Full wwPDB X-ray Structure Validation Report ⓘ

Apr 2, 2025 – 04:06 PM EDT

PDB ID	:	9N26 / pdb_00009n26
Title	:	DNA gyrase complexed with uncleaved DNA and Compound 148 to 1.96 A resolution
Authors	:	Bell, C.E.; McElroy, C.A.; Ratigan, S.C.
Deposited on	:	2025-01-27
Resolution	:	1.96 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:

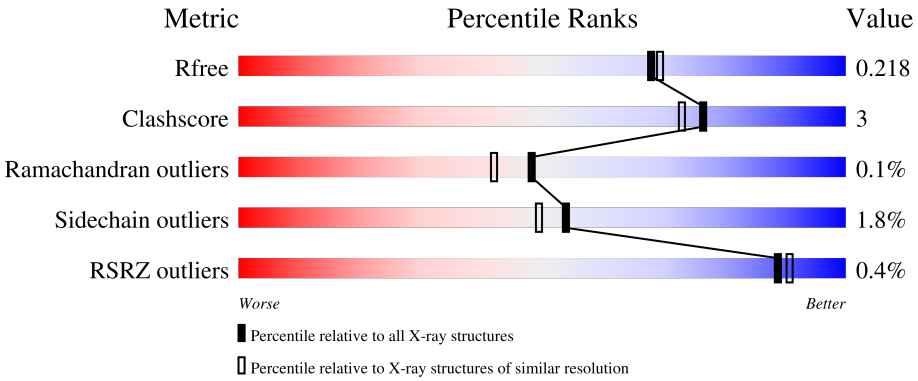
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 1.96 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}	164625	3187 (1.96-1.96)
Clashscore	180529	3412 (1.96-1.96)
Ramachandran outliers	177936	3390 (1.96-1.96)
Sidechain outliers	177891	3390 (1.96-1.96)
RSRZ outliers	164620	3186 (1.96-1.96)

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	693	% 90% 6% • •
1	B	693	90% 6% • •
2	C	20	45% 50% 5%
2	D	20	50% 45% 5%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 12100 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 DNA gyrase subunit B fusion with DNA gyrase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	672	Total	C	N	O	S	0	0	0
			5322	3319	959	1019	25			
1	B	670	Total	C	N	O	S	0	0	0
			5308	3311	955	1017	25			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	408	GLY	-	expression tag	UNP P0A0K8
A	409	MET	-	expression tag	UNP P0A0K8
A	?	-	LEU	deletion	UNP P0A0K8
A	?	-	TYR	deletion	UNP P0A0K8
A	?	-	LYS	deletion	UNP P0A0K8
A	?	-	LEU	deletion	UNP P0A0K8
A	?	-	THR	deletion	UNP P0A0K8
A	?	-	GLN	deletion	UNP P0A0K8
A	?	-	GLY	deletion	UNP P0A0K8
A	?	-	LYS	deletion	UNP P0A0K8
A	?	-	GLN	deletion	UNP P0A0K8
A	?	-	LYS	deletion	UNP P0A0K8
A	?	-	TYR	deletion	UNP P0A0K8
A	?	-	TYR	deletion	UNP P0A0K8
A	?	-	VAL	deletion	UNP P0A0K8
A	?	-	TYR	deletion	UNP P0A0K8
A	?	-	ASN	deletion	UNP P0A0K8
A	?	-	ASP	deletion	UNP P0A0K8
A	?	-	ARG	deletion	UNP P0A0K8
A	?	-	GLU	deletion	UNP P0A0K8
A	?	-	LEU	deletion	UNP P0A0K8
A	?	-	ASP	deletion	UNP P0A0K8
A	?	-	LYS	deletion	UNP P0A0K8
A	?	-	LEU	deletion	UNP P0A0K8
A	?	-	LYS	deletion	UNP P0A0K8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	SER	deletion	UNP P0A0K8
A	?	-	GLU	deletion	UNP P0A0K8
A	?	-	LEU	deletion	UNP P0A0K8
A	?	-	ASN	deletion	UNP P0A0K8
A	?	-	PRO	deletion	UNP P0A0K8
A	?	-	THR	deletion	UNP P0A0K8
A	?	-	PRO	deletion	UNP P0A0K8
A	?	-	LYS	deletion	UNP P0A0K8
A	?	-	TRP	deletion	UNP P0A0K8
A	?	-	SER	deletion	UNP P0A0K8
A	?	-	ILE	deletion	UNP P0A0K8
A	544	THR	ALA	conflict	UNP P0A0K8
A	545	GLY	ARG	conflict	UNP P0A0K8
A	1123	PHE	TYR	conflict	UNP P20831
A	1457	THR	ALA	conflict	UNP P20831
B	408	GLY	-	expression tag	UNP P0A0K8
B	409	MET	-	expression tag	UNP P0A0K8
B	?	-	LEU	deletion	UNP P0A0K8
B	?	-	TYR	deletion	UNP P0A0K8
B	?	-	LYS	deletion	UNP P0A0K8
B	?	-	LEU	deletion	UNP P0A0K8
B	?	-	THR	deletion	UNP P0A0K8
B	?	-	GLN	deletion	UNP P0A0K8
B	?	-	GLY	deletion	UNP P0A0K8
B	?	-	LYS	deletion	UNP P0A0K8
B	?	-	GLN	deletion	UNP P0A0K8
B	?	-	LYS	deletion	UNP P0A0K8
B	?	-	TYR	deletion	UNP P0A0K8
B	?	-	TYR	deletion	UNP P0A0K8
B	?	-	VAL	deletion	UNP P0A0K8
B	?	-	TYR	deletion	UNP P0A0K8
B	?	-	ASN	deletion	UNP P0A0K8
B	?	-	ASP	deletion	UNP P0A0K8
B	?	-	ARG	deletion	UNP P0A0K8
B	?	-	GLU	deletion	UNP P0A0K8
B	?	-	LEU	deletion	UNP P0A0K8
B	?	-	ASP	deletion	UNP P0A0K8
B	?	-	LYS	deletion	UNP P0A0K8
B	?	-	LEU	deletion	UNP P0A0K8
B	?	-	LYS	deletion	UNP P0A0K8
B	?	-	SER	deletion	UNP P0A0K8
B	?	-	GLU	deletion	UNP P0A0K8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	LEU	deletion	UNP P0A0K8
B	?	-	ASN	deletion	UNP P0A0K8
B	?	-	PRO	deletion	UNP P0A0K8
B	?	-	THR	deletion	UNP P0A0K8
B	?	-	PRO	deletion	UNP P0A0K8
B	?	-	LYS	deletion	UNP P0A0K8
B	?	-	TRP	deletion	UNP P0A0K8
B	?	-	SER	deletion	UNP P0A0K8
B	?	-	ILE	deletion	UNP P0A0K8
B	544	THR	ALA	conflict	UNP P0A0K8
B	545	GLY	ARG	conflict	UNP P0A0K8
B	1123	PHE	TYR	conflict	UNP P20831
B	1457	THR	ALA	conflict	UNP P20831

