



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2022 – 02:05 PM EDT

PDB ID : 6MG0  
Title : Crystal structure of a 5-domain construct of LgrA in the thiolation state  
Authors : Reimer, J.M.; Eivaskhani, M.; Harb, I.; Schmeing, T.M.  
Deposited on : 2018-09-12  
Resolution : 6.00 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](mailto: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>.

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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 : 2.29  
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) : 2.29

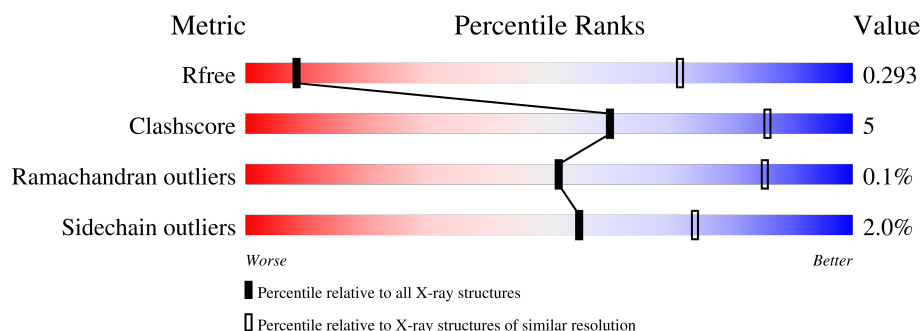
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 6.00 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	1000 (8.00-3.88)
Clashscore	141614	1049 (8.00-3.90)
Ramachandran outliers	138981	1016 (8.00-3.86)
Sidechain outliers	138945	1017 (8.00-3.82)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	1728	 85% 12% ..
1	B	1728	 87% 11% .

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 27074 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 Linear gramicidin synthase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1692	Total	C	N	O	S	0	0	0
			13501	8621	2308	2514	58			
1	B	1687	Total	C	N	O	S	0	0	0
			13473	8601	2307	2507	58			

There are 26 discrepancies between the modelled and reference sequences:

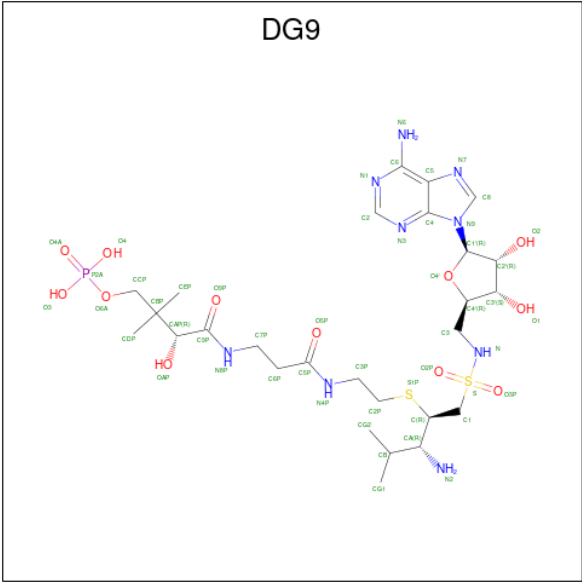
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q70LM7
A	0	ALA	-	expression tag	UNP Q70LM7
A	1	MET	-	expression tag	UNP Q70LM7
A	2	GLY	-	expression tag	UNP Q70LM7
A	1718	ALA	-	expression tag	UNP Q70LM7
A	1719	ALA	-	expression tag	UNP Q70LM7
A	1720	ALA	-	expression tag	UNP Q70LM7
A	1721	GLU	-	expression tag	UNP Q70LM7
A	1722	ASN	-	expression tag	UNP Q70LM7
A	1723	LEU	-	expression tag	UNP Q70LM7
A	1724	TYR	-	expression tag	UNP Q70LM7
A	1725	PHE	-	expression tag	UNP Q70LM7
A	1726	GLN	-	expression tag	UNP Q70LM7
B	-1	GLY	-	expression tag	UNP Q70LM7
B	0	ALA	-	expression tag	UNP Q70LM7
B	1	MET	-	expression tag	UNP Q70LM7
B	2	GLY	-	expression tag	UNP Q70LM7
B	1718	ALA	-	expression tag	UNP Q70LM7
B	1719	ALA	-	expression tag	UNP Q70LM7
B	1720	ALA	-	expression tag	UNP Q70LM7
B	1721	GLU	-	expression tag	UNP Q70LM7
B	1722	ASN	-	expression tag	UNP Q70LM7
B	1723	LEU	-	expression tag	UNP Q70LM7
B	1724	TYR	-	expression tag	UNP Q70LM7
B	1725	PHE	-	expression tag	UNP Q70LM7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1726	GLN	-	expression tag	UNP Q70LM7

- Molecule 2 is 5'-([[(2R,3R)-3-amino-2-{[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-{[oxido(oxo)phosphonio]oxy}butanoyl]-beta-alanyl}amino)ethyl]sulfanyl}-4-methylpentyl]sulfonyl}amino)-5'-deoxyadenosine (three-letter code: DG9) (formula: C<sub>27</sub>H<sub>48</sub>N<sub>9</sub>O<sub>12</sub>PS<sub>2</sub>).

