Full wwPDB X-ray Structure Validation Report (i)

Jun 25, 2024 – 02:56 AM EDT

PDB ID	:	6O0E
Title	:	Saxiphilin:STX complex, soaking
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Deposited on	:	2019-02-16
Resolution	:	2.50 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 (i) 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 (i)) were used in the production of this report:

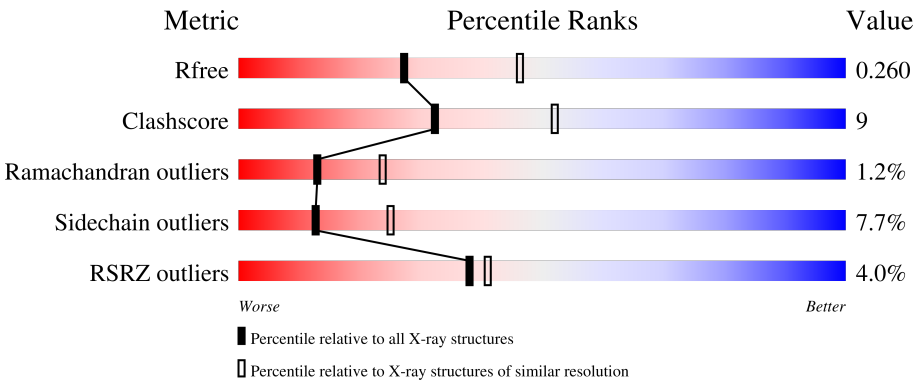
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 <=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	5% 68% 21% • 6%
1	B	853	2% 75% 18% • •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 12541 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.

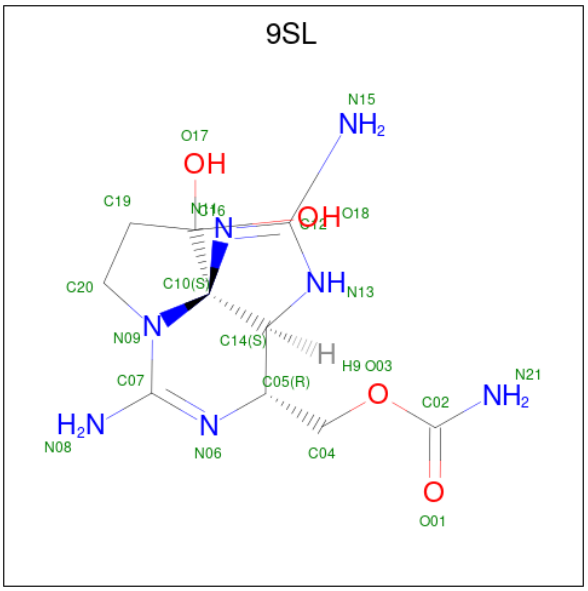
- Molecule 1 is a protein called Saxiphilin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	799	6169	3856	1065	1189	59	0	0	0
1	B	815	6289	3927	1086	1217	59	0	0	0

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
			Total	C	N	O		
2	A	1	21	10	7	4	0	0
			Total	C	N	O		
2	B	1	21	10	7	4	0	0

- Molecule 3 is water.

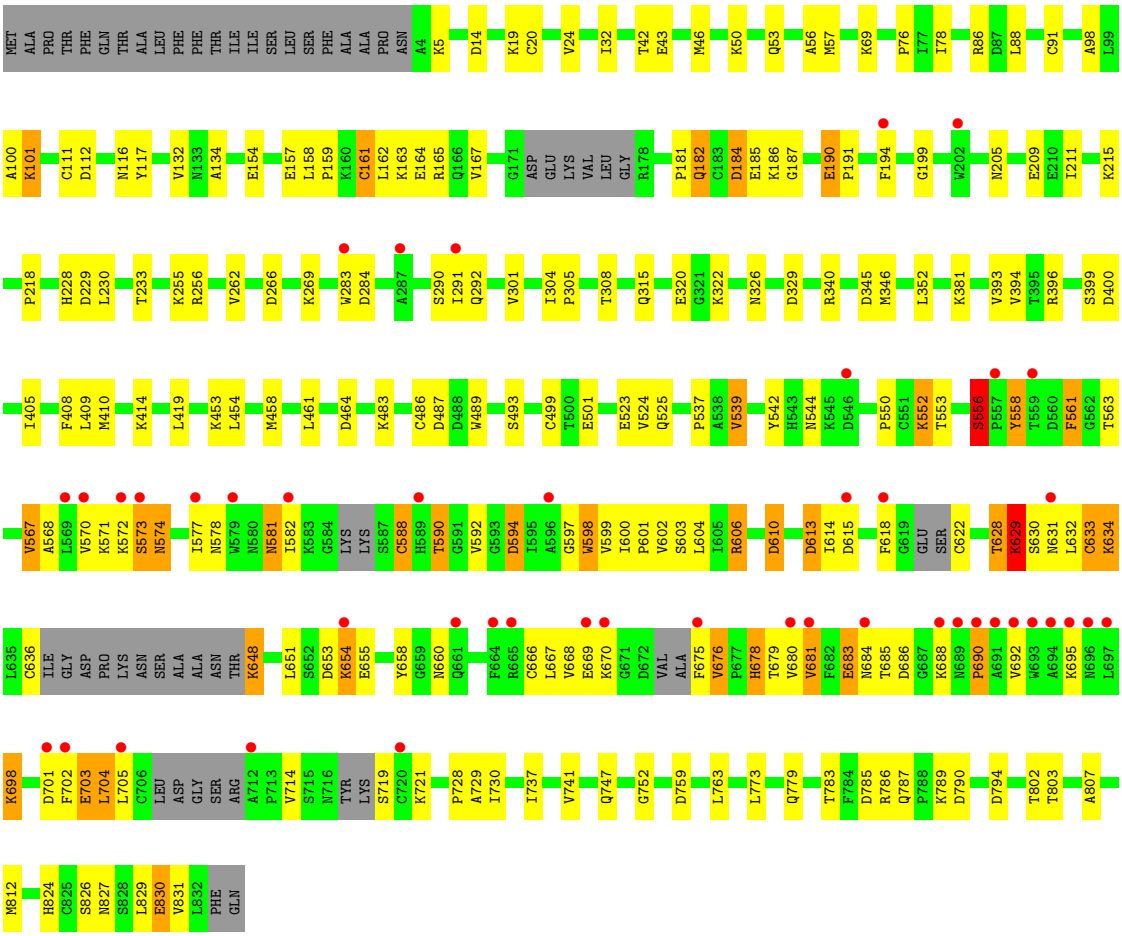
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	24	24	24	0	0
			Total	O		
3	B	17	17	17	0	0

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.

