



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:14 AM UTC

PDB ID : 6MG0 / pdb_00006mg0
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

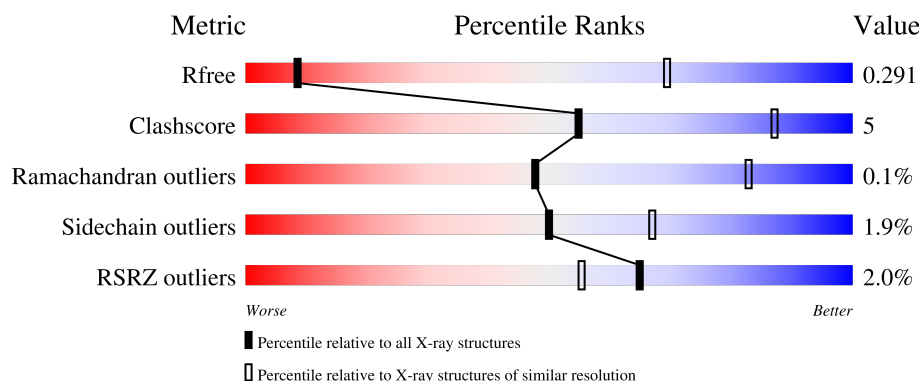
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1143 (8.00-4.00)
Clashscore	190562	1210 (8.00-4.00)
Ramachandran outliers	187476	1034 (8.00-4.00)
Sidechain outliers	187428	1000 (8.00-4.00)
RSRZ outliers	180081	1136 (8.00-4.00)

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

Mol	Chain	Length	Quality of chain
1	A	1728	 2% 85% 12% ..
1	B	1728	 2% 86% 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:

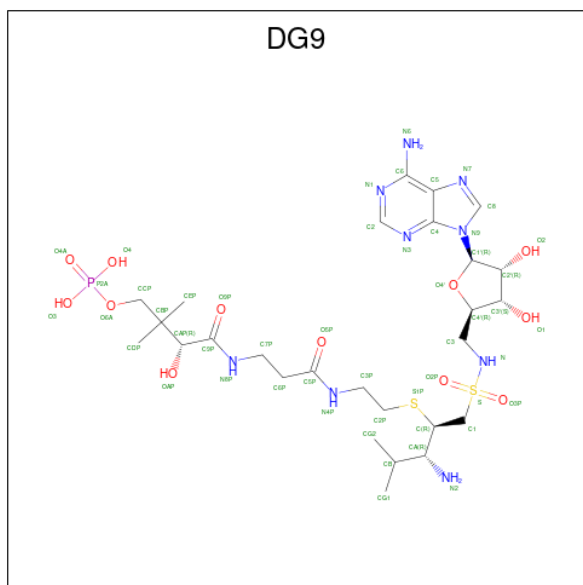
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q70LM7
A	0	ALA	-	expression tag	UNP Q70LM7
A	1	MET	-	expression tag	UNP Q70LM7
A	2	GLY	-	expression tag	UNP Q70LM7
A	1718	ALA	-	expression tag	UNP Q70LM7
A	1719	ALA	-	expression tag	UNP Q70LM7
A	1720	ALA	-	expression tag	UNP 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

Continued on next page...

Continued from previous page...

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

- Molecule 2 is 5'-(5-((2R,3R)-3-amino-2-((2S)-2-((2R)-2-hydroxy-3,3-dimethyl-4-oxo-5-oxo-5H-tetrazol-5-yl)butanoyl)-beta-alanyl)amino)ethyl)sulfanyl)-4-methylpentyl)sulfonyl)amin o)-5'-deoxyadenosine (CCD ID: DG9) (formula: $C_{27}H_{48}N_9O_{12}PS_2$).