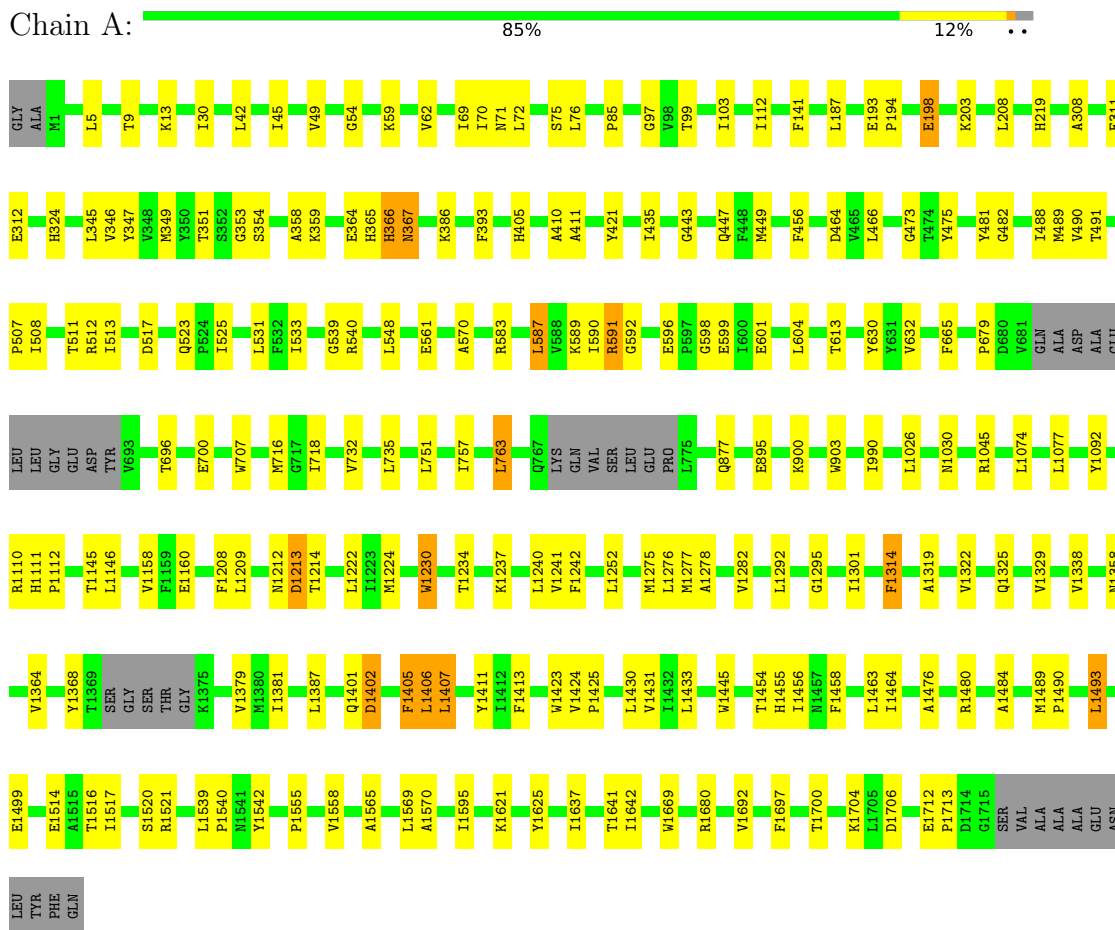


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			50	27	9	11	1	2		
2	B	1	Total	C	N	O	P	S	0	0
			50	27	9	11	1	2		

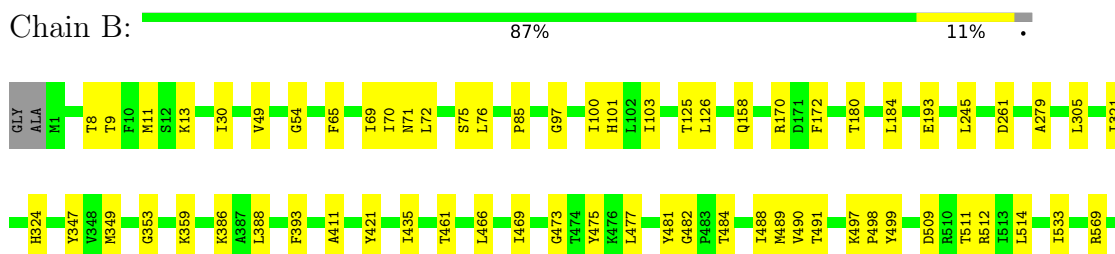
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: Linear gramicidin synthase subunit A



- Molecule 1: Linear gramicidin synthase subunit A



L581		P1112	K1377	I1595	L1636	D1652	L1659	L1663	L1674	R1675	L1678	Y1685	M1686	I1687	F1691	G1715	SER	VAL	ALA	ALA	ALA	GLU	ASN	LEU	TYR	PHE	GLN																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	161.55Å 212.89Å 253.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	78.44 – 6.00 78.44 – 6.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (78.44-6.00) 98.5 (78.44-6.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.58 (at 6.18Å)	Xtriage
Refinement program	PHENIX (dev_3092: ???)	Depositor
R, $R_{free}$	0.244 , 0.294 0.244 , 0.293	Depositor DCC
$R_{free}$ test set	1125 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	280.3	Xtriage
Anisotropy	0.440	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 353.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	27074	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	379.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DG9

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	0/13798	0.44	0/18728
1	B	0.27	0/13769	0.43	0/18682
All	All	0.27	0/27567	0.44	0/37410

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	13501	0	13437	147	0
1	B	13473	0	13418	102	0
2	A	50	0	46	7	0
2	B	50	0	46	8	0
All	All	27074	0	26947	248	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 5.

