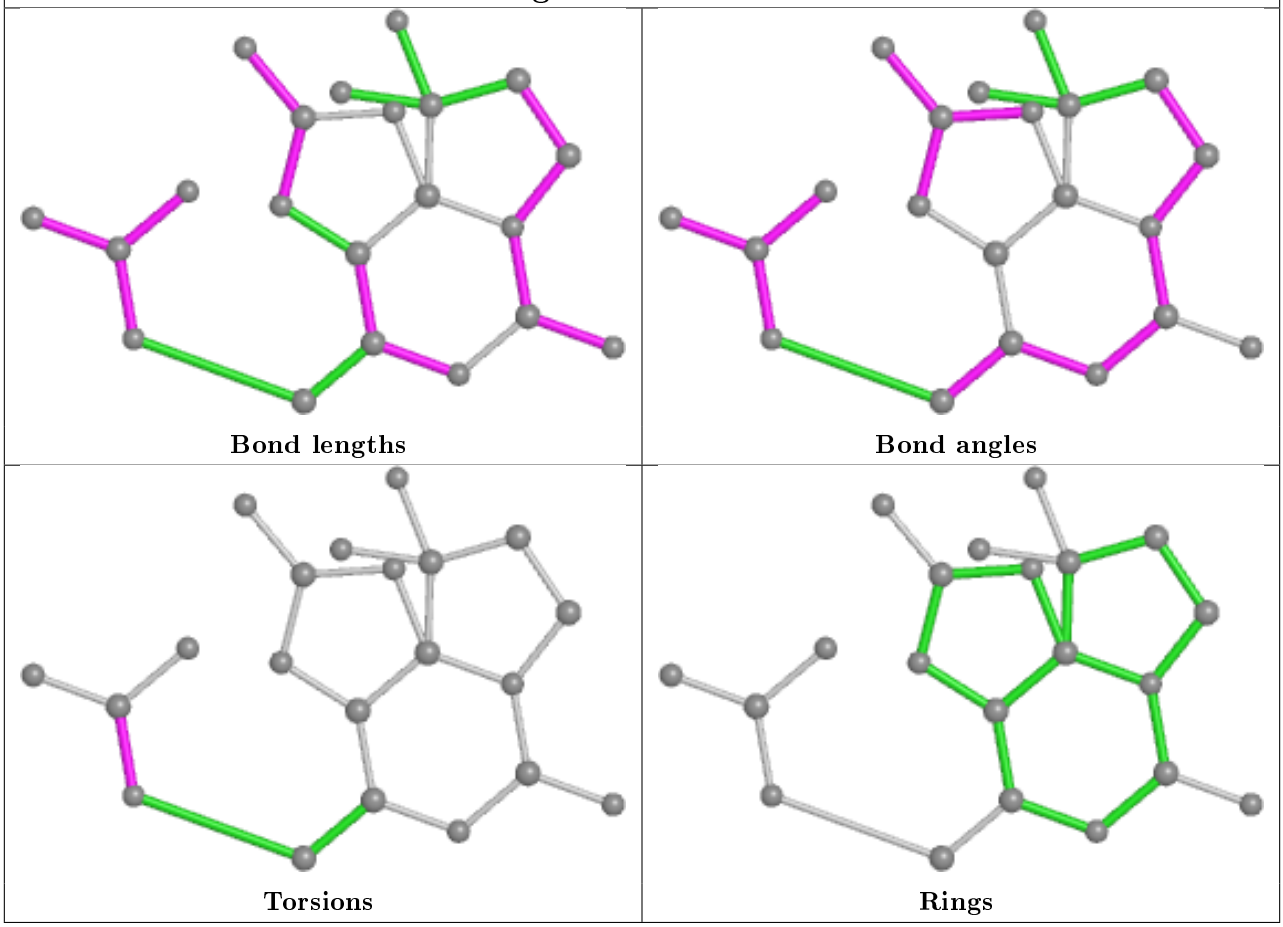
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	901	9SL	1	0
2	A	901	9SL	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.