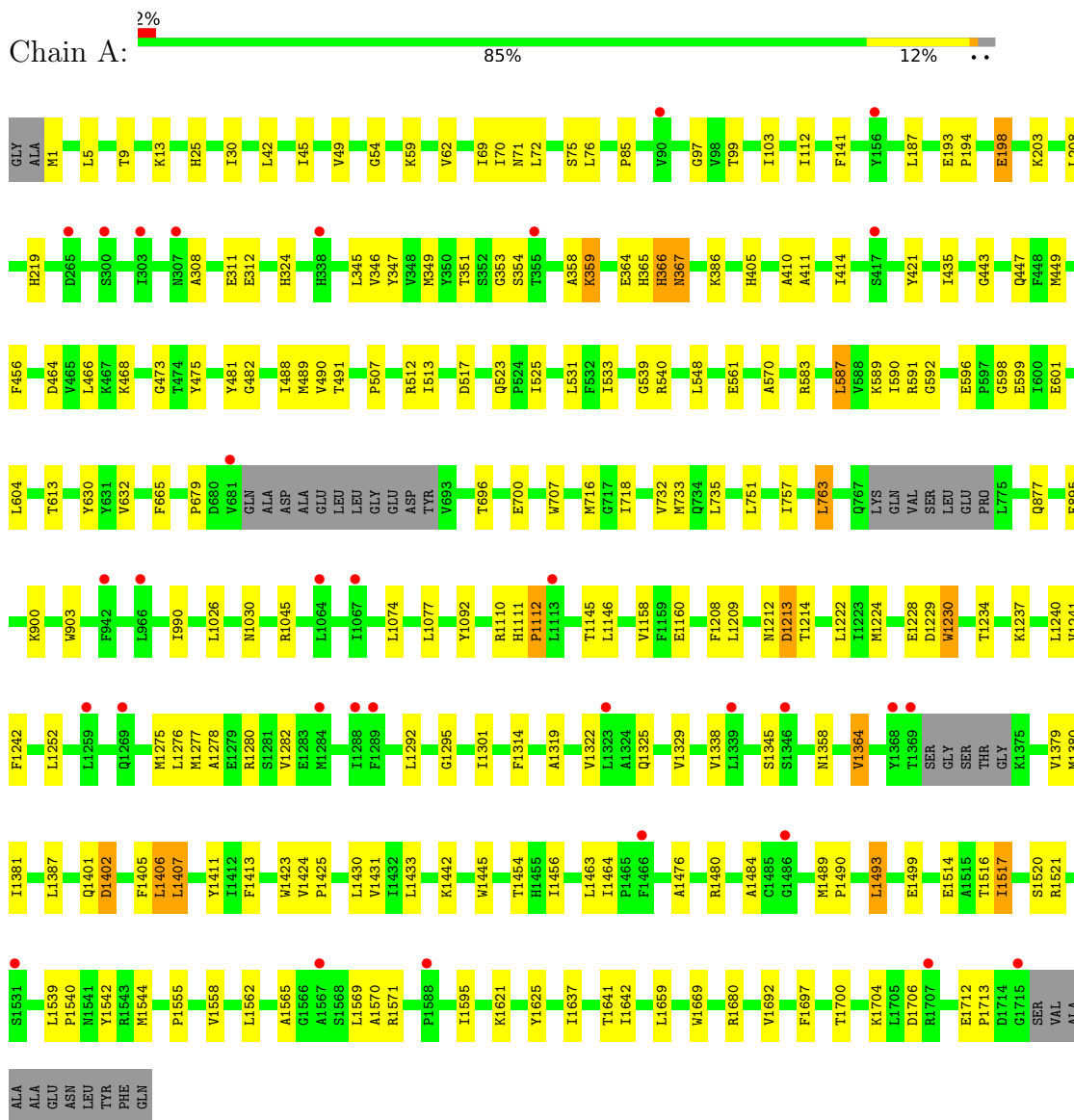


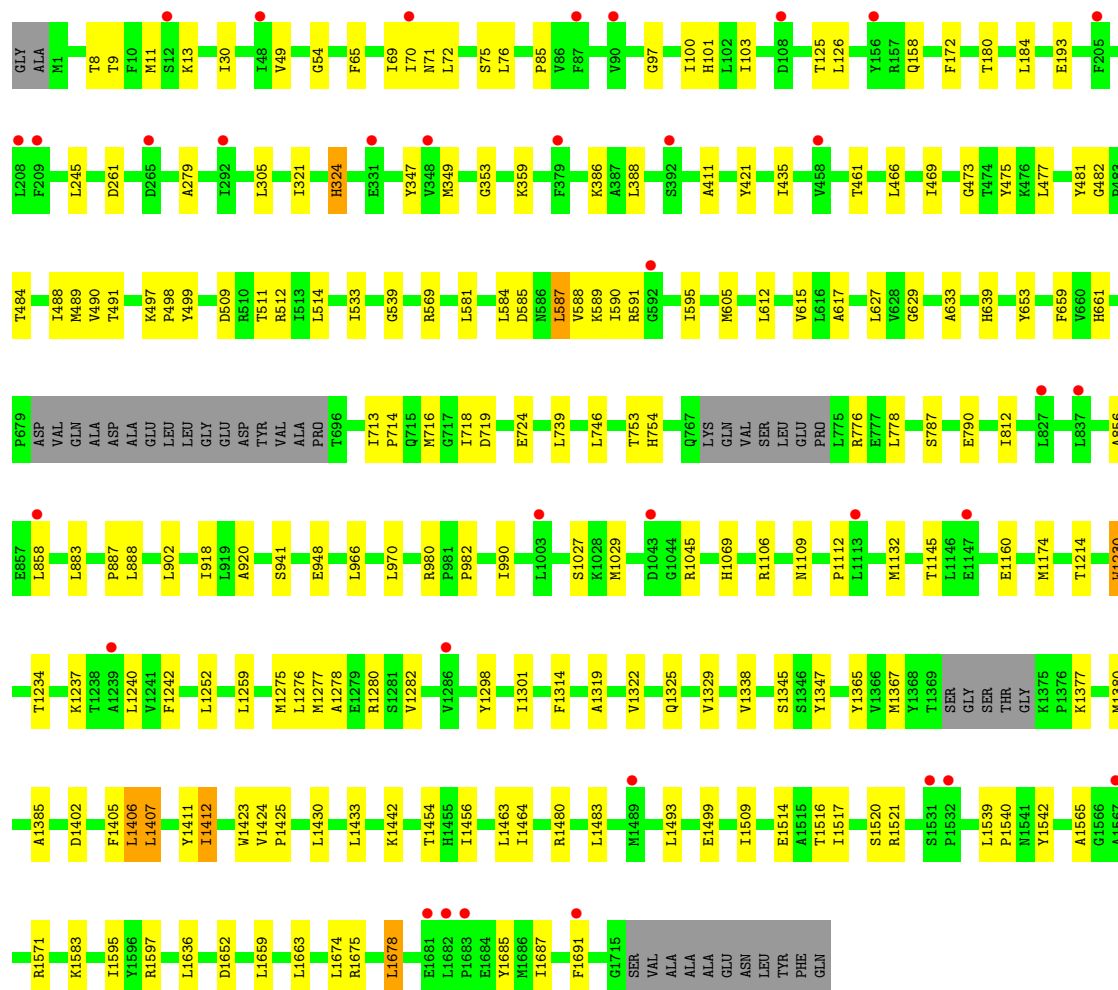
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 50	C 27	N 9	O 11	P 1	S 2	0	0
2	B	1	Total 50	C 27	N 9	O 11	P 1	S 2	0	0

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 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: Linear gramicidin synthase subunit A





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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) 98.4 (78.44-6.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 6.18Å)	Xtriage
Refinement program	PHENIX (dev_3092: ???)	Depositor
R, R_{free}	0.244 , 0.294 0.246 , 0.291	Depositor DCC
R_{free} test set	1125 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	280.3	Xtriage
Anisotropy	0.440	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 383.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.22	0/13798	0.40	5/18728 (0.0%)
1	B	0.21	0/13769	0.37	3/18682 (0.0%)
All	All	0.22	0/27567	0.39	8/37410 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1412	ILE	N-CA-C	-8.18	104.60	112.29
1	A	1229	ASP	CA-C-N	-6.58	110.08	121.66
1	A	1229	ASP	C-N-CA	-6.58	110.08	121.66
1	A	1228	GLU	O-C-N	5.83	128.30	122.12
1	B	539	GLY	CA-C-N	-5.83	111.46	120.31
1	B	539	GLY	C-N-CA	-5.83	111.46	120.31
1	A	1112	PRO	N-CA-C	5.08	122.00	113.78
1	A	1517	ILE	N-CA-C	-5.00	98.93	109.34