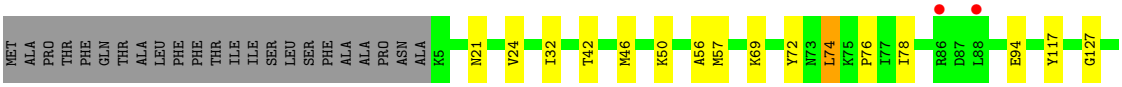
- Molecule 1: Saxiphilin

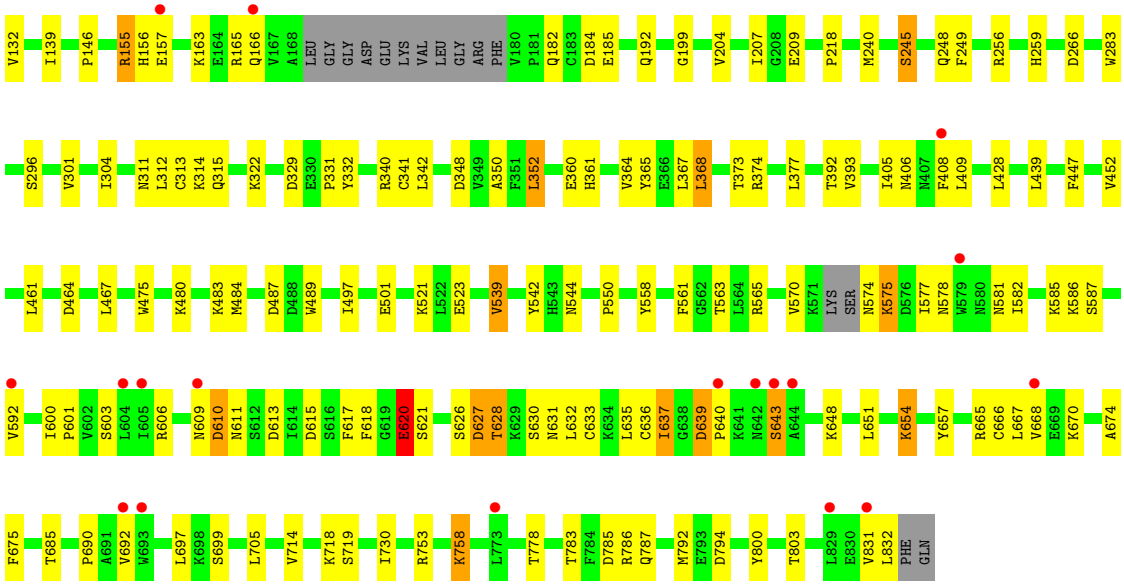
Chain A:



- Molecule 1: Saxiphilin

Chain B:




V132 I139 P146 R155 H156 E157 K163 E164 R165 Q166 V167 A168 LEU GLY GLY ASP GLU LYS VAL LEU GLY ARG PHE V180 P181 Q182 C183 D184 E185 Q192 G199 V204 I207 G208 E209 P218 M240 S245 Q248 F249 R256 H259 D266 W283
S296 V301 I304 N311 L312 C313 K314 Q315 K322 D329 E330 P331 Y332 R340 C341 L342 D348 V349 A350 F351 L352 E360 H361 V364 Y365 E366 L367 L368 T373 R374 L377 T392 V393 I405 N406 M407 F408 L409 L428 L439 F447 V452
L461 D464 L467 W475 K480 K483 M484 D487 D488 W489 I497 E501 K521 L522 E523 V539 Y542 H543 N544 P550 Y558 F561 G562 T563 L564 R565 V570 K571 LYS SER N574 K576 D576 I577 N578 W579 N580 N581 I582 K585 K586 S587
V592 I600 P601 V602 S603 L604 I605 R606 N609 D610 N611 S612 D613 I614 D615 S616 F617 F618 G619 E620 S621 S626 D627 T628 K629 S630 N631 L632 C633 K634 L635 C636 I637 G638 D639 P640 K641 N642 S643 A644 K648 L651 K654 Y657 R665 C666 L667 V668 E669 K670 A674
F675 T685 P690 A691 V692 W693 L697 K698 S699 L705 V714 K718 S719 I730 R753 K758 L773 T778 T783 F784 D785 R786 Q787 M792 E793 D794 Y800 T803 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	96.38Å 110.76Å 254.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.19 – 2.50 48.19 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.19-2.50) 99.6 (48.19-2.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.30 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.12_2829)	Depositor
R, R_{free}	0.237 , 0.262 0.234 , 0.260	Depositor DCC
R_{free} test set	4702 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	62.7	Xtriage
Anisotropy	0.694	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 58.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12541	wwPDB-VP
Average B, all atoms (Å^2)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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 (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	0.27	0/6287	0.50	0/8476
1	B	0.28	0/6413	0.49	0/8655
All	All	0.27	0/12700	0.50	0/17131

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	A	0	3
1	B	0	2
All	All	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	556	SER	Peptide
1	A	573	SER	Peptide
1	A	610	ASP	Peptide
1	B	610	ASP	Peptide
1	B	639	ASP	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6169	0	6029	129	1
1	B	6289	0	6153	89	0
2	A	21	0	0	0	0
2	B	21	0	0	1	0
3	A	24	0	0	3	0
3	B	17	0	0	0	0
All	All	12541	0	12182	218	1

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 9.