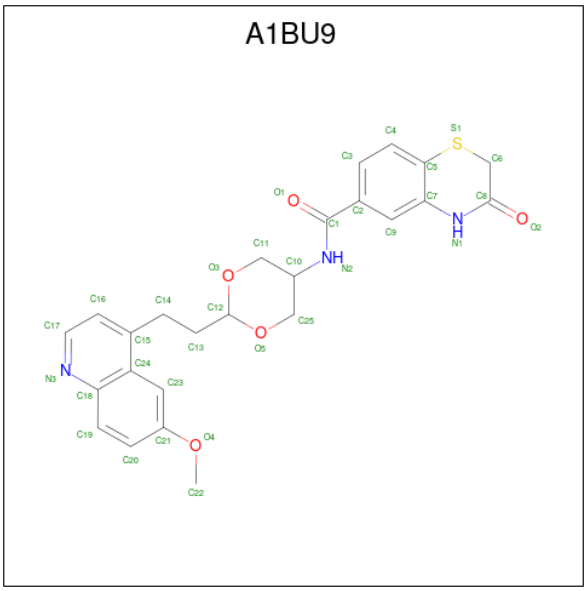
- Molecule 2 is a DNA chain called DNA (5'-D(*AP*GP*CP*CP*GP*TP*AP*GP*GP*GP*CP*CP*CP*TP*AP*CP*GP*GP*CP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	20	Total	C	N	O	P	0	0	0
			407	193	77	118	19			
2	D	20	Total	C	N	O	P	0	0	0
			390	183	75	113	19			

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		
3	B	1	Total	Mn	0	0
			1	1		

- Molecule 4 is N-{(2r,5r)-2-[2-(6-methoxyquinolin-4-yl)ethyl]-1,3-dioxan-5-yl}-3-oxo-3,4-dihydro-2H-1,4-benzothiazine-6-carboxamide (CCD ID: A1BU9) (formula: $C_{25}H_{25}N_3O_5S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C N O S 68 50 6 10 2	0	1

- Molecule 5 is water.

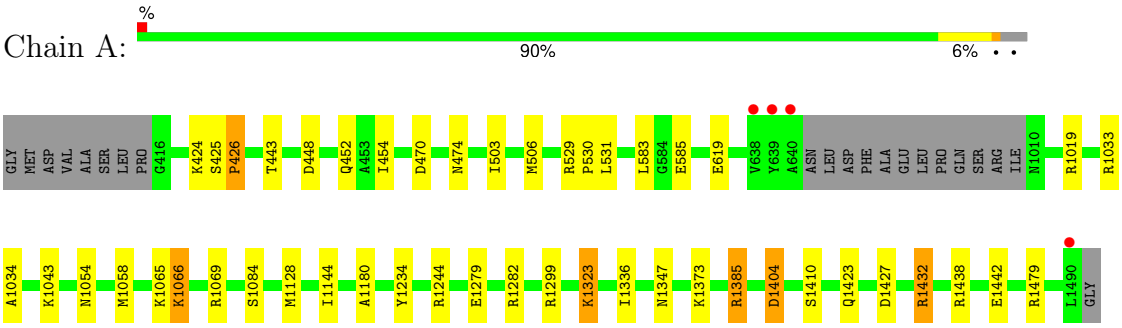
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	269	Total O 269 269	0	0
5	B	262	Total O 262 262	0	0
5	C	39	Total O 39 39	0	0
5	D	33	Total O 33 33	0	0

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.