All (248) 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:1214:THR:HB	1:A:1540:PRO:HA	1.58	0.85
1:A:604:LEU:HG	1:A:613:THR:HG21	1.65	0.76
1:B:639:HIS:ND1	1:B:724:GLU:HG2	2.03	0.73
1:A:513:ILE:HG12	1:A:533:ILE:CD1	2.19	0.73
1:B:980:ARG:NH1	1:B:1109:ASN:O	2.23	0.71
1:B:245:LEU:HD21	1:B:305:LEU:HD21	1.75	0.69
1:A:763:LEU:HD13	1:A:763:LEU:O	1.92	0.69
1:B:581:LEU:O	1:B:581:LEU:HG	1.92	0.69
1:A:1692:VAL:HG22	1:A:1713:PRO:HB3	1.73	0.69
1:A:696:THR:HB	1:A:1092:TYR:HE2	1.58	0.69
1:B:1565:ALA:HB2	1:B:1595:ILE:HG22	1.76	0.68
1:A:513:ILE:HG12	1:A:533:ILE:HD13	1.75	0.66
1:B:595:ILE:HD11	1:B:627:LEU:HD11	1.78	0.66
1:B:421:TYR:HE1	2:B:2000:DG9:HDP	1.60	0.66
1:A:1565:ALA:HB2	1:A:1595:ILE:HG22	1.76	0.66
1:A:482:GLY:HA3	1:A:489:MET:HA	1.78	0.65
1:A:604:LEU:CG	1:A:613:THR:HG21	2.27	0.64
1:B:388:LEU:HG	1:B:435:ILE:HG21	1.78	0.64
1:A:513:ILE:HG23	1:A:531:LEU:CD2	2.27	0.64
1:A:194:PRO:HB2	1:A:198:GLU:HG2	1.79	0.64
1:A:482:GLY:O	2:A:2000:DG9:N2	2.31	0.64
1:A:5:LEU:HD22	1:A:45:ILE:HD13	1.80	0.63
1:B:490:VAL:HG21	1:B:533:ILE:HD13	1.81	0.63
1:B:76:LEU:HD13	1:B:97:GLY:HA3	1.80	0.62
1:B:421:TYR:CE1	2:B:2000:DG9:HDP	2.35	0.62
1:A:513:ILE:HG23	1:A:531:LEU:HD23	1.82	0.62
1:B:1234:THR:HB	1:B:1237:LYS:HG2	1.81	0.62
1:B:126:LEU:HD11	1:B:184:LEU:HD22	1.81	0.61
1:B:482:GLY:O	2:B:2000:DG9:N2	2.34	0.60
1:A:1490:PRO:HD2	1:A:1493:LEU:HD22	1.84	0.60
1:A:1516:THR:HG22	1:A:1516:THR:O	2.01	0.60
1:B:856:ALA:HB1	1:B:887:PRO:HD3	1.84	0.60
1:A:531:LEU:CD2	1:A:533:ILE:HD11	2.32	0.59
1:A:346:VAL:HA	1:A:365:HIS:CE1	2.38	0.59
1:A:1111:HIS:HB3	1:A:1112:PRO:HD2	1.85	0.59
1:B:615:VAL:HG12	1:B:629:GLY:HA2	1.85	0.58
1:A:367:ASN:OD1	1:A:367:ASN:N	2.36	0.58
1:A:1292:LEU:HD21	1:A:1364:VAL:HG23	1.85	0.58
1:B:590:ILE:HG22	1:B:591:ARG:HG3	1.86	0.58
1:A:630:TYR:OH	1:A:679:PRO:O	2.19	0.57
1:A:589:LYS:HG3	2:A:2000:DG9:O4'	2.04	0.57
1:A:1275:MET:HB3	1:A:1322:VAL:HG22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:481:TYR:CE1	2:B:2000:DG9:H2'	2.40	0.56
1:B:812:ILE:HG12	1:B:1132:MET:HG2	1.87	0.56
1:A:364:GLU:HB2	1:A:367:ASN:OD1	2.04	0.56
2:A:2000:DG9:N	2:A:2000:DG9:S1P	2.79	0.56
2:B:2000:DG9:N	2:B:2000:DG9:S1P	2.78	0.56
1:B:1275:MET:HB3	1:B:1322:VAL:HG22	1.88	0.55
1:A:1234:THR:HG22	1:A:1237:LYS:CB	2.37	0.55
1:B:718:ILE:HG13	1:B:719:ASP:N	2.21	0.55
1:A:1208:PHE:HA	1:A:1212:ASN:CB	2.37	0.55
1:A:531:LEU:HD12	1:A:570:ALA:CB	2.38	0.54
1:A:587:LEU:HD23	1:A:596:GLU:HG2	1.91	0.53
1:B:1385:ALA:O	1:B:1516:THR:HG21	2.09	0.53
1:A:1401:GLN:HG3	1:A:1402:ASP:N	2.22	0.53
1:A:1680:ARG:HG3	1:B:982:PRO:CG	2.39	0.53
1:B:193:GLU:HA	1:B:512:ARG:HD2	1.90	0.53
1:A:367:ASN:ND2	1:A:539:GLY:HA2	2.25	0.52
1:B:1675:ARG:HA	1:B:1678:LEU:HD12	1.90	0.52
1:A:1641:THR:HG21	1:A:1669:TRP:HZ2	1.75	0.52
1:B:1514:GLU:OE1	1:B:1514:GLU:N	2.40	0.52
1:A:507:PRO:HG3	1:A:513:ILE:HD12	1.92	0.52
1:A:718:ILE:HG23	1:A:757:ILE:HB	1.91	0.52
1:A:735:LEU:HD23	1:A:751:LEU:HD11	1.92	0.51
1:B:8:THR:OG1	1:B:11:MET:HB2	2.11	0.51
1:A:877:GLN:HB3	1:A:903:TRP:CH2	2.46	0.51
1:A:1680:ARG:HG3	1:B:982:PRO:HG3	1.93	0.51
1:B:9:THR:OG1	1:B:54:GLY:N	2.29	0.51
1:B:966:LEU:HA	1:B:970:LEU:HD21	1.92	0.51
1:A:353:GLY:HA2	1:A:359:LYS:HE3	1.93	0.51
1:A:732:VAL:HG13	1:A:751:LEU:HD12	1.92	0.51
1:A:604:LEU:CD2	1:A:613:THR:HG21	2.41	0.51
1:A:49:VAL:HG22	1:A:70:ILE:HD11	1.93	0.51
1:A:1445:TRP:HH2	1:A:1476:ALA:HB2	1.76	0.50
1:B:739:LEU:HD13	1:B:746:LEU:HD12	1.92	0.50
1:A:71:ASN:HB2	1:A:103:ILE:HD11	1.92	0.50
1:B:466:LEU:HD21	1:B:477:LEU:HD21	1.91	0.50
1:A:1240:LEU:HD11	1:A:1252:LEU:HD13	1.93	0.50
1:A:1405:PHE:HD1	1:A:1406:LEU:H	1.59	0.50
1:B:125:THR:HA	1:B:180:THR:HA	1.93	0.50
1:A:481:TYR:CE1	2:A:2000:DG9:H2'	2.47	0.50
1:A:346:VAL:HB	1:A:365:HIS:CE1	2.47	0.50