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	13501	0	13437	152	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	13473	0	13418	109	0
2	A	50	0	46	7	0
2	B	50	0	46	8	0
All	All	27074	0	26947	260	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 (260) 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:421:TYR:HD1	1:A:733:MET:HE2	1.70	0.57
1:A:1275:MET:HB3	1:A:1322:VAL:HG22	1.87	0.56
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:366:HIS:C	1:A:366:HIS:CD2	2.86	0.53
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:517:ASP:HB3	1:A:523:GLN:CD	2.34	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:1401:GLN:HG3	1:A:1402:ASP:N	2.22	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:1:MET:HE1	1:A:25:HIS:HB2	1.92	0.51
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:589:LYS:HZ3	2:B:2000:DG9:HN	1.60	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: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: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: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:920:ALA:HB1	1:B:1132:MET:HE1	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:1029:MET:HE1	1:B:1174:MET:HG2	1.95	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:B:1380:MET:HE3	1:B:1571:ARG:HG3	1.95	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
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:1209:LEU:HD12	1:A:1213:ASP:OD2	2.16	0.46
1:A:449:MET:HE1	1:A:468:LYS:C	2.40	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:707:TRP:HE3	1:A:716:MET:HE2	1.81	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:B:1385:ALA:C	1:B:1516:THR:HG21	2.41	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:421:TYR:CD1	1:A:733:MET:HE2	2.50	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
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:1380:MET:HE3	1:A:1571:ARG:HG3	2.00	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:B:585:ASP:C	1:B:587:LEU:H	2.26	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
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:B:605:MET:HE2	1:B:612:LEU:HA	2.01	0.42
1:B:718:ILE:HG13	1:B:719:ASP:H	1.83	0.42
1:B:1583:LYS:NZ	1:B:1597:ARG:O	2.44	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:B:324:HIS:ND1	1:B:324:HIS:C	2.77	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:449:MET:HE1	1:A:468:LYS:O	2.19	0.41
1:A:1544:MET:HE2	1:A:1562:LEU:HD11	2.02	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: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
1:A:587:LEU:H	1:A:587:LEU:HG	1.59	0.40
1:B:1367:MET:HE3	1:B:1367:MET:HB3	1.95	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1684/1728 (98%)	1628 (97%)	54 (3%)	2 (0%)	48	83

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	1679/1728 (97%)	1626 (97%)	51 (3%)	2 (0%)	48 83
All	All	3363/3456 (97%)	3254 (97%)	105 (3%)	4 (0%)	48 83

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 ⓘ

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%)	47 65
1	B	1451/1490 (97%)	1426 (98%)	25 (2%)	53 69
All	All	2905/2980 (98%)	2850 (98%)	55 (2%)	50 67

All (55) 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	359	LYS
1	A	366	HIS
1	A	367	ASN
1	A	414	ILE
1	A	466	LEU
1	A	583	ARG
1	A	587	LEU
1	A	763	LEU
1	A	1213	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1224	MET
1	A	1230	TRP
1	A	1280	ARG
1	A	1345	SER
1	A	1364	VAL
1	A	1402	ASP
1	A	1406	LEU
1	A	1407	LEU
1	A	1411	TYR
1	A	1442	LYS
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	1659	LEU
1	A	1697	PHE
1	B	101	HIS
1	B	158	GLN
1	B	261	ASP
1	B	324	HIS
1	B	587	LEU
1	B	716	MET
1	B	990	ILE
1	B	1230	TRP
1	B	1280	ARG
1	B	1345	SER
1	B	1377	LYS
1	B	1402	ASP
1	B	1406	LEU
1	B	1407	LEU
1	B	1411	TYR
1	B	1412	ILE
1	B	1442	LYS
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	1678	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1685	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	HIS
1	A	36	HIS
1	A	211	GLN
1	A	366	HIS
1	A	370	ASN
1	A	447	GLN
1	A	829	GLN
1	A	834	HIS
1	A	1134	HIS
1	A	1541	ASN
1	A	1552	GLN
1	A	1651	ASN
1	B	206	HIS
1	B	235	ASN
1	B	472	ASN
1	B	834	HIS
1	B	1552	GLN

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 ⓘ

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	46,52,53	3.19	21 (45%)	59,75,78	2.46	12 (20%)
2	DG9	B	2000	1	46,52,53	3.14	19 (41%)	59,75,78	2.48	15 (25%)

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	-	13/47/68/69	0/3/3/3
2	DG9	B	2000	1	-	12/47/68/69	0/3/3/3