All (218) 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:69:LYS:NZ	1:A:464:ASP:OD2	1.85	1.08
1:A:396:ARG:NH1	1:A:400:ASP:OD1	1.94	0.99
1:B:69:LYS:NZ	1:B:464:ASP:OD2	2.03	0.91
1:B:609:ASN:HD22	1:B:617:PHE:HE1	1.19	0.90
1:A:698:LYS:NZ	1:A:701:ASP:OD2	2.05	0.89
1:A:578:ASN:OD1	1:A:581:ASN:ND2	2.09	0.85
1:A:654:LYS:HB2	1:A:654:LYS:NZ	2.02	0.74
1:A:570:VAL:HG12	1:A:571:LYS:H	1.54	0.72
1:A:86:ARG:NH1	1:A:228:HIS:O	2.22	0.72
1:B:578:ASN:OD1	1:B:581:ASN:ND2	2.22	0.72
1:A:301:VAL:HG22	1:A:315:GLN:HG2	1.72	0.71
1:A:636:CYS:HB2	1:A:648:LYS:NZ	2.06	0.70
1:A:88:LEU:HD23	1:A:186:LYS:HE2	1.73	0.69
1:B:245:SER:HB2	1:B:374:ARG:HH22	1.56	0.69
1:A:262:VAL:HG22	1:A:304:ILE:HG22	1.75	0.68
1:B:657:TYR:HD2	1:B:666:CYS:HB2	1.58	0.68
1:A:381:LYS:NZ	1:A:827:ASN:OD1	2.19	0.68
1:B:753:ARG:NH1	1:B:778:THR:O	2.27	0.67
1:A:603:SER:OG	1:A:803:THR:O	2.11	0.67
1:A:572:LYS:O	1:A:574:ASN:N	2.28	0.67
1:A:615:ASP:O	1:A:631:ASN:ND2	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:ARG:NE	1:B:157:GLU:OE2	2.29	0.66
1:A:602:VAL:HG13	1:A:606:ARG:NH1	2.10	0.66
1:A:98:ALA:HA	1:A:101:LYS:HD2	1.76	0.66
1:B:620:GLU:HB3	1:B:635:LEU:HD11	1.78	0.64
1:A:578:ASN:H	1:A:581:ASN:HD21	1.45	0.64
1:B:609:ASN:ND2	1:B:617:PHE:HE1	1.95	0.63
1:A:597:GLY:O	1:A:599:VAL:N	2.30	0.63
1:A:56:ALA:HB2	1:A:405:ILE:HD13	1.81	0.63
1:A:558:TYR:HD1	1:A:558:TYR:H	1.47	0.63
1:B:654:LYS:NZ	1:B:654:LYS:HB3	2.13	0.63
1:B:636:CYS:HB2	1:B:648:LYS:HG3	1.80	0.62
1:A:489:TRP:HE1	1:A:747:GLN:HG2	1.65	0.61
1:A:552:LYS:NZ	1:A:552:LYS:HB2	2.15	0.61
1:B:72:TYR:HB3	1:B:74:LEU:HD22	1.81	0.61
1:A:592:VAL:HG12	1:A:651:LEU:HD21	1.83	0.61
1:A:829:LEU:O	1:A:831:VAL:N	2.27	0.60
1:A:561:PHE:HB3	1:A:563:THR:HG23	1.84	0.60
1:A:568:ALA:HB2	1:A:675:PHE:CE1	2.36	0.60
1:A:752:GLY:HA2	1:A:763:LEU:H	1.65	0.60
1:A:790:ASP:O	1:A:794:ASP:N	2.31	0.60
1:A:161:CYS:SG	1:A:162:LEU:N	2.74	0.60
1:A:292:GLN:OE1	1:A:308:THR:N	2.25	0.60
1:A:648:LYS:NZ	1:A:655:GLU:OE1	2.35	0.60
1:A:567:VAL:HG11	1:A:704:LEU:HD12	1.83	0.60
1:A:262:VAL:HG23	1:A:305:PRO:O	2.03	0.59
1:A:606:ARG:HH12	1:A:613:ASP:HB3	1.66	0.59
1:B:78:ILE:HD13	1:B:409:LEU:HD12	1.85	0.59
1:B:301:VAL:HG22	1:B:315:GLN:HG2	1.84	0.58
1:B:155:ARG:HG2	1:B:157:GLU:HG3	1.85	0.58
1:A:636:CYS:HB2	1:A:648:LYS:HZ1	1.68	0.58
1:A:550:PRO:HG2	1:A:558:TYR:HB3	1.85	0.57
1:A:19:LYS:NZ	3:A:1003:HOH:O	2.36	0.57
1:A:681:VAL:HG21	1:A:714:VAL:HG21	1.88	0.56
1:B:570:VAL:HG13	1:B:705:LEU:HD11	1.86	0.56
1:B:361:HIS:HB3	1:B:365:TYR:CD2	2.40	0.56
1:B:794:ASP:OD1	2:B:901:9SL:N15	2.38	0.56
1:A:539:VAL:HG23	1:A:730:ILE:HB	1.88	0.56
1:B:603:SER:OG	1:B:803:THR:O	2.24	0.56
1:A:628:THR:C	1:A:629:LYS:HD3	2.27	0.55
1:A:606:ARG:NH1	1:A:606:ARG:HB3	2.22	0.55
1:B:249:PHE:N	1:B:368:LEU:HD21	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:537:PRO:HB3	1:A:729:ALA:HB1	1.88	0.55
1:B:94:GLU:OE1	1:B:117:TYR:OH	2.26	0.54
1:B:542:TYR:CZ	1:B:544:ASN:HB3	2.43	0.54
1:A:396:ARG:HH11	1:A:396:ARG:HB2	1.72	0.54
1:B:32:ILE:HG21	1:B:408:PHE:HB2	1.89	0.54
1:A:340:ARG:NH1	3:A:1002:HOH:O	2.35	0.54
1:B:332:TYR:CG	1:B:341:CYS:HB2	2.43	0.54
1:A:322:LYS:HD3	1:A:329:ASP:HB3	1.89	0.53
1:B:21:ASN:HA	1:B:24:VAL:HG12	1.91	0.53
1:A:570:VAL:HG11	1:A:577:ILE:HB	1.90	0.53
1:A:571:LYS:NZ	1:A:667:LEU:O	2.40	0.52
1:A:654:LYS:HB2	1:A:654:LYS:HZ3	1.73	0.52
1:B:304:ILE:HD12	1:B:312:LEU:HD13	1.90	0.52
1:A:590:THR:OG1	1:A:594:ASP:OD2	2.24	0.52
1:B:621:SER:HB2	1:B:632:LEU:HA	1.90	0.52
1:A:100:ALA:HB1	1:A:414:LYS:HE2	1.91	0.52
1:A:786:ARG:HD2	1:A:794:ASP:OD2	2.09	0.52
1:A:668:VAL:HG13	1:A:669:GLU:OE2	2.10	0.51
1:A:32:ILE:HG21	1:A:408:PHE:HB2	1.93	0.51
1:A:230:LEU:HD11	1:A:826:SER:HB2	1.93	0.51
1:A:269:LYS:HZ2	1:A:458:MET:HE1	1.75	0.51
1:B:199:GLY:HA3	1:B:218:PRO:HG3	1.93	0.51
1:B:620:GLU:HB3	1:B:635:LEU:CD1	2.42	0.50
1:A:256:ARG:NH2	1:A:345:ASP:O	2.41	0.50
1:A:588:CYS:HB3	1:A:622:CYS:N	2.27	0.50
1:B:207:ILE:HD11	1:B:209:GLU:OE2	2.12	0.50
1:A:190:GLU:HG3	1:A:191:PRO:HD2	1.93	0.50
1:A:581:ASN:H	1:A:581:ASN:HD22	1.60	0.50
1:A:802:THR:HG22	1:A:807:ALA:HB2	1.93	0.50
1:A:630:SER:O	1:A:634:LYS:HD3	2.11	0.49
1:A:489:TRP:HE1	1:A:747:GLN:CG	2.24	0.49
1:A:737:ILE:O	1:A:741:VAL:HG12	2.12	0.49
1:B:565:ARG:HH12	1:B:718:LYS:HG3	1.77	0.49
1:B:301:VAL:HG23	1:B:314:LYS:HB3	1.95	0.49
1:B:550:PRO:HG2	1:B:558:TYR:HB3	1.95	0.49
1:B:667:LEU:HB2	1:B:674:ALA:HB2	1.94	0.49
1:B:699:SER:HB2	1:B:714:VAL:HG11	1.93	0.49
1:A:182:GLN:OE1	1:A:194:PHE:N	2.40	0.49
1:B:475:TRP:CZ2	1:B:730:ILE:HD12	2.48	0.49
1:B:592:VAL:HG12	1:B:651:LEU:HD21	1.95	0.49
1:B:606:ARG:HB2	1:B:611:ASN:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:615:ASP:OD1	1:B:630:SER:OG	2.26	0.48
1:A:165:ARG:HD3	1:A:181:PRO:O	2.13	0.48
1:A:704:LEU:HD22	1:A:714:VAL:HA	1.95	0.48
1:B:240:MET:HE2	1:B:352:LEU:HD11	1.94	0.48
1:A:628:THR:O	1:A:630:SER:N	2.45	0.48
1:B:256:ARG:NH2	1:B:348:ASP:OD1	2.41	0.48