1:A:1381:ILE:HG12	1:A:1570:ALA:CB	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1277:MET:HB3	1:B:1301:ILE:HB	1.93	0.50
1:A:193:GLU:HA	1:A:512:ARG:HD2	1.92	0.50
1:A:490:VAL:HG13	1:A:491:THR:HG23	1.94	0.50
1:B:1230:TRP:NE1	1:B:1424:VAL:O	2.44	0.50
1:B:1424:VAL:N	1:B:1425:PRO:HD2	2.27	0.50
1:A:421:TYR:HE1	2:A:2000:DG9:HDP	1.77	0.49
1:B:589:LYS:HZ3	2:B:2000:DG9:HN	1.58	0.49
1:B:633:ALA:O	1:B:661:HIS:NE2	2.37	0.49
1:A:1277:MET:HB3	1:A:1301:ILE:HB	1.94	0.49
1:B:1659:LEU:HD23	1:B:1659:LEU:H	1.78	0.49
1:A:596:GLU:HB3	1:A:599:GLU:HB3	1.93	0.49
1:A:13:LYS:HG2	1:A:30:ILE:HG21	1.94	0.49
1:A:590:ILE:HG22	1:A:591:ARG:HG2	1.94	0.49
1:A:632:VAL:HG21	1:A:665:PHE:HD2	1.77	0.49
1:B:812:ILE:HD12	1:B:902:LEU:HD23	1.95	0.49
1:A:346:VAL:CA	1:A:365:HIS:CE1	2.96	0.49
1:A:359:LYS:HZ2	1:A:548:LEU:HD21	1.78	0.49
1:A:366:HIS:C	1:A:366:HIS:CD2	2.86	0.48
1:A:1424:VAL:N	1:A:1425:PRO:HD2	2.27	0.48
1:B:1405:PHE:HD1	1:B:1406:LEU:H	1.59	0.48
1:A:354:SER:H	1:A:359:LYS:HE3	1.78	0.48
1:B:1678:LEU:HD13	1:B:1687:ILE:HG23	1.94	0.48
1:A:517:ASP:HB3	1:A:523:GLN:CD	2.34	0.48
1:A:1214:THR:HB	1:A:1540:PRO:CA	2.38	0.48
1:A:1276:LEU:O	1:A:1301:ILE:N	2.46	0.48
1:A:59:LYS:HA	1:A:62:VAL:HG12	1.94	0.48
1:B:776:ARG:NH2	1:B:948:GLU:OE1	2.47	0.48
1:A:1230:TRP:HA	1:A:1230:TRP:CE3	2.48	0.48
1:B:1240:LEU:HD11	1:B:1252:LEU:HD13	1.96	0.48
1:B:279:ALA:HB1	1:B:347:TYR:HA	1.96	0.47
1:A:72:LEU:HD21	1:A:141:PHE:CD1	2.49	0.47
1:A:405:HIS:HB3	1:A:410:ALA:HB3	1.96	0.47
1:A:193:GLU:OE2	1:A:561:GLU:OE2	2.32	0.47
1:A:1329:VAL:HG13	1:A:1338:VAL:HG11	1.95	0.47
1:B:787:SER:OG	1:B:790:GLU:HG3	2.13	0.47
1:A:1230:TRP:HA	1:A:1230:TRP:HE3	1.80	0.47
1:B:1027:SER:OG	1:B:1069:HIS:NE2	2.46	0.47
1:A:513:ILE:CG2	1:A:531:LEU:CD2	2.93	0.47
1:A:1208:PHE:HA	1:A:1212:ASN:HB3	1.96	0.47
1:A:1445:TRP:CH2	1:A:1476:ALA:HB2	2.50	0.47
1:A:1700:THR:HG21	1:A:1706:ASP:OD2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:591:ARG:HH22	1:B:653:TYR:HA	1.80	0.47
1:A:1145:THR:HB	1:A:1160:GLU:HB3	1.97	0.47
1:B:353:GLY:HA2	1:B:359:LYS:HE3	1.96	0.47
1:B:1406:LEU:HD22	1:B:1456:ILE:HG23	1.96	0.47
1:B:497:LYS:HE2	1:B:499:TYR:CE1	2.50	0.47
1:A:1026:LEU:O	1:A:1030:ASN:ND2	2.35	0.46
1:B:482:GLY:HA3	1:B:489:MET:HA	1.96	0.46
1:B:1106:ARG:HG2	1:B:1112:PRO:HG3	1.96	0.46
1:A:464:ASP:OD2	1:A:592:GLY:N	2.48	0.46
1:B:71:ASN:HB2	1:B:103:ILE:HD11	1.98	0.46
1:B:473:GLY:HA3	1:B:475:TYR:CE2	2.50	0.46
1:B:1407:LEU:O	1:B:1433:LEU:HB3	2.15	0.46
1:A:707:TRP:HE3	1:A:716:MET:HE2	1.80	0.46
1:A:1209:LEU:HD12	1:A:1213:ASP:OD2	2.16	0.46
1:A:1484:ALA:HB3	1:A:1489:MET:CE	2.46	0.46
1:B:484:THR:N	2:B:2000:DG9:O2P	2.34	0.46
1:B:589:LYS:NZ	2:B:2000:DG9:HN	2.14	0.46
1:B:1636:LEU:HD13	1:B:1663:LEU:HD21	1.97	0.46
1:A:1407:LEU:O	1:A:1433:LEU:HB3	2.16	0.46
1:A:42:LEU:HA	1:A:45:ILE:HD12	1.98	0.46
1:A:700:GLU:HB3	1:A:718:ILE:HD11	1.97	0.46
1:A:1208:PHE:HA	1:A:1212:ASN:HB2	1.97	0.46
1:A:1712:GLU:HG2	1:A:1713:PRO:HD2	1.97	0.45
1:B:778:LEU:HG	1:B:941:SER:HA	1.98	0.45
1:A:1406:LEU:HD22	1:A:1456:ILE:HG23	1.98	0.45
1:B:1145:THR:HB	1:B:1160:GLU:HB3	1.99	0.45
1:B:1423:TRP:NE1	1:B:1430:LEU:HD22	2.31	0.45
1:A:1074:LEU:HA	1:A:1077:LEU:HD12	1.98	0.45
1:A:1423:TRP:NE1	1:A:1430:LEU:HD22	2.31	0.45
1:A:99:THR:HG23	1:A:112:ILE:HG23	1.99	0.45
1:A:1637:ILE:HG23	1:A:1642:ILE:HG22	1.99	0.45
1:B:49:VAL:HG22	1:B:70:ILE:HD11	1.99	0.45
1:B:386:LYS:HG2	1:B:411:ALA:HB3	1.99	0.45
1:B:918:ILE:HD11	1:B:1045:ARG:NH2	2.32	0.45
1:B:1314:PHE:CE1	1:B:1319:ALA:HB3	2.52	0.45
1:B:1539:LEU:O	1:B:1542:TYR:HB2	2.17	0.45
1:A:386:LYS:HG2	1:A:411:ALA:HB3	1.99	0.44
1:B:753:THR:HG23	1:B:754:HIS:CD2	2.52	0.44
1:B:1276:LEU:O	1:B:1301:ILE:N	2.49	0.44
1:B:1652:ASP:OD1	1:B:1652:ASP:N	2.42	0.44
1:A:366:HIS:CD2	1:A:366:HIS:O	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1514:GLU:OE1	1:A:1514:GLU:N	2.42	0.44