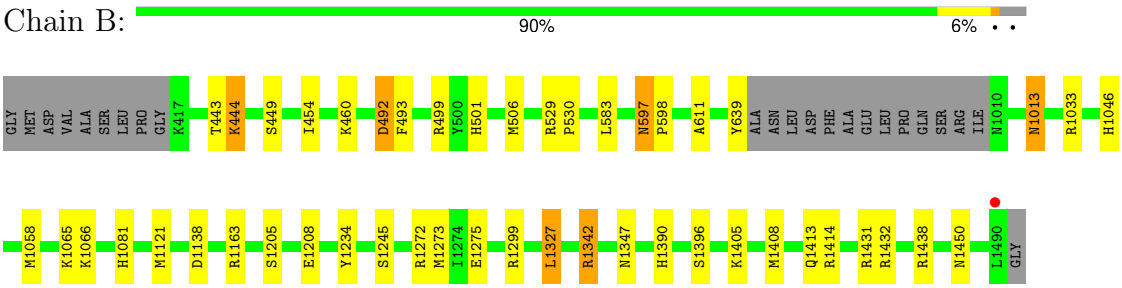
• Molecule 1: DNA gyrase subunit B fusion with DNA gyrase subunit A

Chain A:



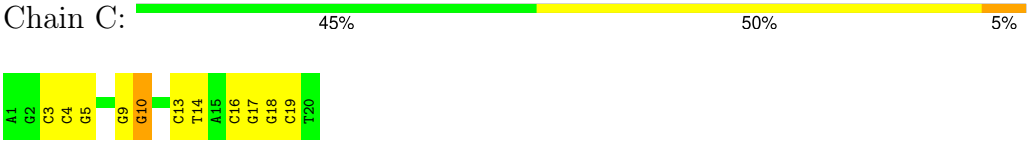
• Molecule 1: DNA gyrase subunit B fusion with DNA gyrase subunit A

Chain B:



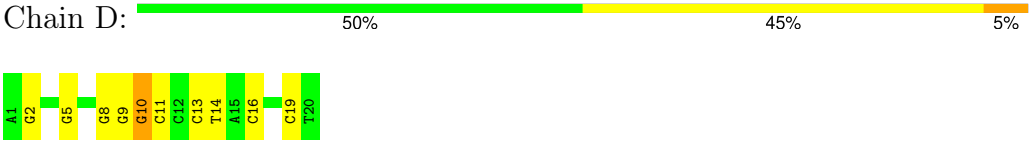
• Molecule 2: DNA (5'-D(*AP*GP*CP*CP*GP*TP*AP*GP*GP*GP*CP*CP*CP*TP*AP*CP *GP*GP*CP*T)-3')

Chain C:



• Molecule 2: DNA (5'-D(*AP*GP*CP*CP*GP*TP*AP*GP*GP*GP*CP*CP*CP*TP*AP*CP *GP*GP*CP*T)-3')

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	92.94Å 92.94Å 405.76Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.70 – 1.96 29.70 – 1.96	Depositor EDS
% Data completeness (in resolution range)	99.4 (29.70-1.96) 99.4 (29.70-1.96)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.14 (at 1.96Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.171 , 0.217 0.175 , 0.218	Depositor DCC
R_{free} test set	7112 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	44.4	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 26.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.088 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	12100	wwPDB-VP
Average B, all atoms (Å^2)	53.0	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.*

[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: MN, A1BU9

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	0.41	0/5394	0.83	3/7266 (0.0%)
1	B	0.41	0/5380	0.82	2/7249 (0.0%)
2	C	0.70	0/456	1.79	17/702 (2.4%)
2	D	0.77	0/437	1.69	15/674 (2.2%)
All	All	0.44	0/11667	0.94	37/15891 (0.2%)