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2000	DG9	C3'-C2'	-9.81	1.26	1.53
2	A	2000	DG9	C3'-C2'	-9.77	1.26	1.53
2	A	2000	DG9	C5P-N4P	7.44	1.51	1.33
2	B	2000	DG9	C5P-N4P	7.29	1.50	1.33
2	A	2000	DG9	O4'-C1'	-6.13	1.27	1.42
2	B	2000	DG9	O4'-C1'	-5.97	1.28	1.42
2	A	2000	DG9	C9P-N8P	5.63	1.46	1.33
2	A	2000	DG9	C6-N6	5.43	1.48	1.34
2	B	2000	DG9	C9P-N8P	5.41	1.46	1.33
2	B	2000	DG9	C6-N6	5.41	1.48	1.34
2	B	2000	DG9	C3-C4'	-5.03	1.40	1.52
2	A	2000	DG9	C3-C4'	-5.02	1.40	1.52
2	A	2000	DG9	S-N	4.57	1.72	1.61
2	B	2000	DG9	O4'-C4'	4.53	1.55	1.45
2	B	2000	DG9	S-N	4.46	1.72	1.61
2	A	2000	DG9	O4'-C4'	4.39	1.54	1.45
2	A	2000	DG9	C2'-C1'	4.26	1.66	1.53
2	B	2000	DG9	C2'-C1'	4.24	1.66	1.53
2	A	2000	DG9	CCP-CBP	4.02	1.59	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2000	DG9	CCP-CBP	3.96	1.59	1.52
2	A	2000	DG9	C3-N	3.94	1.53	1.47
2	B	2000	DG9	C3-N	3.88	1.53	1.47
2	A	2000	DG9	C2P-S1P	3.52	1.86	1.81
2	B	2000	DG9	C2P-S1P	3.36	1.86	1.81
2	A	2000	DG9	C8-N9	-3.18	1.32	1.37
2	B	2000	DG9	C8-N9	-3.10	1.32	1.37
2	A	2000	DG9	O1-C3'	3.04	1.50	1.43
2	B	2000	DG9	O1-C3'	3.02	1.50	1.43
2	B	2000	DG9	C8-N7	2.54	1.36	1.31
2	A	2000	DG9	C8-N7	2.48	1.36	1.31
2	A	2000	DG9	OAP-CAP	-2.46	1.38	1.42
2	A	2000	DG9	O2P-S	2.38	1.46	1.43
2	A	2000	DG9	O5P-C5P	-2.37	1.18	1.23
2	B	2000	DG9	O2P-S	2.31	1.46	1.43
2	B	2000	DG9	OAP-CAP	-2.31	1.38	1.42
2	B	2000	DG9	O5P-C5P	-2.28	1.18	1.23
2	B	2000	DG9	O9P-C9P	-2.20	1.19	1.23
2	A	2000	DG9	O9P-C9P	-2.19	1.19	1.23
2	A	2000	DG9	CDP-CBP	2.10	1.58	1.53
2	A	2000	DG9	O3P-S	2.08	1.46	1.43

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2000	DG9	O3P-S-O2P	-13.60	100.32	119.34
2	A	2000	DG9	O3P-S-O2P	-13.52	100.42	119.34
2	A	2000	DG9	C5-C4-N3	-5.21	119.54	126.72
2	B	2000	DG9	C5-C4-N3	-5.14	119.64	126.72
2	B	2000	DG9	N3-C2-N1	-4.36	121.98	128.58
2	A	2000	DG9	N3-C2-N1	-4.33	122.03	128.58
2	A	2000	DG9	N3-C4-N9	3.66	133.39	127.17
2	A	2000	DG9	C2-N3-C4	3.52	120.43	111.83
2	B	2000	DG9	C2-N3-C4	3.51	120.41	111.83
2	B	2000	DG9	N3-C4-N9	3.45	133.04	127.17
2	A	2000	DG9	C3'-C2'-C1'	3.29	107.69	101.46
2	B	2000	DG9	C3'-C2'-C1'	3.23	107.58	101.46
2	A	2000	DG9	N9-C8-N7	-3.06	109.60	113.94
2	B	2000	DG9	C4-C5-N7	-2.99	107.16	110.58
2	A	2000	DG9	C4-C5-N7	-2.96	107.20	110.58
2	B	2000	DG9	N9-C8-N7	-2.96	109.74	113.94
2	A	2000	DG9	O3P-S-C1	2.93	112.48	107.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2000	DG9	C5-N7-C8	2.91	108.02	103.45
2	B	2000	DG9	C5-N7-C8	2.84	107.92	103.45
2	B	2000	DG9	O3P-S-C1	2.73	112.16	107.86
2	B	2000	DG9	C6P-C7P-N8P	-2.64	106.38	112.00
2	A	2000	DG9	O3P-S-N	2.27	112.17	107.02
2	A	2000	DG9	C4-N9-C8	2.26	108.11	105.74
2	B	2000	DG9	C2P-C3P-N4P	-2.19	107.84	112.41
2	B	2000	DG9	O2P-S-C1	2.14	111.24	107.86
2	B	2000	DG9	O3P-S-N	2.12	111.81	107.02
2	B	2000	DG9	C4-N9-C8	2.03	107.87	105.74

There are no chirality outliers.