1:A:1278:ALA:HB1	1:A:1325:GLN:HG3	1.98	0.44
1:A:1314:PHE:CE1	1:A:1319:ALA:HB3	2.52	0.44
1:A:1413:PHE:HZ	1:A:1704:LYS:HE3	1.82	0.44
1:A:1242:PHE:HD2	1:A:1282:VAL:HG23	1.82	0.44
1:A:1539:LEU:O	1:A:1542:TYR:HB2	2.17	0.44
1:B:172:PHE:HZ	1:B:514:LEU:HD13	1.82	0.44
1:B:1518:TYR:O	1:B:1542:TYR:OH	2.36	0.44
1:A:9:THR:OG1	1:A:54:GLY:N	2.43	0.44
1:A:345:LEU:HD21	1:A:540:ARG:HD3	2.00	0.44
1:A:421:TYR:CE1	2:A:2000:DG9:HDP	2.53	0.44
1:A:592:GLY:O	2:A:2000:DG9:N4P	2.50	0.44
1:A:598:GLY:HA2	1:A:601:GLU:HG3	2.00	0.44
1:A:1110:ARG:HD2	1:A:1625:TYR:CE1	2.52	0.44
1:A:1208:PHE:O	1:A:1212:ASN:HB3	2.18	0.44
1:B:858:LEU:HD23	1:B:858:LEU:HA	1.88	0.44
1:A:203:LYS:HD2	1:A:208:LEU:HD21	1.99	0.44
1:A:1045:ARG:O	1:A:1045:ARG:HG3	2.17	0.44
1:B:1329:VAL:HG13	1:B:1338:VAL:HG11	1.98	0.44
1:A:1234:THR:CG2	1:A:1237:LYS:CB	2.96	0.44
1:B:588:VAL:HG21	1:B:617:ALA:CB	2.48	0.44
1:A:69:ILE:HG12	1:A:103:ILE:HD12	2.00	0.44
1:A:346:VAL:HB	1:A:365:HIS:CG	2.53	0.44
1:A:443:GLY:O	1:A:447:GLN:HG2	2.17	0.44
1:A:531:LEU:CD2	1:A:533:ILE:CD1	2.95	0.44
1:B:13:LYS:HG2	1:B:30:ILE:HG21	2.00	0.44
1:B:347:TYR:CD1	1:B:349:MET:HG3	2.53	0.44
1:A:1413:PHE:CZ	1:A:1704:LYS:HE3	2.53	0.43
1:A:347:TYR:CD1	1:A:349:MET:HG3	2.54	0.43
1:B:1674:LEU:HD22	1:B:1691:PHE:CZ	2.53	0.43
1:A:895:GLU:HG3	1:A:900:LYS:HG2	2.01	0.43
1:B:305:LEU:HD23	1:B:321:ILE:HB	2.00	0.43
1:A:587:LEU:CD2	1:A:596:GLU:HG2	2.48	0.43
1:A:75:SER:HB3	1:A:85:PRO:HB2	1.99	0.43
1:A:351:THR:O	1:A:358:ALA:HB1	2.18	0.43
1:B:75:SER:HB3	1:B:85:PRO:HB2	2.00	0.43
1:B:1454:THR:HG23	1:B:1480:ARG:CB	2.48	0.43
1:A:1569:LEU:HD23	1:A:1569:LEU:HA	1.84	0.43
1:B:1214:THR:HB	1:B:1540:PRO:HA	2.01	0.43
1:B:569:ARG:HH11	1:B:584:LEU:HD21	1.84	0.43
1:A:1222:LEU:HA	1:A:1387:LEU:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:883:LEU:HA	1:B:888:LEU:HD21	2.00	0.43
1:A:1555:PRO:HG2	1:A:1558:VAL:HG21	2.01	0.42
1:B:72:LEU:HD23	1:B:100:ILE:HG12	2.01	0.42
1:B:469:ILE:HD13	1:B:498:PRO:HB3	2.00	0.42
1:A:508:ILE:O	1:A:511:THR:OG1	2.34	0.42
1:B:718:ILE:HG13	1:B:719:ASP:H	1.83	0.42
1:A:1295:GLY:HA2	1:A:1358:ASN:ND2	2.34	0.42
1:A:311:GLU:HG3	1:A:312:GLU:N	2.35	0.42
1:B:1483:LEU:HB3	1:B:1509:ILE:HG13	2.02	0.42
1:A:359:LYS:HZ2	1:A:548:LEU:CD2	2.32	0.42
1:B:1278:ALA:HB1	1:B:1325:GLN:HG3	2.01	0.42
1:A:354:SER:O	1:A:596:GLU:HG3	2.20	0.42
1:A:449:MET:HB2	1:A:449:MET:HE2	1.98	0.42
1:A:490:VAL:HG21	1:A:533:ILE:HD12	2.02	0.42
1:A:76:LEU:HD13	1:A:97:GLY:HA3	2.02	0.41
1:A:1379:VAL:HG12	1:A:1381:ILE:HG13	2.02	0.41
1:B:639:HIS:CD2	1:B:659:PHE:HD2	2.38	0.41
1:B:1298:TYR:CE1	1:B:1365:TYR:HB3	2.55	0.41
1:A:990:ILE:HG23	1:A:1158:VAL:HG13	2.01	0.41
1:A:1454:THR:HG23	1:A:1480:ARG:CB	2.50	0.41
1:A:435:ILE:HG22	1:A:456:PHE:CE1	2.54	0.41
1:A:1621:LYS:HA	1:A:1625:TYR:O	2.20	0.41
1:B:461:THR:HG21	1:B:466:LEU:HD22	2.03	0.41
1:A:1146:LEU:HA	1:A:1146:LEU:HD23	1.84	0.41
1:B:481:TYR:HB3	1:B:491:THR:OG1	2.20	0.41
1:A:1680:ARG:HG3	1:B:982:PRO:HG2	2.03	0.41
1:B:595:ILE:CD1	1:B:627:LEU:HD11	2.49	0.41
1:B:1242:PHE:HD2	1:B:1282:VAL:HG23	1.86	0.41
1:A:1241:VAL:HB	1:A:1431:VAL:HG22	2.02	0.41
1:B:509:ASP:O	1:B:511:THR:HG23	2.21	0.41
1:A:473:GLY:HA3	1:A:475:TYR:CE2	2.55	0.41
1:A:513:ILE:CG2	1:A:531:LEU:HD21	2.51	0.41
1:B:588:VAL:HG21	1:B:617:ALA:HB2	2.03	0.41
1:B:1259:LEU:HD13	1:B:1347:TYR:CE2	2.56	0.41
1:B:1385:ALA:C	1:B:1516:THR:HG21	2.41	0.41
1:A:187:LEU:HB2	1:A:525:ILE:HG13	2.02	0.41
1:A:308:ALA:O	1:A:311:GLU:HG2	2.20	0.41
1:A:346:VAL:HB	1:A:365:HIS:CD2	2.55	0.41
1:A:596:GLU:O	1:A:599:GLU:HG2	2.21	0.41
1:B:65:PHE:HB2	1:B:69:ILE:HD11	2.03	0.41
1:B:713:ILE:HA	1:B:714:PRO:HD3	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:587:LEU:H	1:A:587:LEU:HG	1.59	0.40