1:B:601:PRO:HB3	1:B:675:PHE:CD1	2.49	0.48
1:A:76:PRO:HA	1:A:394:VAL:HG12	1.94	0.48
1:A:326:ASN:ND2	3:A:1006:HOH:O	2.46	0.48
1:A:572:LYS:HB2	1:A:703:GLU:OE1	2.13	0.48
1:B:582:ILE:HD11	1:B:705:LEU:HD22	1.94	0.47
1:A:199:GLY:HA3	1:A:218:PRO:HG3	1.96	0.47
1:A:489:TRP:O	1:A:493:SER:HB3	2.15	0.47
1:A:568:ALA:HB2	1:A:675:PHE:CD1	2.50	0.47
1:B:665:ARG:HA	1:B:668:VAL:HG12	1.95	0.47
1:A:42:THR:O	1:A:46:MET:HG3	2.14	0.47
1:A:57:MET:O	1:A:393:VAL:HA	2.15	0.47
1:B:577:ILE:HD12	1:B:585:LYS:HG2	1.96	0.47
1:A:678:HIS:O	1:A:681:VAL:HG13	2.15	0.47
1:B:21:ASN:O	1:B:24:VAL:HG12	2.14	0.47
1:B:127:GLY:HA3	1:B:146:PRO:HG3	1.97	0.47
1:A:182:GLN:HE21	1:A:182:GLN:HB3	1.51	0.47
1:B:615:ASP:O	1:B:631:ASN:ND2	2.30	0.47
1:A:598:TRP:O	1:A:602:VAL:HB	2.16	0.46
1:B:259:HIS:CD2	1:B:304:ILE:HG12	2.50	0.46
1:B:539:VAL:HG12	1:B:730:ILE:HG13	1.98	0.46
1:A:163:LYS:O	1:A:167:VAL:HG23	2.14	0.46
1:A:622:CYS:N	1:A:632:LEU:HB3	2.30	0.46
1:A:205:ASN:HD21	1:A:209:GLU:HG2	1.80	0.46
1:B:184:ASP:OD1	1:B:185:GLU:N	2.49	0.46
1:B:831:VAL:HG22	1:B:831:VAL:O	2.15	0.46
1:A:632:LEU:O	1:A:634:LYS:N	2.49	0.46
1:A:592:VAL:HG23	1:A:598:TRP:CE2	2.51	0.45
1:A:600:ILE:HB	1:A:601:PRO:HD3	1.98	0.45
1:B:342:LEU:HB2	1:B:350:ALA:HB2	1.98	0.45
1:A:570:VAL:HG12	1:A:571:LYS:N	2.26	0.45
1:A:685:THR:HG23	1:A:686:ASP:OD1	2.16	0.45
1:B:301:VAL:CG2	1:B:314:LYS:HB3	2.47	0.45
1:A:542:TYR:CZ	1:A:544:ASN:HB3	2.52	0.45
1:A:688:LYS:O	1:A:690:PRO:HD3	2.17	0.45
1:B:575:LYS:HB2	1:B:575:LYS:NZ	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:TRP:CZ2	1:A:291:ILE:HG12	2.52	0.45
1:A:604:LEU:HD12	1:A:604:LEU:HA	1.83	0.45
1:B:322:LYS:HD3	1:B:329:ASP:HB3	1.99	0.45
1:B:296:SER:HB2	1:B:311:ASN:OD1	2.17	0.45
1:A:489:TRP:NE1	1:A:747:GLN:HG2	2.31	0.44
1:B:447:PHE:CZ	1:B:452:VAL:HG12	2.52	0.44
1:A:86:ARG:NH1	1:A:229:ASP:OD1	2.50	0.44
1:A:542:TYR:O	1:A:779:GLN:N	2.50	0.44
1:A:785:ASP:OD1	1:A:785:ASP:N	2.49	0.44
1:B:312:LEU:O	1:B:313:CYS:HB2	2.17	0.44
1:B:600:ILE:HD11	1:B:800:TYR:CD2	2.52	0.44
1:A:571:LYS:HE3	1:A:702:PHE:CE1	2.53	0.44
1:A:606:ARG:HB3	1:A:606:ARG:HH11	1.82	0.44
1:A:453:LYS:HE2	1:A:453:LYS:HB3	1.85	0.44
1:A:483:LYS:HE3	1:A:487:ASP:OD2	2.17	0.44
1:A:653:ASP:HA	1:A:658:TYR:HB3	1.99	0.43
1:B:56:ALA:HB2	1:B:405:ILE:HD13	2.00	0.43
1:B:296:SER:O	1:B:311:ASN:ND2	2.51	0.43
1:A:719:SER:HB2	1:A:721:LYS:HG2	2.00	0.43
1:B:654:LYS:HB3	1:B:654:LYS:HZ2	1.83	0.43
1:B:758:LYS:HE2	1:B:758:LYS:HB3	1.85	0.43
1:B:331:PRO:HB3	1:B:340:ARG:HH12	1.84	0.43
1:B:574:ASN:OD1	1:B:575:LYS:NZ	2.51	0.43
1:B:165:ARG:O	1:B:166:GLN:HB2	2.18	0.43
1:A:582:ILE:HG22	1:A:618:PHE:CE1	2.54	0.43
1:B:406:ASN:OD1	1:B:439:LEU:HB2	2.19	0.43
1:A:134:ALA:HB2	1:A:157:GLU:HA	2.00	0.42
1:A:215:LYS:H	1:A:215:LYS:HG2	1.59	0.42
1:A:553:THR:O	1:A:556:SER:OG	2.37	0.42
1:A:629:LYS:O	1:A:629:LYS:NZ	2.49	0.42
1:B:561:PHE:HB3	1:B:563:THR:HG23	2.01	0.42
1:B:617:PHE:HD2	1:B:618:PHE:CD1	2.37	0.42
1:B:155:ARG:HG2	1:B:157:GLU:CG	2.50	0.42
1:A:486:CYS:HB2	1:A:773:LEU:HD11	2.01	0.42
1:A:787:GLN:HB2	1:A:789:LYS:HE2	2.01	0.42
1:B:57:MET:O	1:B:393:VAL:HA	2.19	0.42
1:B:718:LYS:HE3	1:B:718:LYS:HB2	1.87	0.42
1:A:91:CYS:HB2	1:A:117:TYR:CE1	2.54	0.42
1:A:594:ASP:N	1:A:594:ASP:OD1	2.53	0.42
1:A:632:LEU:C	1:A:634:LYS:H	2.23	0.42
1:B:301:VAL:HG21	1:B:314:LYS:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:ASN:H	1:A:581:ASN:ND2	2.14	0.42
1:A:20:CYS:O	1:A:24:VAL:HG23	2.19	0.42
1:A:91:CYS:HB2	1:A:117:TYR:CD1	2.54	0.42
1:A:523:GLU:OE2	1:A:728:PRO:HG3	2.20	0.42
1:A:550:PRO:HG3	1:A:556:SER:O	2.19	0.42
1:A:112:ASP:OD2	1:A:116:ASN:HB2	2.19	0.41
1:B:785:ASP:OD1	1:B:785:ASP:N	2.49	0.41
1:A:159:PRO:HG3	1:A:187:GLY:HA3	2.02	0.41
1:B:42:THR:O	1:B:46:MET:HG3	2.20	0.41
1:A:269:LYS:NZ	1:A:458:MET:HE1	2.35	0.41
1:B:483:LYS:HD3	1:B:501:GLU:HG3	2.02	0.41
1:B:627:ASP:O	1:B:628:THR:HB	2.20	0.41
1:B:78:ILE:HB	1:B:393:VAL:HB	2.01	0.41
1:B:367:LEU:HG	1:B:377:LEU:HD23	2.02	0.41
1:B:668:VAL:HG21	1:B:697:LEU:HD21	2.02	0.41
1:A:615:ASP:OD1	1:A:630:SER:HB3	2.20	0.41
1:B:483:LYS:HE2	1:B:487:ASP:OD1	2.21	0.41
1:A:205:ASN:ND2	1:A:209:GLU:HG2	2.35	0.41
1:A:483:LYS:HD3	1:A:501:GLU:HG3	2.03	0.41
1:A:679:THR:O	1:A:683:GLU:HG3	2.21	0.41
1:B:76:PRO:HB3	1:B:392:THR:HG21	2.03	0.41
1:B:360:GLU:O	1:B:361:HIS:CG	2.73	0.41
1:A:184:ASP:OD1	1:A:185:GLU:N	2.54	0.41
1:A:78:ILE:HB	1:A:393:VAL:HB	2.02	0.40
1:B:428:LEU:HD23	1:B:428:LEU:HA	1.84	0.40
1:B:654:LYS:HB3	1:B:654:LYS:HZ3	1.86	0.40
1:A:539:VAL:HG12	1:A:783:THR:HA	2.03	0.40
1:B:480:LYS:O	1:B:484:MET:HG3	2.21	0.40
1:A:676:VAL:HG21	1:A:680:VAL:HG11	2.02	0.40
1:A:552:LYS:HB2	1:A:552:LYS:HZ3	1.86	0.40
1:A:588:CYS:HB3	1:A:622:CYS:HB3	2.04	0.40
1:B:489:TRP:CE2	1:B:497:ILE:HG13	2.57	0.40
1:B:139:ILE:HD11	1:B:156:HIS:HE1	1.87	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:GLN:NE2	1:A:154:GLU:OE2[4_555]	2.05	0.15