All (25) torsion outliers are listed below:

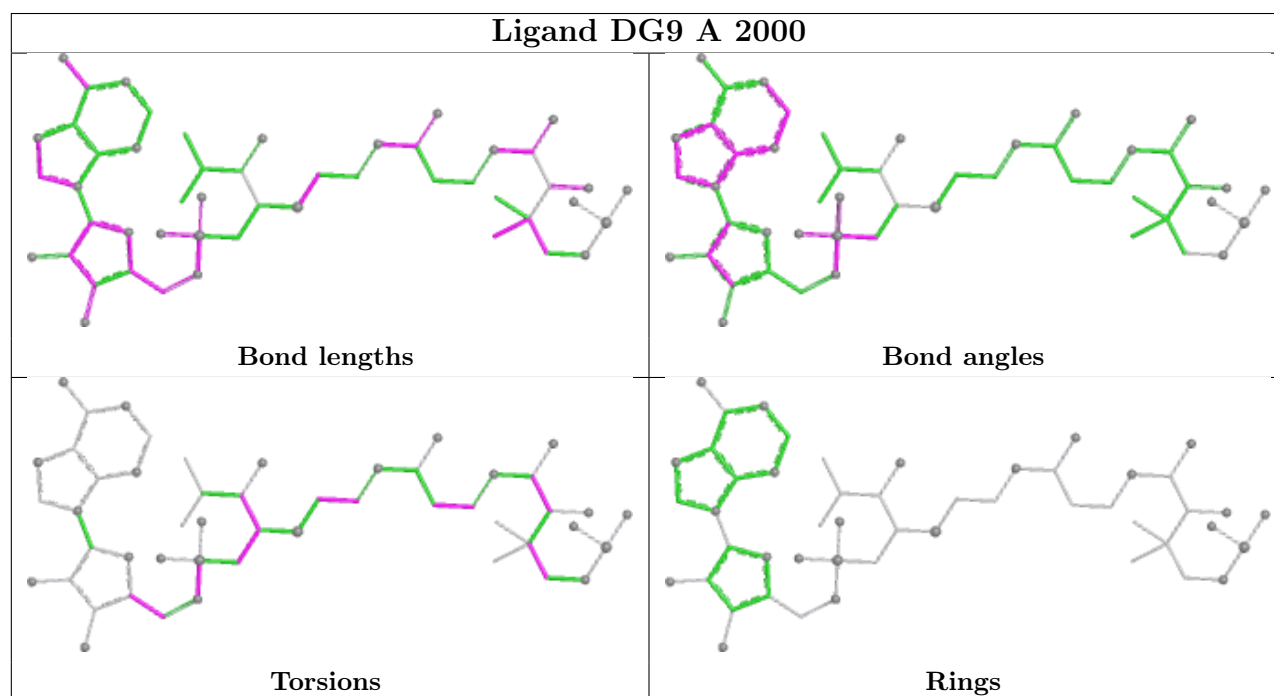
Mol	Chain	Res	Type	Atoms
2	A	2000	DG9	C1-C-CA-N2
2	A	2000	DG9	C3-N-S-C1
2	A	2000	DG9	C3-N-S-O2P
2	A	2000	DG9	N-C3-C4'-C3'
2	A	2000	DG9	N-C3-C4'-O4'
2	A	2000	DG9	S1P-C2P-C3P-N4P
2	A	2000	DG9	C5P-C6P-C7P-N8P
2	B	2000	DG9	C1-C-CA-N2
2	B	2000	DG9	C3-N-S-C1
2	B	2000	DG9	C3-N-S-O2P
2	B	2000	DG9	N-C3-C4'-C3'
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	CA-C-C1-S
2	B	2000	DG9	CA-C-C1-S
2	A	2000	DG9	O9P-C9P-CAP-CBP
2	B	2000	DG9	O9P-C9P-CAP-CBP
2	B	2000	DG9	N8P-C9P-CAP-CBP
2	A	2000	DG9	CDP-CBP-CCP-O6A
2	A	2000	DG9	N8P-C9P-CAP-OAP
2	B	2000	DG9	N8P-C9P-CAP-OAP