There are no symmetry-related clashes.

## 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	1684/1728 (98%)	1628 (97%)	54 (3%)	2 (0%)	51	85
1	B	1679/1728 (97%)	1626 (97%)	51 (3%)	2 (0%)	51	85
All	All	3363/3456 (97%)	3254 (97%)	105 (3%)	4 (0%)	51	85

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1517	Ile
1	A	1517	Ile
1	A	488	Ile
1	B	488	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	1454/1490 (98%)	1424 (98%)	30 (2%)	53	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	1451/1490 (97%)	1422 (98%)	29 (2%)	55	74
All	All	2905/2980 (98%)	2846 (98%)	59 (2%)	55	74

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	198	GLU
1	A	219	HIS
1	A	324	HIS
1	A	366	HIS
1	A	367	ASN
1	A	393	PHE
1	A	466	LEU
1	A	583	ARG
1	A	587	LEU
1	A	591	ARG
1	A	763	LEU
1	A	1213	ASP
1	A	1224	MET
1	A	1230	TRP
1	A	1314	PHE
1	A	1368	TYR
1	A	1402	ASP
1	A	1405	PHE
1	A	1406	LEU
1	A	1407	LEU
1	A	1411	TYR
1	A	1455	HIS
1	A	1458	PHE
1	A	1463	LEU
1	A	1464	ILE
1	A	1493	LEU
1	A	1499	GLU
1	A	1520	SER
1	A	1521	ARG
1	A	1697	PHE
1	B	101	HIS
1	B	158	GLN
1	B	170	ARG
1	B	261	ASP
1	B	324	HIS
1	B	393	PHE

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Mol	Chain	Res	Type
1	B	587	LEU
1	B	990	ILE
1	B	1230	TRP
1	B	1314	PHE
1	B	1368	TYR
1	B	1377	LYS
1	B	1402	ASP
1	B	1405	PHE
1	B	1406	LEU
1	B	1407	LEU
1	B	1411	TYR
1	B	1412	ILE
1	B	1427	ARG
1	B	1455	HIS
1	B	1458	PHE
1	B	1463	LEU
1	B	1464	ILE
1	B	1493	LEU
1	B	1499	GLU
1	B	1520	SER
1	B	1521	ARG
1	B	1568	SER
1	B	1685	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	366	HIS

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry

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	DG9	A	2000	1	41,52,53	3.62	18 (43%)	45,75,78	2.44	6 (13%)
2	DG9	B	2000	1	41,52,53	3.56	17 (41%)	45,75,78	2.46	9 (20%)

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	DG9	A	2000	1	-	10/43/68/69	0/3/3/3
2	DG9	B	2000	1	-	10/43/68/69	0/3/3/3

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2000	DG9	C3'-C2'	-9.71	1.26	1.53
2	A	2000	DG9	C3'-C2'	-9.67	1.26	1.53
2	A	2000	DG9	O4'-C1'	-9.48	1.27	1.41
2	B	2000	DG9	O4'-C1'	-9.22	1.28	1.41
2	A	2000	DG9	C2'-C1'	8.65	1.66	1.53
2	B	2000	DG9	C2'-C1'	8.60	1.66	1.53
2	A	2000	DG9	C5P-N4P	7.76	1.51	1.33
2	B	2000	DG9	C5P-N4P	7.61	1.50	1.33
2	A	2000	DG9	C9P-N8P	6.05	1.46	1.33
2	B	2000	DG9	C9P-N8P	5.81	1.46	1.33
2	B	2000	DG9	C3-C4'	-4.91	1.40	1.52
2	A	2000	DG9	C3-C4'	-4.90	1.40	1.52
2	B	2000	DG9	O4'-C4'	4.50	1.55	1.45
2	A	2000	DG9	S-N	4.46	1.72	1.61
2	A	2000	DG9	O4'-C4'	4.36	1.54	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2000	DG9	S-N	4.35	1.72	1.61
2	A	2000	DG9	C2P-S1P	3.88	1.86	1.81
2	A	2000	DG9	C6-N6	3.84	1.48	1.34
2	B	2000	DG9	C6-N6	3.82	1.48	1.34
2	B	2000	DG9	C2P-S1P	3.70	1.86	1.81
2	A	2000	DG9	C3-N	3.63	1.53	1.47
2	B	2000	DG9	C3-N	3.57	1.53	1.47
2	A	2000	DG9	O1-C3'	3.19	1.50	1.43
2	B	2000	DG9	O1-C3'	3.17	1.50	1.43
2	A	2000	DG9	OAP-CAP	-2.36	1.38	1.42
2	A	2000	DG9	C2-N3	2.36	1.35	1.32
2	A	2000	DG9	O5P-C5P	-2.32	1.18	1.23
2	B	2000	DG9	C2-N3	2.29	1.35	1.32
2	A	2000	DG9	O2P-S	2.29	1.46	1.43
2	B	2000	DG9	O5P-C5P	-2.23	1.18	1.23
2	B	2000	DG9	O2P-S	2.22	1.46	1.43
2	B	2000	DG9	OAP-CAP	-2.21	1.38	1.42
2	B	2000	DG9	O9P-C9P	-2.13	1.19	1.23
2	A	2000	DG9	O9P-C9P	-2.11	1.19	1.23
2	A	2000	DG9	O3P-S	2.01	1.46	1.43

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2000	DG9	O3P-S-O2P	-13.14	100.32	119.35
2	A	2000	DG9	O3P-S-O2P	-13.06	100.42	119.35
2	A	2000	DG9	C3'-C2'-C1'	4.46	107.69	100.98
2	B	2000	DG9	C3'-C2'-C1'	4.38	107.58	100.98
2	B	2000	DG9	N3-C2-N1	-4.29	121.98	128.68
2	A	2000	DG9	N3-C2-N1	-4.25	122.03	128.68
2	A	2000	DG9	O3P-S-C1	2.92	112.48	107.87
2	B	2000	DG9	C6P-C7P-N8P	-2.73	106.38	111.90
2	B	2000	DG9	O3P-S-C1	2.72	112.16	107.87
2	A	2000	DG9	O3P-S-N	2.28	112.17	106.97
2	B	2000	DG9	C2P-C3P-N4P	-2.18	107.84	112.42
2	B	2000	DG9	C4-C5-N7	-2.15	107.16	109.40
2	B	2000	DG9	O2P-S-C1	2.13	111.24	107.87
2	B	2000	DG9	O3P-S-N	2.13	111.81	106.97
2	A	2000	DG9	C4-C5-N7	-2.11	107.20	109.40

There are no chirality outliers.