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	4
All	All	0	7

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	19	DC	O5'-P-OP1	13.00	126.30	110.70
2	C	4	DC	O5'-P-OP2	-12.52	94.44	105.70
2	D	10	DG	O5'-P-OP2	-12.14	94.77	105.70
2	C	10	DG	O5'-P-OP2	-11.24	95.58	105.70
2	C	13	DC	O5'-P-OP1	9.56	122.17	110.70
2	C	14	DT	O5'-P-OP2	-8.88	97.71	105.70
2	C	13	DC	O5'-P-OP2	-8.67	97.90	105.70
2	D	14	DT	O5'-P-OP2	-8.03	98.47	105.70
2	C	5	DG	O5'-P-OP2	-7.56	98.90	105.70
2	D	10	DG	O5'-P-OP1	7.35	119.53	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	13	DC	O4'-C4'-C3'	-7.01	101.70	104.50
2	C	13	DC	O4'-C4'-C3'	-6.73	101.81	104.50
2	C	18	DG	O3'-P-O5'	-6.70	91.27	104.00
2	D	13	DC	O5'-P-OP2	-6.65	99.72	105.70
2	C	19	DC	O4'-C4'-C3'	-6.46	101.92	104.50
2	C	3	DC	OP2-P-O3'	6.28	119.02	105.20
1	A	1385	ARG	NE-CZ-NH1	6.19	123.40	120.30
2	C	13	DC	C4'-C3'-C2'	-6.14	97.57	103.10
2	D	19	DC	O5'-P-OP1	6.13	118.05	110.70
2	D	11	DC	OP2-P-O3'	6.04	118.50	105.20
2	D	9	DG	O3'-P-O5'	6.04	115.47	104.00
2	C	10	DG	O5'-P-OP1	5.96	117.85	110.70
2	D	2	DG	C4-N9-C1'	-5.94	118.78	126.50
1	B	1033	ARG	NE-CZ-NH2	-5.85	117.38	120.30
2	D	16	DC	C1'-O4'-C4'	-5.83	104.27	110.10
2	D	14	DT	O4'-C4'-C3'	-5.75	102.20	104.50
2	D	5	DG	O3'-P-O5'	-5.71	93.15	104.00
2	D	2	DG	C8-N9-C1'	5.67	134.37	127.00
1	A	1385	ARG	NE-CZ-NH2	-5.58	117.51	120.30
2	C	17	DG	O4'-C1'-N9	-5.56	104.11	108.00
2	C	16	DC	C1'-O4'-C4'	-5.49	104.61	110.10
2	C	9	DG	O3'-P-O5'	5.24	113.96	104.00
1	B	1438	ARG	NE-CZ-NH2	5.22	122.91	120.30
2	D	14	DT	C4'-C3'-C2'	-5.17	98.45	103.10
1	A	1244	ARG	CB-CA-C	5.14	120.68	110.40
2	D	19	DC	C1'-O4'-C4'	-5.14	104.96	110.10
2	C	14	DT	C4'-C3'-C2'	-5.06	98.54	103.10

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1069	ARG	Sidechain
1	A	1385	ARG	Sidechain
1	A	1432	ARG	Sidechain
1	B	1163	ARG	Sidechain
1	B	1342	ARG	Sidechain
1	B	1432	ARG	Sidechain
1	B	499	ARG	Sidechain

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	5322	0	5374	30	0
1	B	5308	0	5350	35	0
2	C	407	0	225	1	0
2	D	390	0	209	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	C	68	0	0	2	0
5	A	269	0	0	5	1
5	B	262	0	0	13	1
5	C	39	0	0	0	0
5	D	33	0	0	0	0
All	All	12100	0	11158	64	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 3.