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	783/853 (92%)	735 (94%)	38 (5%)	10 (1%)	12	21
1	B	809/853 (95%)	759 (94%)	41 (5%)	9 (1%)	14	26
All	All	1592/1706 (93%)	1494 (94%)	79 (5%)	19 (1%)	13	24

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	573	SER
1	A	598	TRP
1	A	629	LYS
1	A	692	VAL
1	A	830	GLU
1	B	628	THR
1	B	640	PRO
1	A	633	CYS
1	B	637	ILE
1	B	692	VAL
1	A	284	ASP
1	A	610	ASP
1	B	613	ASP
1	B	690	PRO
1	A	684	ASN
1	B	627	ASP
1	B	643	SER
1	B	620	GLU
1	A	690	PRO

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	687/731 (94%)	621 (90%)	66 (10%)	8 16
1	B	701/731 (96%)	660 (94%)	41 (6%)	20 38
All	All	1388/1462 (95%)	1281 (92%)	107 (8%)	13 25

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	14	ASP
1	A	43	GLU
1	A	50	LYS
1	A	101	LYS
1	A	111	CYS
1	A	132	VAL
1	A	158	LEU
1	A	161	CYS
1	A	164	GLU
1	A	182	GLN
1	A	184	ASP
1	A	190	GLU
1	A	211	ILE
1	A	233	THR
1	A	255	LYS
1	A	266	ASP
1	A	290	SER
1	A	320	GLU
1	A	346	MET
1	A	352	LEU
1	A	399	SER
1	A	409	LEU
1	A	410	MET
1	A	419	LEU
1	A	454	LEU
1	A	461	LEU
1	A	499	CYS
1	A	524	VAL
1	A	525	GLN
1	A	539	VAL
1	A	552	LYS
1	A	556	SER