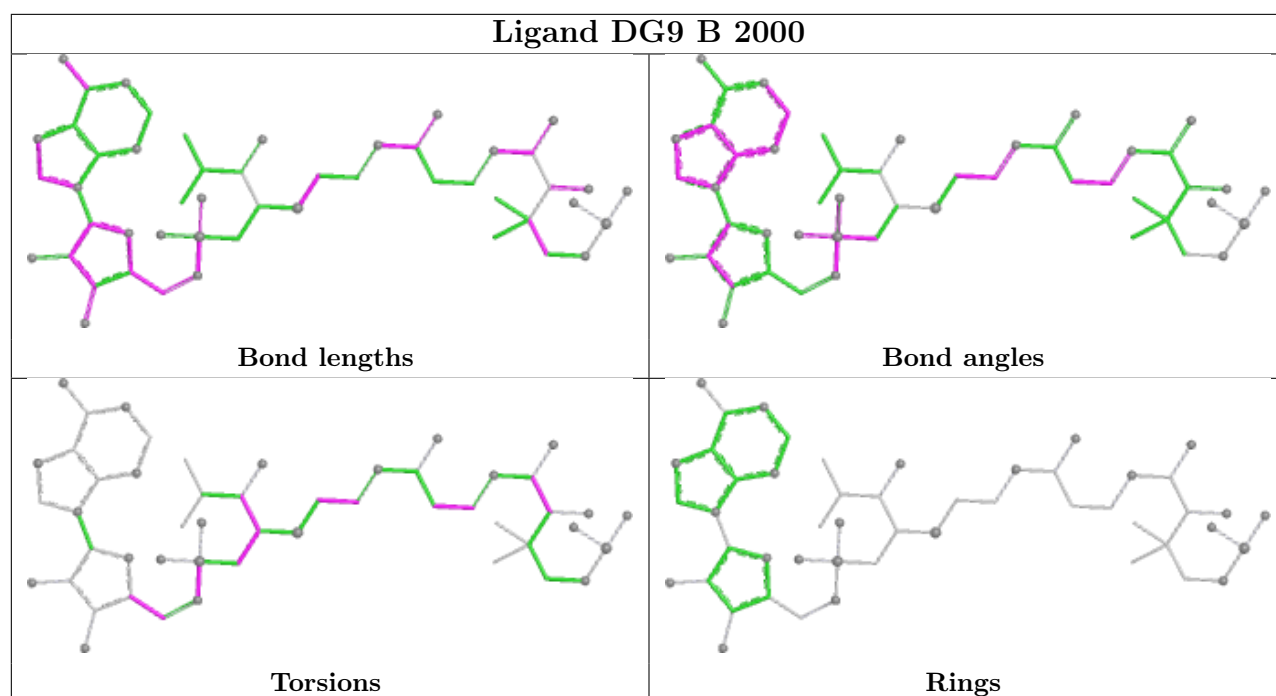
There are no ring outliers.

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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1692/1728 (97%)	0.13	32 (1%) 66 56	234, 335, 411, 568	0
1	B	1687/1728 (97%)	0.14	35 (2%) 63 54	300, 406, 557, 648	0
All	All	3379/3456 (97%)	0.13	67 (1%) 65 55	234, 367, 525, 648	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	205	PHE	4.7
1	A	681	VAL	4.5
1	A	1715	GLY	4.4
1	A	265	ASP	4.1
1	A	1567	ALA	3.8
1	B	592	GLY	3.7
1	B	209	PHE	3.6
1	B	1147	GLU	3.5
1	A	1368	TYR	3.4
1	B	827	LEU	3.3
1	B	265	ASP	3.3
1	B	48	ILE	3.2
1	A	1369	THR	3.0
1	B	70	ILE	2.9
1	B	1239	ALA	2.9
1	A	1289	PHE	2.9
1	B	458	VAL	2.8
1	A	338	HIS	2.8
1	A	417	SER	2.8
1	B	1531	SER	2.8
1	A	307	ASN	2.7
1	B	1003	LEU	2.7
1	B	1286	VAL	2.7
1	A	1067	ILE	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	1683	PRO	2.6
1	A	1346	SER	2.6
1	A	1707	ARG	2.6
1	B	1681	GLU	2.6
1	A	1064	LEU	2.6
1	A	1269	GLN	2.6
1	B	1113	LEU	2.6
1	A	1113	LEU	2.6
1	B	1489	MET	2.6
1	A	1284	MET	2.5
1	A	1466	PHE	2.5
1	B	1682	LEU	2.5
1	B	12	SER	2.4
1	B	392	SER	2.4
1	A	942	PHE	2.4
1	B	858	LEU	2.4
1	A	1339	LEU	2.4
1	B	1567	ALA	2.4
1	B	379	PHE	2.3
1	B	1691	PHE	2.3
1	B	292	ILE	2.3
1	A	1259	LEU	2.3
1	A	303	ILE	2.3
1	A	355	THR	2.3
1	A	1288	ILE	2.3
1	B	837	LEU	2.3
1	A	1486	GLY	2.2
1	A	156	TYR	2.2
1	A	1323	LEU	2.2
1	B	1043	ASP	2.2
1	B	208	LEU	2.2
1	A	1531	SER	2.1
1	B	156	TYR	2.1
1	A	966	LEU	2.1
1	A	300	SER	2.1
1	B	331	GLU	2.1
1	B	1532	PRO	2.1
1	A	90	VAL	2.1
1	B	348	VAL	2.1
1	B	90	VAL	2.1
1	B	108	ASP	2.0
1	A	1588	PRO	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	87	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