All (64) 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:B:1138:ASP:OD2	5:B:1601:HOH:O	1.93	0.86
1:A:1084:SER:OG	5:A:1601:HOH:O	1.99	0.80
1:A:1404:ASP:OD2	1:B:1431:ARG:NH2	2.16	0.78
1:B:1273:MET:SD	1:B:1327:LEU:HD13	2.24	0.78
1:B:1413:GLN:HG2	5:B:1624:HOH:O	1.89	0.71
1:A:503:ILE:HD13	1:A:531:LEU:HD21	1.75	0.69
1:B:1390:HIS:NE2	5:B:1602:HOH:O	2.14	0.66
1:A:1066:LYS:HB3	5:A:1764:HOH:O	1.96	0.66
1:B:597:ASN:HD22	1:B:598:PRO:HD2	1.62	0.65
1:B:493:PHE:CE1	1:B:530:PRO:HB2	2.34	0.62
1:A:1279:GLU:HG2	1:A:1282:ARG:HH22	1.63	0.61
1:A:503:ILE:CD1	1:A:531:LEU:HD21	2.31	0.60
1:B:529:ARG:NH2	1:B:611:ALA:HB1	2.17	0.59
1:A:1438:ARG:HH12	1:A:1442:GLU:HG2	1.68	0.58
1:A:1373:LYS:HD3	5:A:1839:HOH:O	2.04	0.58
1:B:1066:LYS:HB3	5:B:1765:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:449:SER:HB2	5:B:1740:HOH:O	2.05	0.56
1:A:1423:GLN:OE1	1:B:1431:ARG:NH1	2.38	0.53
1:A:1438:ARG:HH12	1:A:1442:GLU:CG	2.23	0.52
1:A:424:LYS:O	1:A:426:PRO:HD3	2.09	0.52
1:B:1081:HIS:HD2	2:D:8:DG:OP1	1.93	0.51
1:B:1081:HIS:HE1	5:B:1794:HOH:O	1.93	0.51
1:A:1479:ARG:HD2	5:A:1715:HOH:O	2.10	0.51
4:C:101[A]:A1BU9:C20	2:D:10:DG:C2	2.93	0.51
1:A:443:THR:HG22	1:A:454:ILE:CD1	2.41	0.50
1:A:1323:LYS:HA	1:A:1323:LYS:HE3	1.92	0.50
1:B:460:LYS:HG3	2:D:8:DG:H1'	1.94	0.50
1:A:506:MET:HG2	1:A:583:LEU:HD11	1.94	0.49
1:B:1272:ARG:HG3	1:B:1272:ARG:HH11	1.78	0.49
1:B:1058:MET:HG2	1:B:1065:LYS:CG	2.43	0.49
1:A:448:ASP:H	1:A:452:GLN:NE2	2.10	0.48
1:B:492:ASP:N	1:B:492:ASP:OD1	2.44	0.48
1:B:1245:SER:OG	1:B:1327:LEU:HD12	2.12	0.48
1:B:506:MET:HG2	1:B:583:LEU:HD11	1.96	0.48
1:A:470:ASP:O	1:A:474:ASN:ND2	2.45	0.47
1:B:1058:MET:HG2	1:B:1065:LYS:HG3	1.97	0.47
1:A:1058:MET:HG2	1:A:1065:LYS:HG3	1.96	0.46
1:B:597:ASN:HD22	1:B:598:PRO:CD	2.29	0.46
1:B:1414:ARG:NE	5:B:1618:HOH:O	2.50	0.45
1:A:1427:ASP:OD1	1:B:1431:ARG:NH1	2.27	0.45
1:A:1144:ILE:HD12	1:A:1144:ILE:O	2.17	0.45
1:A:1054:ASN:HA	1:A:1128:MET:CE	2.48	0.44
1:A:1180:ALA:O	1:A:1336:ILE:HD12	2.18	0.44
1:A:1144:ILE:HD12	1:A:1144:ILE:C	2.38	0.43
2:C:10:DG:C2	4:C:101[B]:A1BU9:C20	3.01	0.43
1:B:529:ARG:N	1:B:530:PRO:CD	2.82	0.43
1:A:1438:ARG:NH1	1:A:1442:GLU:HG2	2.31	0.43
1:B:1046:HIS:ND1	5:B:1607:HOH:O	2.36	0.43
1:A:1234:TYR:O	1:A:1347:ASN:HB2	2.20	0.42
1:B:443:THR:HG22	1:B:454:ILE:CD1	2.50	0.42
1:A:529:ARG:N	1:A:530:PRO:CD	2.83	0.42
1:A:585:GLU:O	1:A:585:GLU:HG2	2.19	0.42
1:B:1234:TYR:O	1:B:1347:ASN:HB2	2.18	0.42
1:B:1121:MET:CE	5:B:1798:HOH:O	2.68	0.41
1:B:444:LYS:HD3	5:B:1755:HOH:O	2.20	0.41
1:B:529:ARG:HH21	1:B:611:ALA:HB1	1.84	0.41
1:A:1019:ARG:NH1	5:A:1609:HOH:O	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1390:HIS:CE1	5:B:1602:HOH:O	2.67	0.41
1:A:1279:GLU:HG2	1:A:1282:ARG:NH2	2.32	0.41
1:B:1013:ASN:ND2	5:B:1625:HOH:O	2.53	0.41
1:A:1034:ALA:O	1:A:1043:LYS:HE2	2.20	0.40
1:B:639:TYR:CE1	1:B:1342:ARG:HG2	2.55	0.40
1:B:1138:ASP:HB2	5:B:1601:HOH:O	2.21	0.40
1:B:1205:SER:OG	1:B:1208:GLU:HG3	2.21	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)
5:A:1848:HOH:O	5:B:1851:HOH:O[5_554]	2.16	0.04

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	668/693 (96%)	651 (98%)	16 (2%)	1 (0%)	48	42
1	B	666/693 (96%)	647 (97%)	19 (3%)	0	100	100
All	All	1334/1386 (96%)	1298 (97%)	35 (3%)	1 (0%)	48	42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1033	ARG

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	574/591 (97%)	565 (98%)	9 (2%)	58	55
1	B	572/591 (97%)	560 (98%)	12 (2%)	48	43
All	All	1146/1182 (97%)	1125 (98%)	21 (2%)	54	49

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	425	SER
1	A	426	PRO
1	A	619	GLU
1	A	1066	LYS
1	A	1299	ARG
1	A	1323	LYS
1	A	1404	ASP
1	A	1410	SER
1	A	1432	ARG
1	B	444	LYS
1	B	492	ASP
1	B	501	HIS
1	B	597	ASN
1	B	1013	ASN
1	B	1275	GLU
1	B	1299	ARG
1	B	1327	LEU
1	B	1396	SER
1	B	1405	LYS
1	B	1408	MET
1	B	1450	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	452	GLN
1	A	1413	GLN
1	B	474	ASN
1	B	597	ASN
1	B	1013	ASN

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Mol	Chain	Res	Type
1	B	1081	HIS
1	B	1320	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	$\#\|Z\| > 2$
4	A1BU9	C	101[A]	-	38,38,38	2.10	6 (15%)	47,53,53	2.50	12 (25%)
4	A1BU9	C	101[B]	-	38,38,38	2.02	10 (26%)	47,53,53	2.45	10 (21%)