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Mol	Chain	Res	Type
1	A	558	TYR
1	A	561	PHE
1	A	567	VAL
1	A	574	ASN
1	A	581	ASN
1	A	588	CYS
1	A	590	THR
1	A	594	ASP
1	A	606	ARG
1	A	613	ASP
1	A	614	ILE
1	A	628	THR
1	A	629	LYS
1	A	633	CYS
1	A	634	LYS
1	A	648	LYS
1	A	654	LYS
1	A	660	ASN
1	A	666	CYS
1	A	670	LYS
1	A	676	VAL
1	A	678	HIS
1	A	681	VAL
1	A	683	GLU
1	A	695	LYS
1	A	698	LYS
1	A	703	GLU
1	A	704	LEU
1	A	705	LEU
1	A	759	ASP
1	A	812	MET
1	A	824	HIS
1	A	830	GLU
1	B	50	LYS
1	B	74	LEU
1	B	132	VAL
1	B	155	ARG
1	B	163	LYS
1	B	182	GLN
1	B	192	GLN
1	B	204	VAL
1	B	245	SER

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Mol	Chain	Res	Type
1	B	248	GLN
1	B	266	ASP
1	B	283	TRP
1	B	352	LEU
1	B	364	VAL
1	B	368	LEU
1	B	373	THR
1	B	461	LEU
1	B	467	LEU
1	B	521	LYS
1	B	523	GLU
1	B	539	VAL
1	B	575	LYS
1	B	586	LYS
1	B	587	SER
1	B	610	ASP
1	B	620	GLU
1	B	626	SER
1	B	633	CYS
1	B	637	ILE
1	B	639	ASP
1	B	643	SER
1	B	654	LYS
1	B	670	LYS
1	B	685	THR
1	B	719	SER
1	B	758	LYS
1	B	783	THR
1	B	786	ARG
1	B	787	GLN
1	B	792	MET
1	B	832	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	578	ASN
1	A	580	ASN
1	A	581	ASN
1	B	581	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 monosaccharides 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	6.00	11 (64%)	13,37,37	3.18	8 (61%)
2	9SL	A	901	1	17,23,23	6.09	10 (58%)	13,37,37	3.18	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	-	3/5/53/53	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	9SL	C12-N13	15.86	1.60	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	9SL	C12-N13	15.84	1.60	1.35
2	A	901	9SL	C20-N09	-10.52	1.34	1.47
2	B	901	9SL	C20-N09	-9.93	1.35	1.47
2	B	901	9SL	C19-C20	-8.14	1.37	1.52
2	A	901	9SL	C19-C20	-8.10	1.37	1.52
2	A	901	9SL	C07-N08	7.26	1.47	1.34
2	B	901	9SL	C07-N08	7.12	1.47	1.34
2	B	901	9SL	C02-N21	7.04	1.46	1.33
2	A	901	9SL	C02-N21	6.99	1.46	1.33
2	A	901	9SL	C12-N15	6.05	1.48	1.34
2	B	901	9SL	C12-N15	5.27	1.46	1.34
2	B	901	9SL	C07-N09	4.97	1.44	1.35
2	A	901	9SL	C07-N09	4.92	1.44	1.35
2	B	901	9SL	O03-C02	4.32	1.41	1.35
2	A	901	9SL	O03-C02	4.19	1.41	1.35
2	B	901	9SL	C05-C14	3.07	1.59	1.52
2	A	901	9SL	C05-C14	3.05	1.59	1.52
2	B	901	9SL	C05-N06	-2.43	1.43	1.47
2	A	901	9SL	C05-N06	-2.26	1.43	1.47
2	B	901	9SL	O01-C02	-2.04	1.19	1.21

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	901	9SL	O03-C02-N21	7.29	120.13	111.08
2	A	901	9SL	O03-C02-N21	6.40	119.03	111.08
2	A	901	9SL	C19-C20-N09	4.81	109.26	103.83
2	B	901	9SL	C19-C20-N09	4.38	108.78	103.83
2	A	901	9SL	N13-C12-N11	-4.33	104.47	115.45
2	B	901	9SL	N13-C12-N11	-3.77	105.90	115.45
2	A	901	9SL	N15-C12-N11	3.56	130.90	125.35
2	B	901	9SL	O01-C02-N21	-3.47	119.79	125.51
2	B	901	9SL	O03-C02-O01	-3.16	120.08	123.07
2	A	901	9SL	N09-C07-N06	-3.09	121.11	125.42
2	A	901	9SL	O01-C02-N21	-3.02	120.53	125.51
2	B	901	9SL	N09-C07-N06	-2.81	121.51	125.42
2	A	901	9SL	O03-C02-O01	-2.77	120.45	123.07
2	B	901	9SL	N15-C12-N13	2.53	126.59	122.64
2	A	901	9SL	C04-O03-C02	-2.21	113.04	116.26
2	B	901	9SL	C04-C05-N06	-2.10	105.37	108.57