Ligand 9SL A 901



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	812/853 (95%)	0.43	65 (8%)	12	15	48, 81, 173, 227	0
1	B	816/853 (95%)	0.28	28 (3%)	45	51	51, 83, 153, 244	0
All	All	1628/1706 (95%)	0.35	93 (5%)	23	28	48, 82, 168, 244	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	644	ALA	9.9
1	A	691	ALA	8.4
1	A	690	PRO	6.9
1	B	88	LEU	6.5
1	B	643	SER	6.3
1	A	694	ALA	6.2
1	B	642	ASN	6.1
1	A	697	LEU	6.0
1	A	614	ILE	5.9
1	A	670	LYS	5.7
1	A	693	TRP	5.6
1	A	664	PHE	5.6
1	A	702	PHE	5.0
1	A	582	ILE	5.0
1	A	692	VAL	4.8
1	B	692	VAL	4.7
1	A	569	LEU	4.6
1	A	704	LEU	4.6
1	A	175	VAL	4.6
1	A	579	TRP	4.6
1	A	687	GLY	4.5
1	B	668	VAL	4.5
1	A	714	VAL	4.4
1	A	174	LYS	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	694	ALA	4.1
1	A	701	ASP	4.0
1	A	711	ARG	4.0
1	B	829	LEU	3.9
1	A	577	ILE	3.9
1	A	705	LEU	3.8
1	B	645	ALA	3.8
1	B	693	TRP	3.8
1	A	573	SER	3.8
1	A	684	ASN	3.7
1	A	657	TYR	3.6
1	A	202	TRP	3.5
1	A	572	LYS	3.4
1	A	168	ALA	3.4
1	B	158	LEU	3.4
1	B	619	GLY	3.3
1	A	651	LEU	3.3
1	B	640	PRO	3.2
1	B	831	VAL	3.2
1	A	554	PRO	3.1
1	A	676	VAL	3.1
1	A	194	PHE	3.1
1	B	830	GLU	3.1
1	A	176	LEU	3.1
1	A	689	ASN	3.0
1	A	618	PHE	3.0
1	A	683	GLU	3.0
1	A	698	LYS	3.0
1	A	668	VAL	2.9
1	A	713	PRO	2.9
1	B	10	CYS	2.9
1	A	179	PHE	2.9
1	A	675	PHE	2.9
1	B	629	LYS	2.9
1	A	681	VAL	2.8
1	A	200	TYR	2.8
1	B	157	GLU	2.8
1	B	577	ILE	2.7
1	A	656	ALA	2.6
1	B	703	GLU	2.6
1	A	695	LYS	2.6
1	B	696	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	707	LEU	2.6
1	A	696	ASN	2.6
1	A	166	GLN	2.6
1	A	611	ASN	2.5
1	A	225	CYS	2.4
1	A	598	TRP	2.4
1	B	616	SER	2.4
1	A	570	VAL	2.4
1	B	166	GLN	2.4
1	A	654	LYS	2.4
1	A	631	ASN	2.3
1	B	609	ASN	2.3
1	A	682	PHE	2.2
1	B	697	LEU	2.2
1	A	725	ILE	2.2
1	A	717	TYR	2.2
1	B	646	ASN	2.2
1	A	213	GLY	2.2
1	A	708	ASP	2.1
1	A	665	ARG	2.1
1	A	669	GLU	2.1
1	A	258	CYS	2.1
1	A	715	SER	2.1
1	A	178	ARG	2.1
1	B	664	PHE	2.0
1	A	613	ASP	2.0
1	B	579	TRP	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 carbohydrates 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,

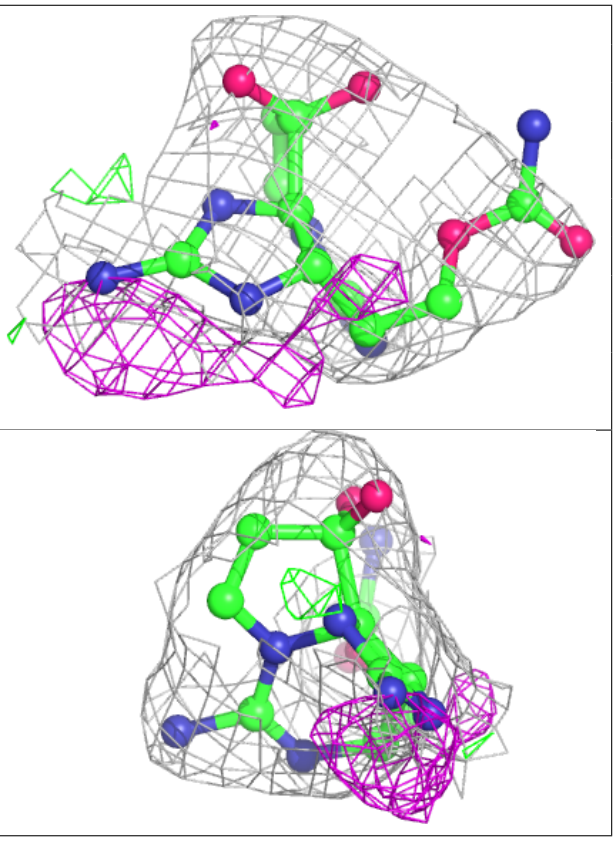
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	9SL	A	901	21/21	0.87	0.16	90,110,127,130	0
2	9SL	B	901	21/21	0.93	0.15	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.