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
4	A1BU9	C	101[A]	-	-	4/15/34/34	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	A1BU9	C	101[B]	-	-	5/15/34/34	1/5/5/5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	101[B]	A1BU9	C19-C18	-6.71	1.30	1.41
4	C	101[A]	A1BU9	C19-C18	-6.67	1.30	1.41
4	C	101[A]	A1BU9	C19-C20	5.39	1.48	1.36
4	C	101[A]	A1BU9	C23-C24	5.28	1.52	1.42
4	C	101[B]	A1BU9	C23-C24	5.23	1.52	1.42
4	C	101[B]	A1BU9	O4-C21	4.66	1.46	1.37
4	C	101[A]	A1BU9	O4-C21	4.49	1.46	1.37
4	C	101[A]	A1BU9	C5-S1	-3.50	1.71	1.76
4	C	101[B]	A1BU9	C5-S1	-3.43	1.71	1.76
4	C	101[B]	A1BU9	C20-C21	-2.78	1.33	1.38
4	C	101[A]	A1BU9	C20-C21	-2.44	1.34	1.38
4	C	101[B]	A1BU9	C8-N1	-2.35	1.32	1.35
4	C	101[B]	A1BU9	C13-C12	2.35	1.55	1.50
4	C	101[B]	A1BU9	C19-C20	2.29	1.41	1.36
4	C	101[B]	A1BU9	C18-N3	-2.21	1.33	1.37
4	C	101[B]	A1BU9	C25-C10	2.09	1.53	1.51

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	101[B]	A1BU9	C19-C18-C24	-9.50	108.89	119.13
4	C	101[A]	A1BU9	C19-C18-C24	-8.58	109.89	119.13
4	C	101[B]	A1BU9	C20-C21-C23	-6.92	111.83	120.83
4	C	101[A]	A1BU9	C20-C21-C23	-6.04	112.98	120.83
4	C	101[B]	A1BU9	C19-C18-N3	5.57	127.51	118.55
4	C	101[A]	A1BU9	C10-N2-C1	5.51	132.98	122.56
4	C	101[A]	A1BU9	C2-C1-N2	-5.07	107.64	117.04
4	C	101[A]	A1BU9	C19-C18-N3	4.70	126.11	118.55
4	C	101[B]	A1BU9	C10-N2-C1	4.12	130.35	122.56
4	C	101[B]	A1BU9	C20-C19-C18	3.78	125.33	120.80
4	C	101[A]	A1BU9	O1-C1-N2	3.65	129.40	122.47
4	C	101[A]	A1BU9	C25-O5-C12	3.50	117.07	112.24
4	C	101[B]	A1BU9	C11-O3-C12	3.41	116.93	112.24
4	C	101[A]	A1BU9	C11-O3-C12	3.29	116.78	112.24
4	C	101[A]	A1BU9	C20-C19-C18	3.19	124.62	120.80
4	C	101[A]	A1BU9	O2-C8-C6	-3.16	117.67	121.38
4	C	101[A]	A1BU9	C6-C8-N1	2.70	120.52	116.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	101[B]	A1BU9	O1-C1-N2	2.54	127.29	122.47
4	C	101[B]	A1BU9	C13-C14-C15	2.40	118.57	112.08
4	C	101[B]	A1BU9	C15-C24-C18	2.14	119.65	117.76
4	C	101[B]	A1BU9	C9-C7-C5	2.11	121.85	119.31
4	C	101[A]	A1BU9	C6-S1-C5	2.07	101.11	97.37

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	101[A]	A1BU9	C25-C10-N2-C1
4	C	101[A]	A1BU9	C12-C13-C14-C15
4	C	101[B]	A1BU9	O5-C12-C13-C14
4	C	101[B]	A1BU9	O3-C12-C13-C14
4	C	101[A]	A1BU9	C13-C14-C15-C16
4	C	101[A]	A1BU9	C13-C14-C15-C24
4	C	101[B]	A1BU9	C13-C14-C15-C24
4	C	101[B]	A1BU9	C13-C14-C15-C16
4	C	101[B]	A1BU9	C25-C10-N2-C1

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	101[B]	A1BU9	C10-C11-C12-C25-O3-O5

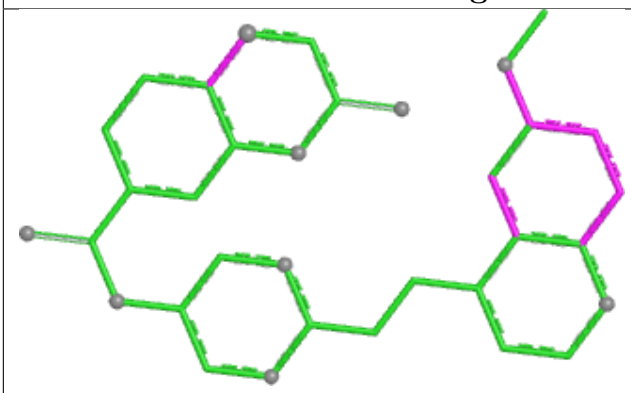
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	101[A]	A1BU9	1	0
4	C	101[B]	A1BU9	1	0