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

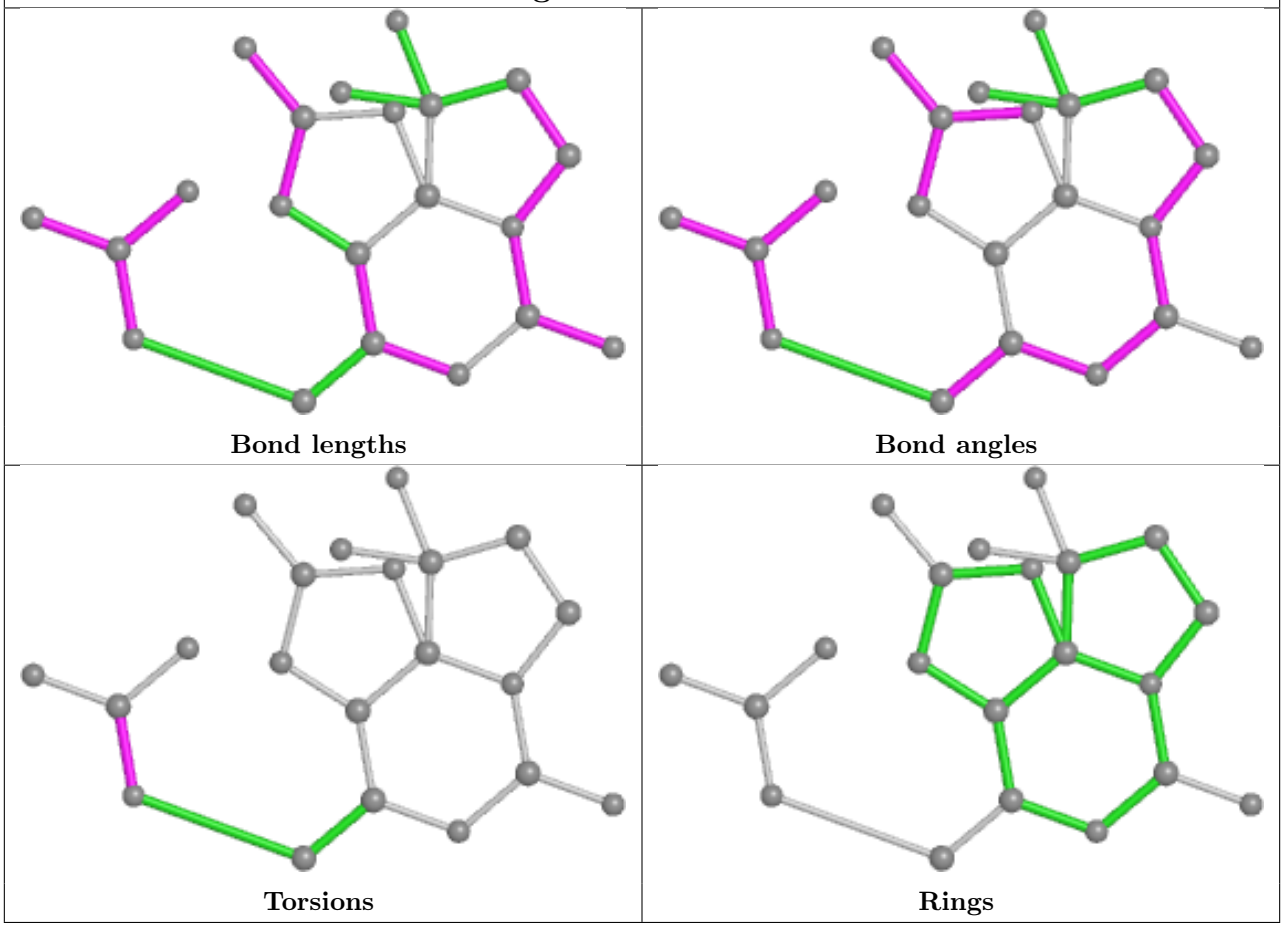
There are no ring outliers.

1 monomer is involved in 1 short contact:

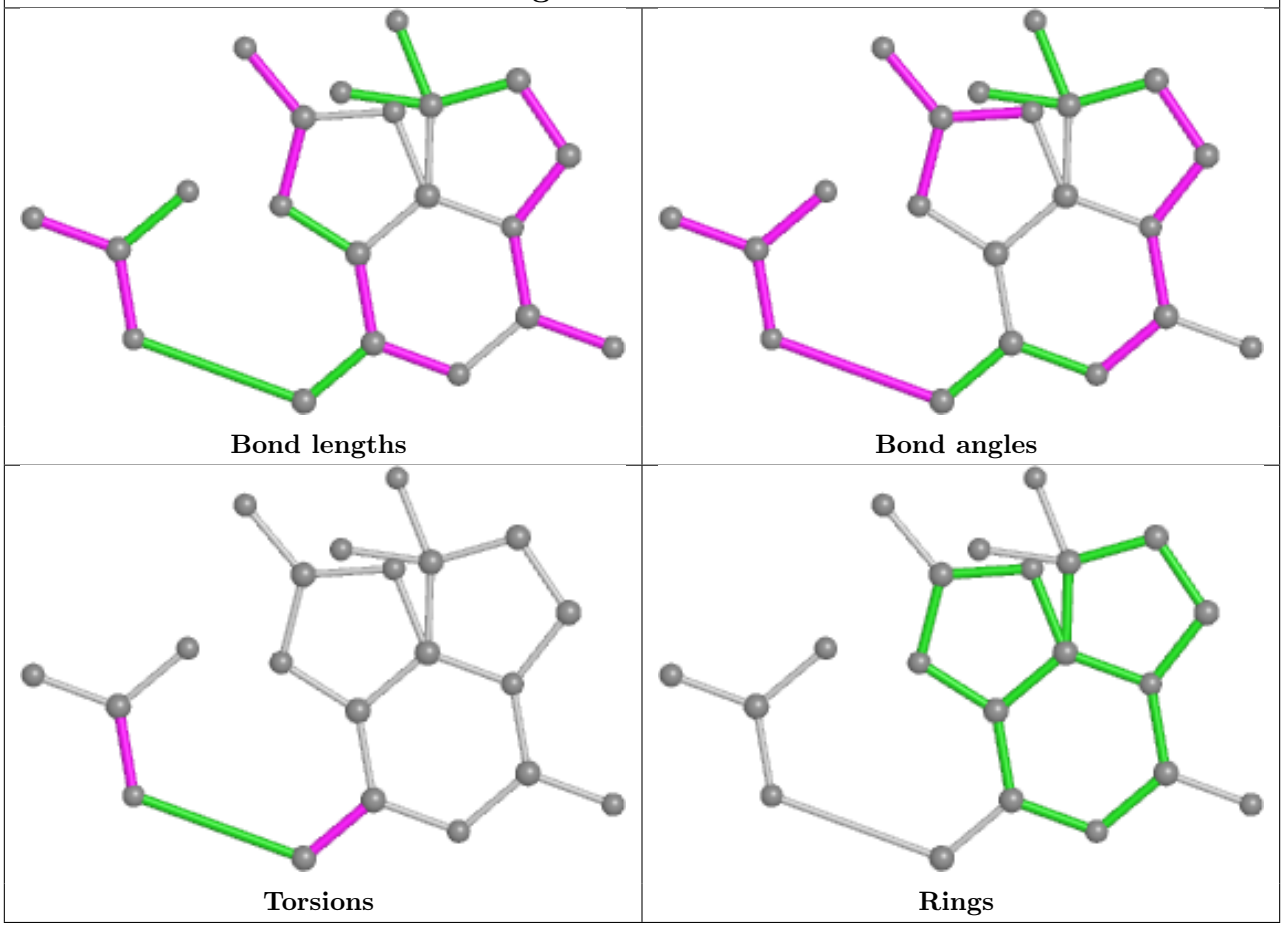
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	901	9SL	1	0

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 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 B 901