All (20) torsion outliers are listed below:

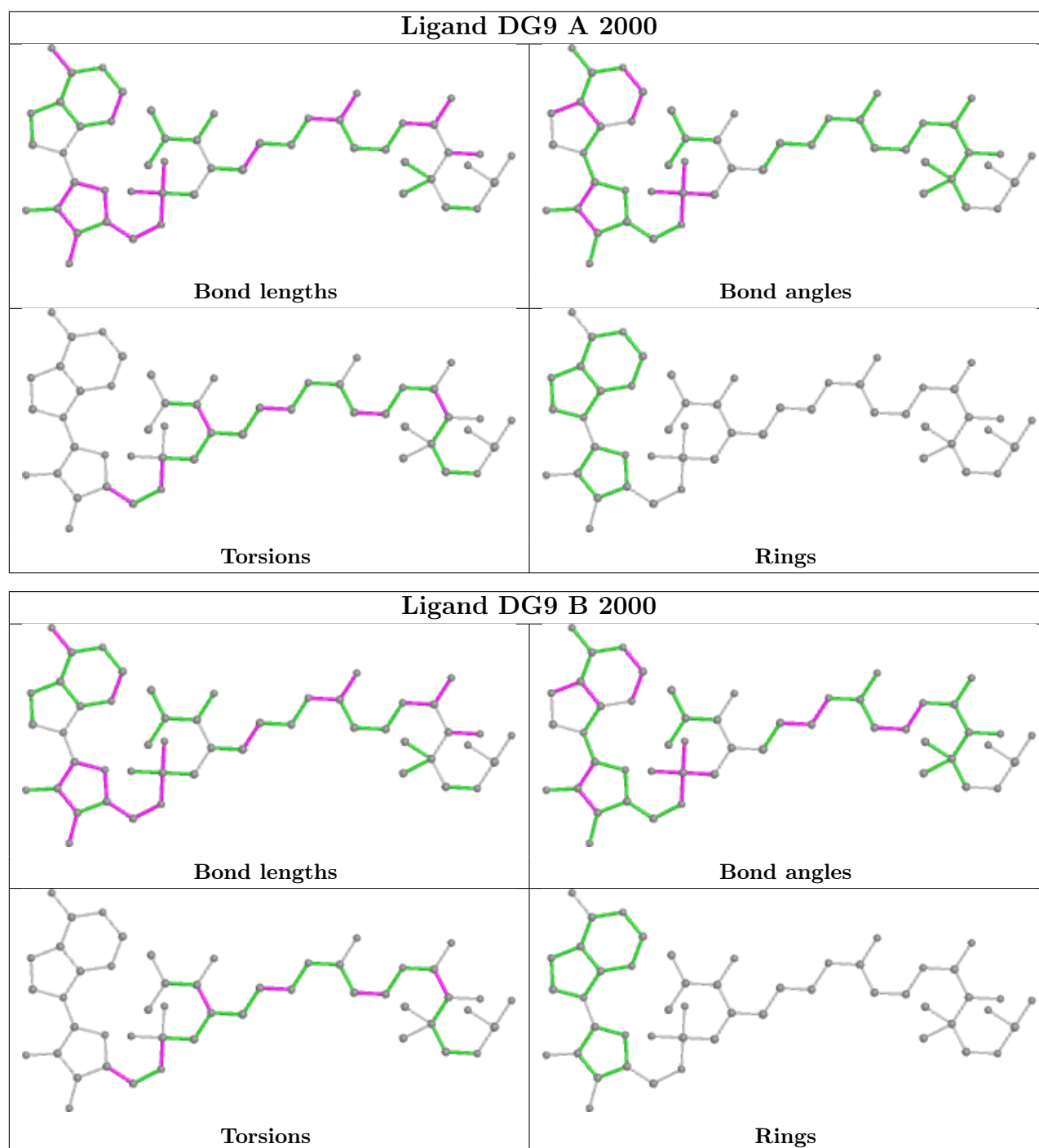
Mol	Chain	Res	Type	Atoms
2	A	2000	DG9	C1-C-CA-N2
2	A	2000	DG9	C3-N-S-C1
2	A	2000	DG9	C3-N-S-O2P
2	A	2000	DG9	N-C3-C4'-C3'
2	A	2000	DG9	N-C3-C4'-O4'
2	A	2000	DG9	S1P-C2P-C3P-N4P
2	A	2000	DG9	C5P-C6P-C7P-N8P
2	B	2000	DG9	C1-C-CA-N2
2	B	2000	DG9	C3-N-S-C1
2	B	2000	DG9	C3-N-S-O2P
2	B	2000	DG9	N-C3-C4'-C3'
2	B	2000	DG9	N-C3-C4'-O4'
2	B	2000	DG9	S1P-C2P-C3P-N4P
2	B	2000	DG9	C5P-C6P-C7P-N8P
2	A	2000	DG9	O9P-C9P-CAP-OAP
2	B	2000	DG9	O9P-C9P-CAP-OAP
2	A	2000	DG9	N8P-C9P-CAP-CBP
2	A	2000	DG9	O9P-C9P-CAP-CBP
2	B	2000	DG9	O9P-C9P-CAP-CBP
2	B	2000	DG9	N8P-C9P-CAP-CBP

There are no ring outliers.