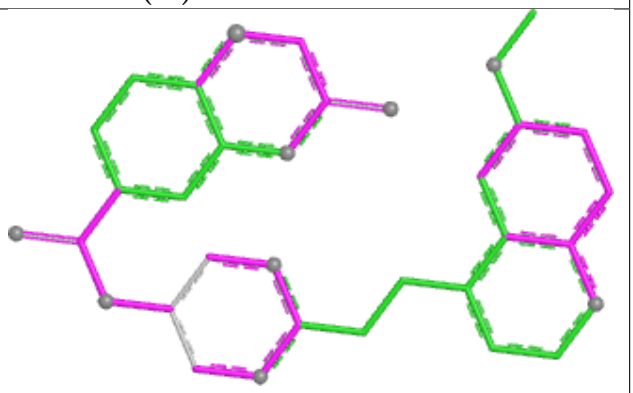
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

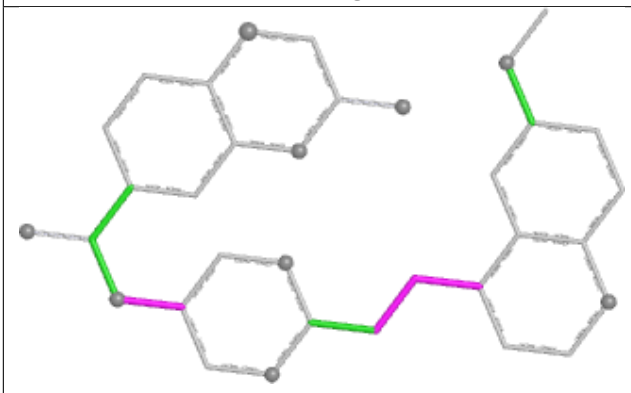
Ligand A1BU9 C 101 (A)