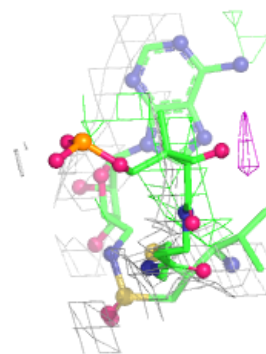
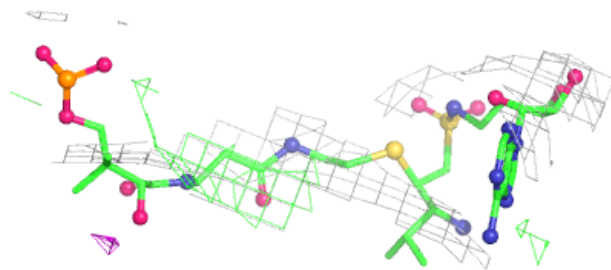
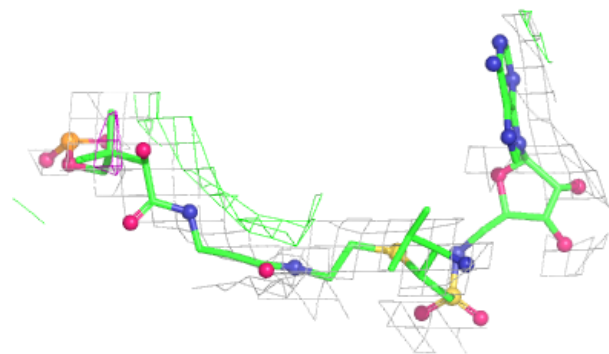
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	DG9	B	2000	50/51	0.85	0.14	334,371,435,460	0
2	DG9	A	2000	50/51	0.90	0.12	266,309,381,385	0

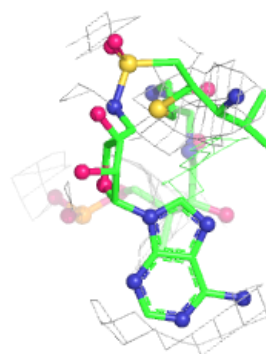
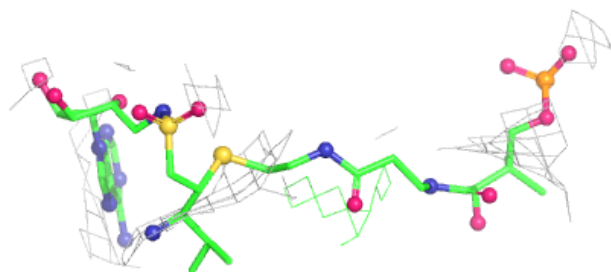
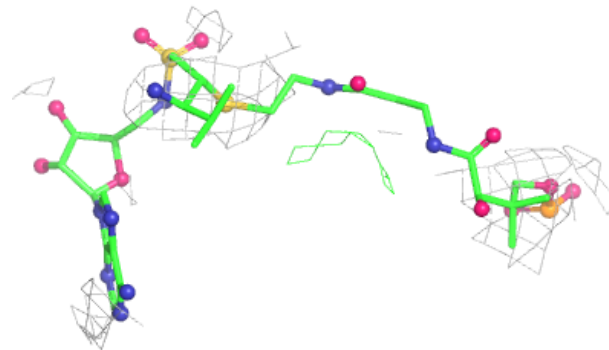
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DG9 B 2000:

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

**Electron density around DG9 A 2000:**

$2mF_o-DF_c$ (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.