2 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2000	DG9	7	0
2	B	2000	DG9	8	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

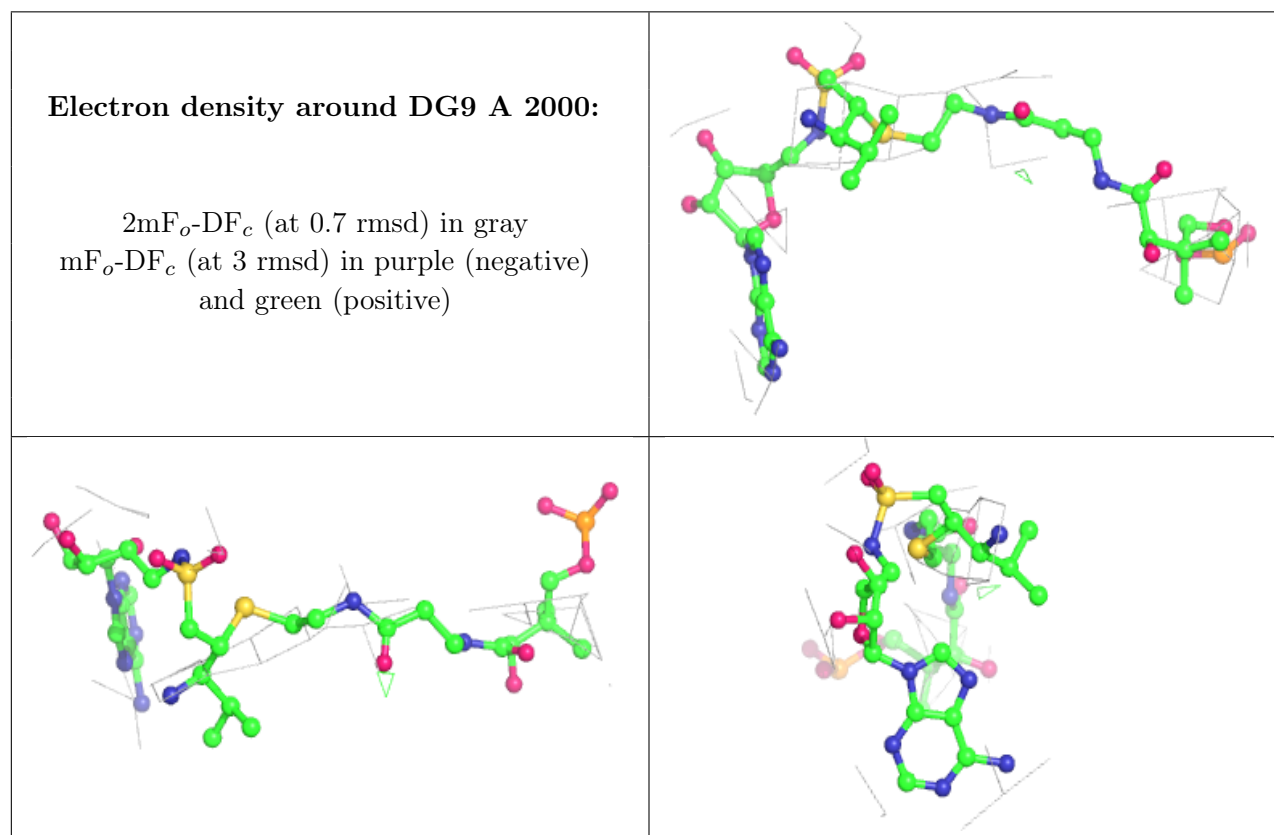
### 6.3 Carbohydrates [i](#)

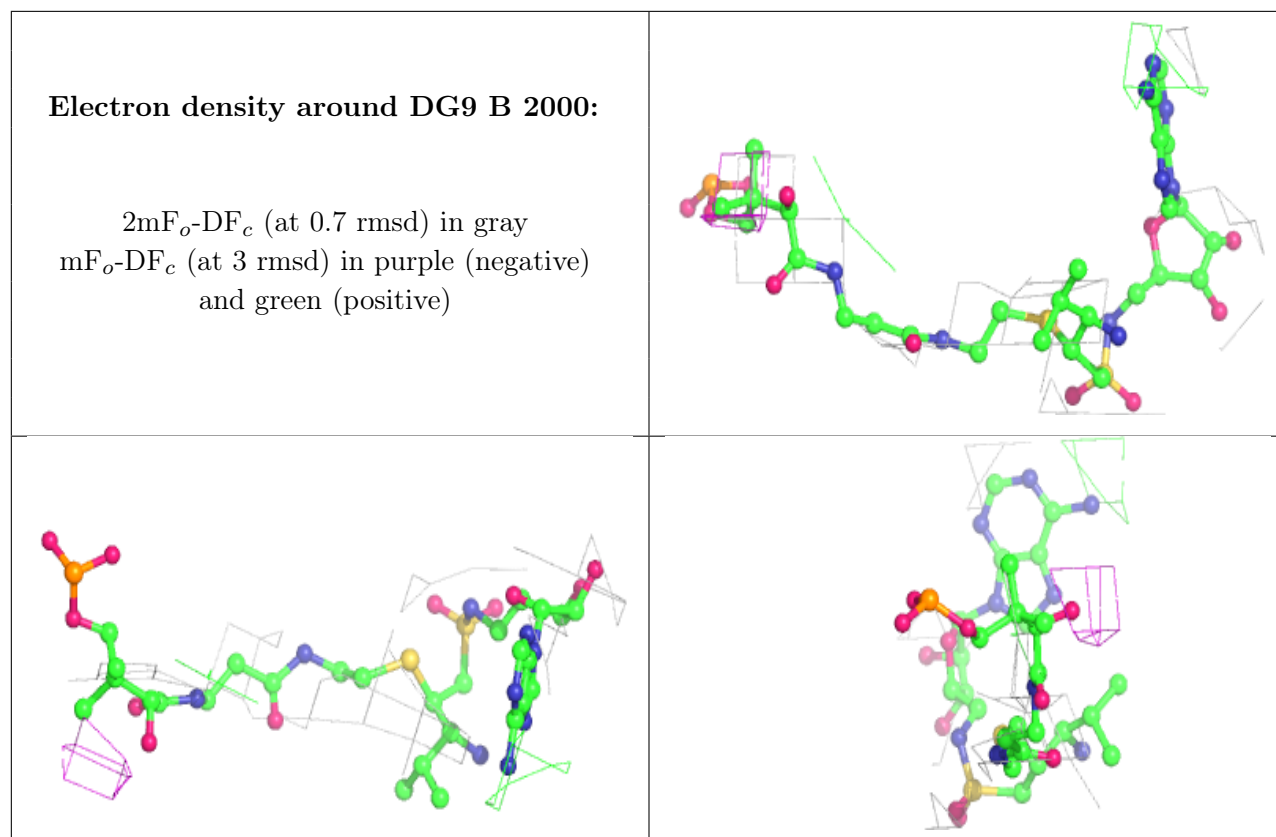
Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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.





## 6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.