Ligand 9SL A 901



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	799/853 (93%)	0.33	45 (5%)	24	25	57, 91, 184, 239	0
1	B	815/853 (95%)	0.21	20 (2%)	57	61	59, 98, 155, 252	0
All	All	1614/1706 (94%)	0.27	65 (4%)	38	41	57, 95, 175, 252	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	690	PRO	9.2
1	B	644	ALA	8.0
1	A	694	ALA	6.4
1	A	692	VAL	6.4
1	A	579	TRP	6.0
1	A	702	PHE	5.8
1	A	691	ALA	5.8
1	A	664	PHE	5.6
1	A	582	ILE	5.4
1	B	692	VAL	5.3
1	B	88	LEU	5.0
1	A	693	TRP	4.8
1	A	675	PHE	4.3
1	A	689	ASN	4.2
1	A	557	PRO	4.2
1	B	642	ASN	4.1
1	A	680	VAL	4.1
1	A	618	PHE	4.1
1	B	831	VAL	3.9
1	A	569	LEU	3.9
1	A	631	ASN	3.9
1	A	684	ASN	3.7
1	A	695	LYS	3.7
1	A	573	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	570	VAL	3.5
1	B	579	TRP	3.4
1	A	681	VAL	3.2
1	B	829	LEU	3.2
1	B	157	GLU	3.1
1	B	773	LEU	3.0
1	A	701	ASP	3.0
1	A	654	LYS	3.0
1	A	661	GLN	3.0
1	A	194	PHE	2.9
1	A	720	CYS	2.9
1	A	546	ASP	2.8
1	B	668	VAL	2.8
1	B	643	SER	2.8
1	A	572	LYS	2.7
1	B	86	ARG	2.7
1	A	688	LYS	2.6
1	A	577	ILE	2.6
1	A	589	HIS	2.5
1	A	697	LEU	2.4
1	A	665	ARG	2.4
1	A	559	THR	2.4
1	B	693	TRP	2.4
1	A	596	ALA	2.3
1	B	592	VAL	2.2
1	A	202	TRP	2.2
1	A	669	GLU	2.2
1	B	605	ILE	2.2
1	A	283	TRP	2.2
1	A	670	LYS	2.1
1	A	696	ASN	2.1
1	A	287	ALA	2.1
1	A	291	ILE	2.1
1	B	609	ASN	2.1
1	A	705	LEU	2.1
1	B	408	PHE	2.1
1	B	604	LEU	2.1
1	A	615	ASP	2.0
1	A	712	ALA	2.0
1	B	166	GLN	2.0
1	B	640	PRO	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

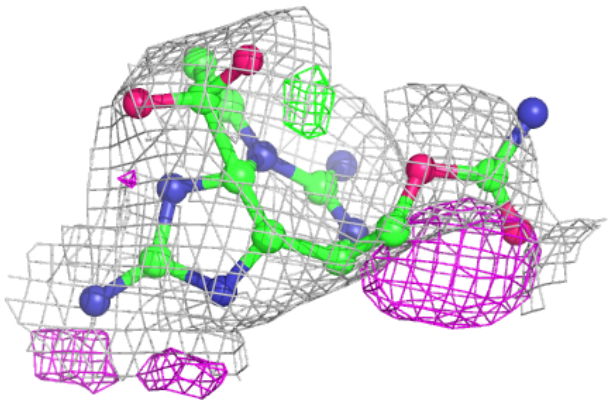
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

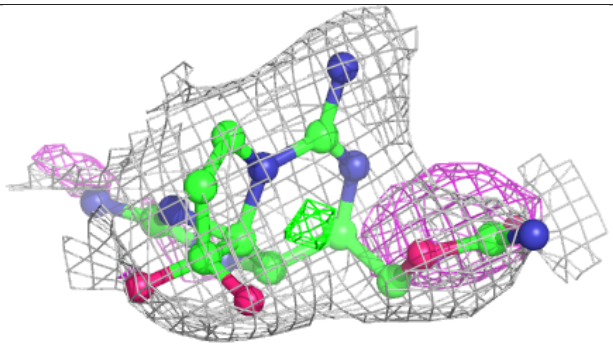
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	9SL	A	901	21/21	0.78	0.21	116,143,156,160	0
2	9SL	B	901	21/21	0.96	0.18	65,84,105,114	0

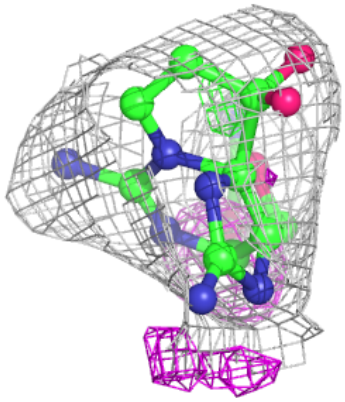
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

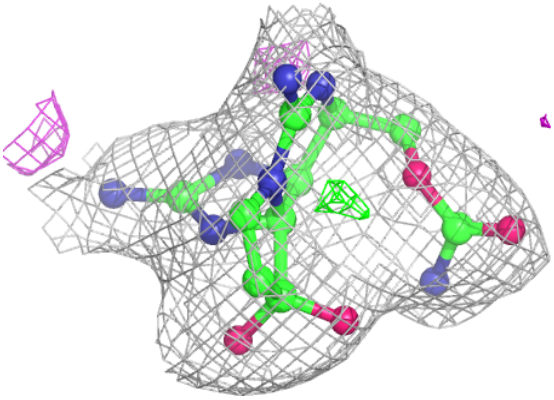


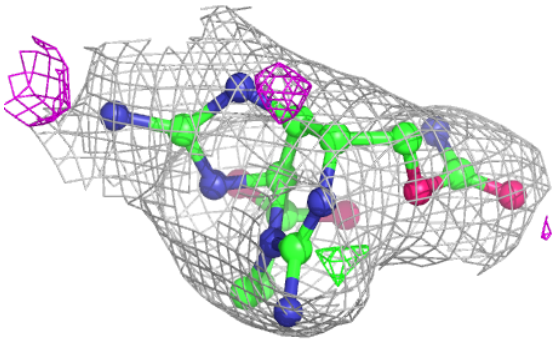


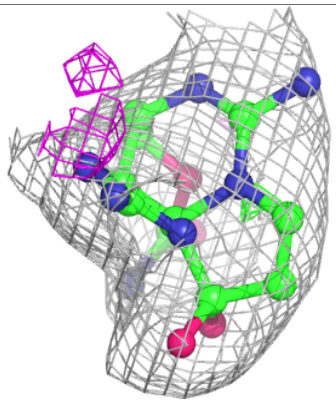


Electron density around 9SL B 901:

$2mF_o$-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.