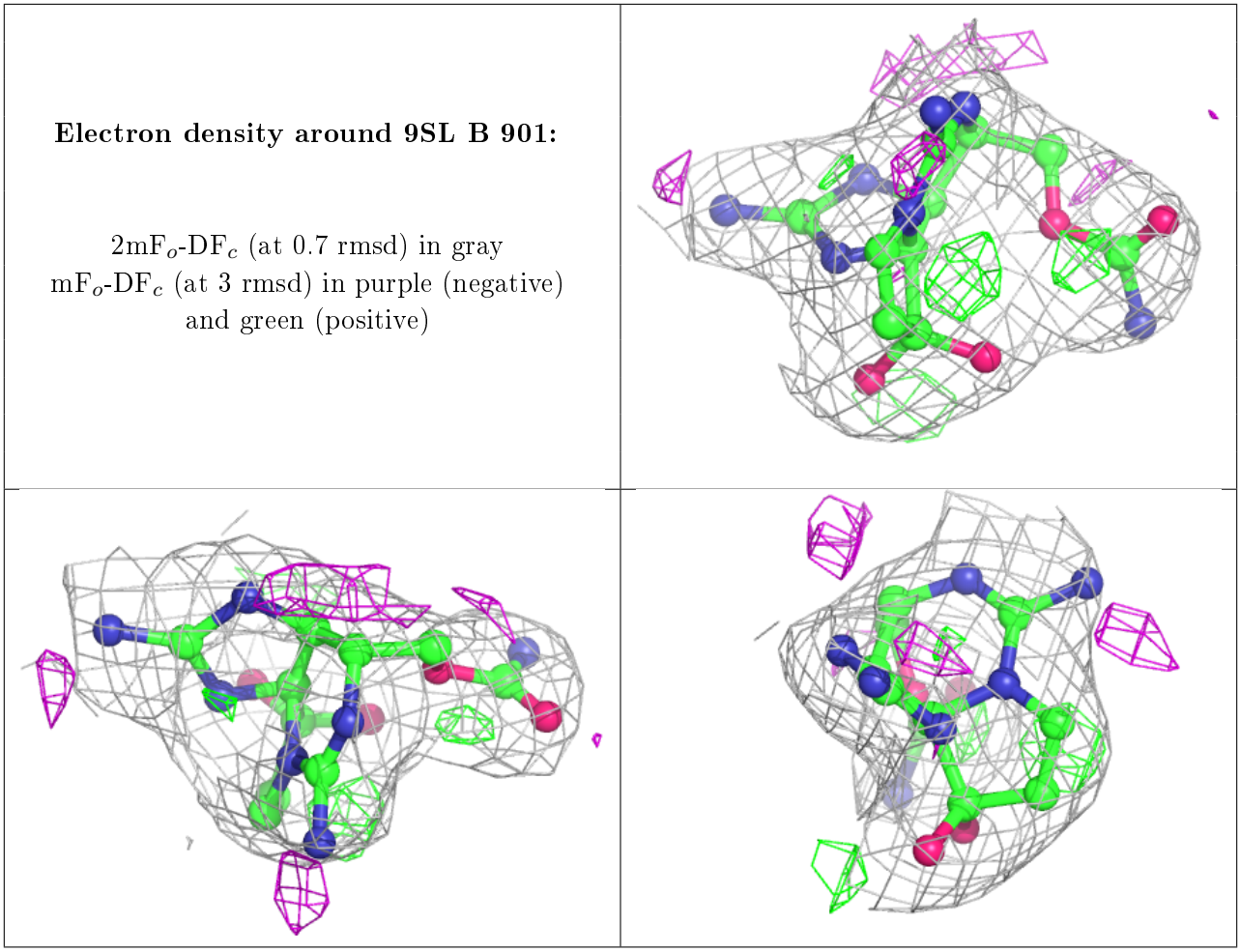
Electron density around 9SL A 901:

$2mF_o$-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.