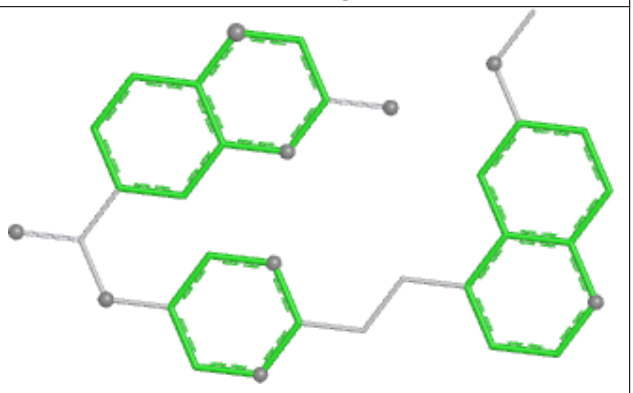
Bond lengths



Bond angles

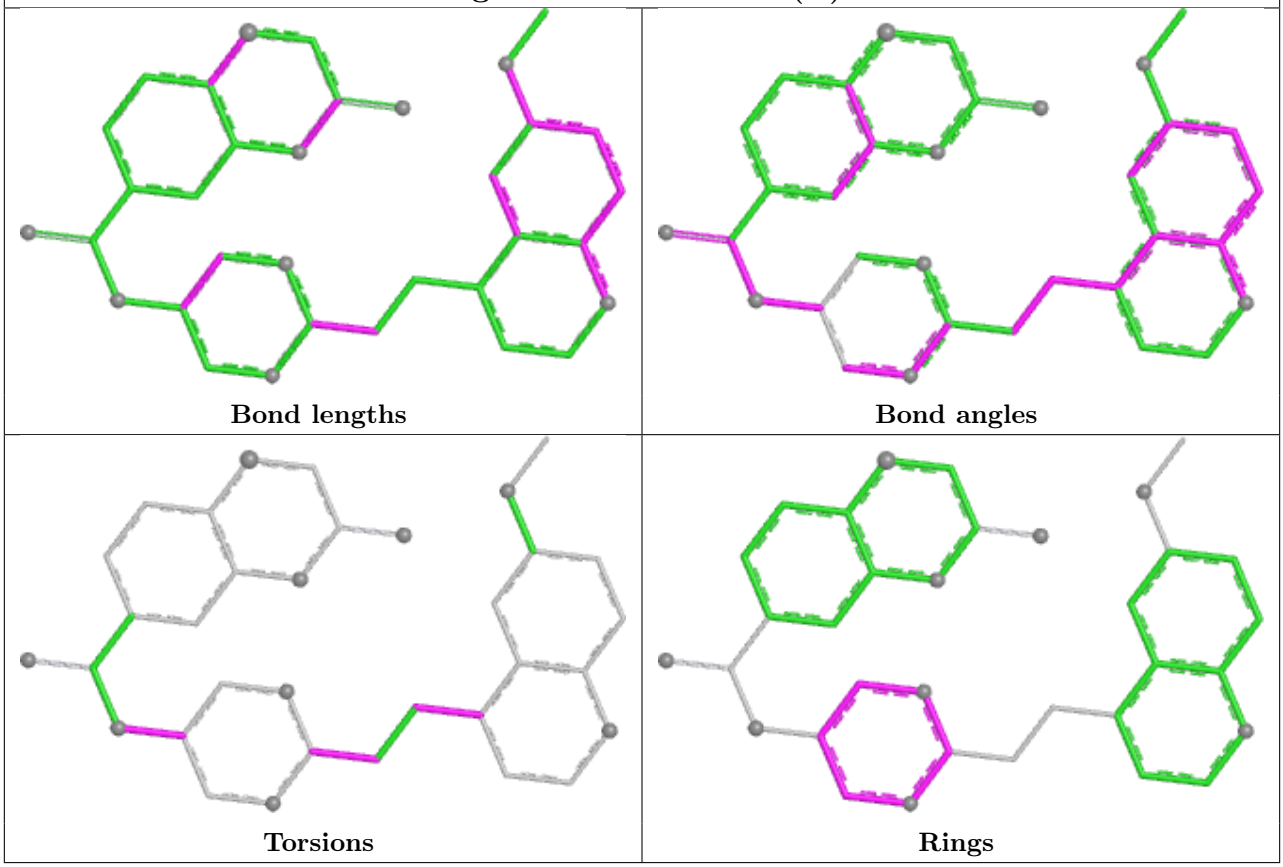


Torsions



Rings

Ligand A1BU9 C 101 (B)



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, 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	672/693 (96%)	-0.39	4 (0%)	85	88	38, 52, 73, 106	0
1	B	670/693 (96%)	-0.42	1 (0%)	92	93	37, 50, 75, 90	0
2	C	20/20 (100%)	-0.97	0	100	100	40, 47, 60, 62	0
2	D	20/20 (100%)	-0.87	0	100	100	40, 49, 79, 94	0
All	All	1382/1426 (96%)	-0.42	5 (0%)	89	91	37, 51, 74, 106	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1490	LEU	3.7
1	A	638	VAL	2.6
1	A	639	TYR	2.4
1	A	1490	LEU	2.3
1	A	640	ALA	2.3

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

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

6.3 Carbohydrates

There are no monosaccharides 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,

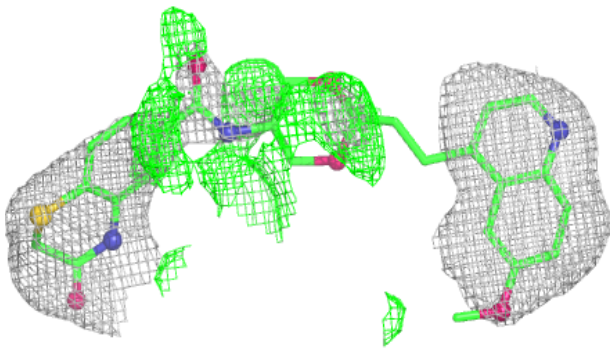
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

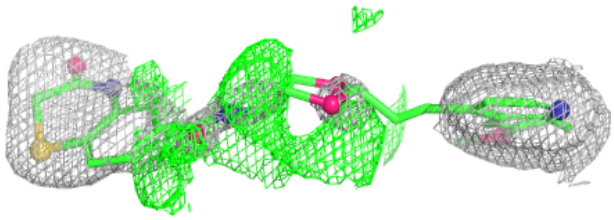
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	A1BU9	C	101[A]	34/34	0.94	0.17	44,53,58,61	34
4	A1BU9	C	101[B]	34/34	0.94	0.17	38,45,56,57	34
3	MN	A	1501	1/1	1.00	0.04	47,47,47,47	0
3	MN	B	1501	1/1	1.00	0.03	46,46,46,46	0

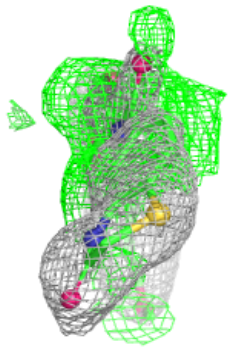
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1BU9 C 101 (A):

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

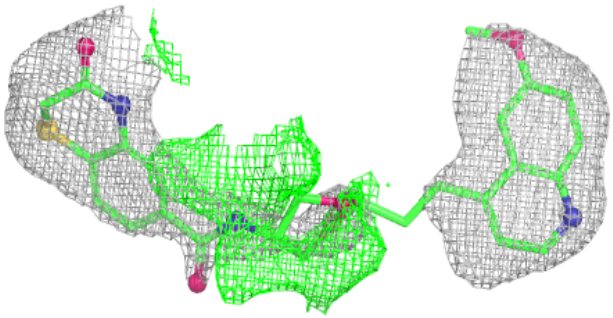


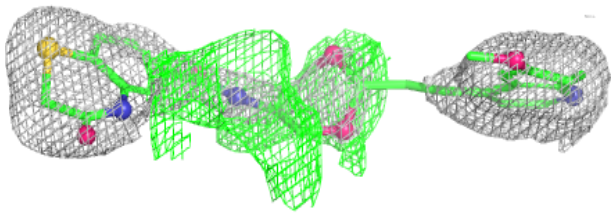


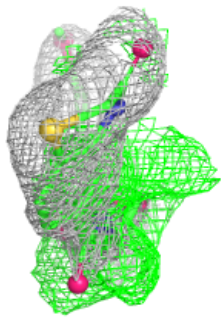


Electron density around A1BU9 C 101 (B):

$2mF_o$-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.