



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:19 PM UTC

PDB ID : 4PLB / pdb_00004plb
Title : Crystal Structure of S.A. gyrase-AM8191 complex
Authors : Lu, J.; Patel, S.; Soisson, S.
Deposited on : 2014-05-16
Resolution : 2.69 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

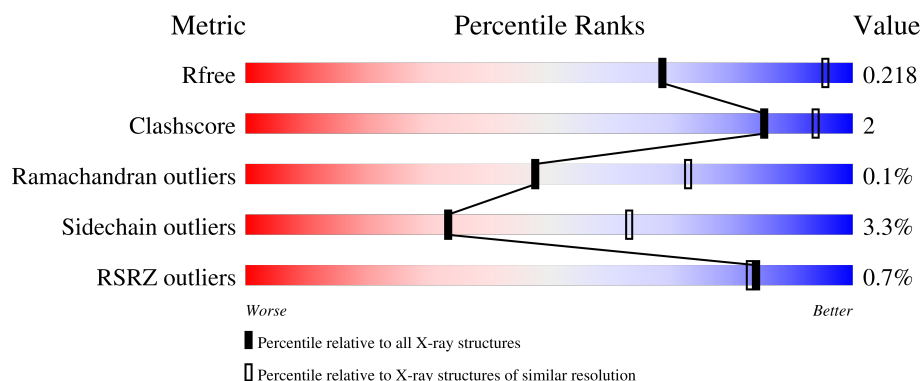
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	E	20	
1	F	20	
2	B	692	
2	D	692	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11503 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 DNA chain called DNA (5'-D(P*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
1	E	20	Total	C	N	O	P	0	0	0
			410	193	77	120	20			
1	F	19	Total	C	N	O	P	0	0	0
			390	183	75	113	19			

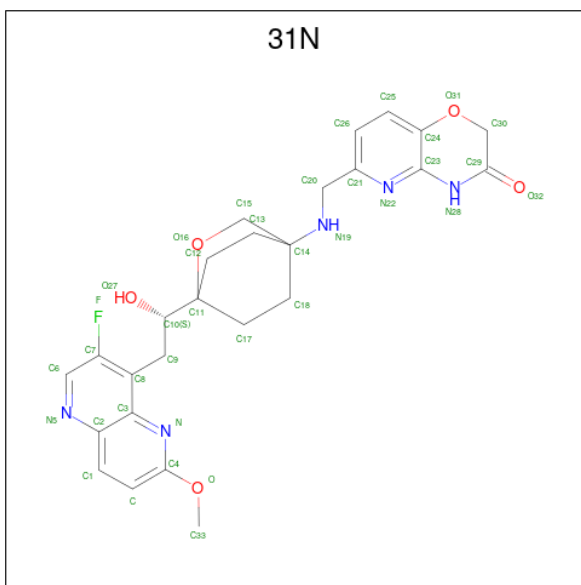
- Molecule 2 is a protein called Chimera protein of DNA gyrase subunits B and A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	672	Total	C	N	O	S	0	1	0
			5279	3288	953	1013	25			
2	D	670	Total	C	N	O	S	0	2	0
			5297	3300	952	1020	25			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	409	PRO	-	expression tag	UNP P0A0K8
B	544	THR	-	linker	UNP P0A0K8
B	545	GLY	-	linker	UNP P0A0K8
B	1123	PHE	TYR	engineered mutation	UNP P20831
B	1457	THR	ALA	engineered mutation	UNP P20831
D	409	PRO	-	expression tag	UNP P0A0K8
D	544	THR	-	linker	UNP P0A0K8
D	545	GLY	-	linker	UNP P0A0K8
D	1123	PHE	TYR	engineered mutation	UNP P20831
D	1457	THR	ALA	engineered mutation	UNP P20831

- Molecule 3 is 6-[(1r,4S)-1-[(1S)-2-(3-fluoro-6-methoxy-1,5-naphthyridin-4-yl)-1-hydroxyethyl]-2-oxabicyclo[2.2.2]oct-4-yl]amino)methyl]-2H-pyrido[3,2-b][1,4]oxazin-3(4H)-one (CCD ID: 31N) (formula: C₂₆H₂₈FN₅O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	F	1	Total	C	F	N	O	0	0
			37	26	1	5	5		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total 1	Mn 1	0	0
5	D	1	Total 1	Mn 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	9	Total 9	O 9	0	0
6	F	5	Total 5	O 5	0	0
6	B	32	Total 32	O 32	0	0
6	D	27	Total 27	O 27	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: DNA (5'-D(P*AP*GP*CP*CP*GP*TP*AP*GP*GP*GP*CP*CP*CP*TP*AP*C P*GP*GP*CP*T)-3')

Chain E: 



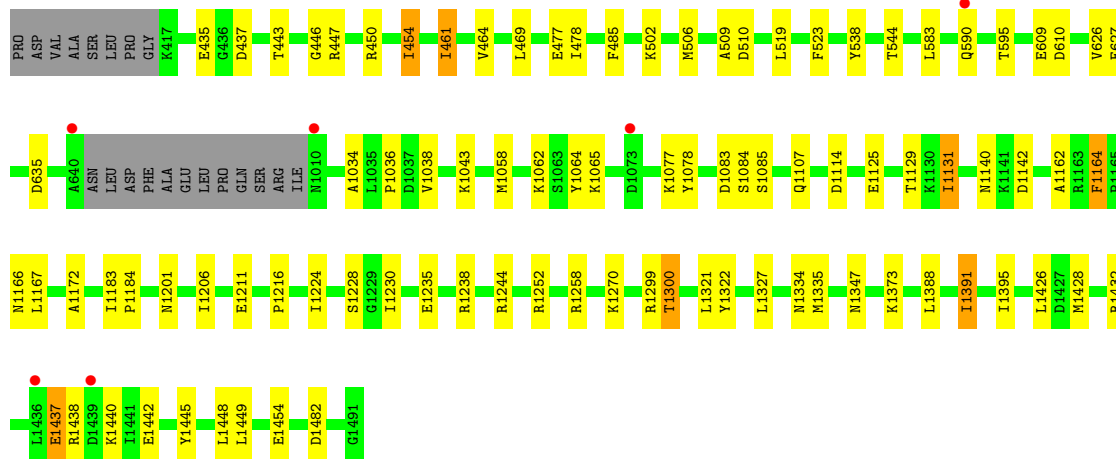
- Molecule 1: DNA (5'-D(P*AP*GP*CP*CP*GP*TP*AP*GP*GP*GP*CP*CP*CP*TP*AP*C P*GP*GP*CP*T)-3')

Chain F: 



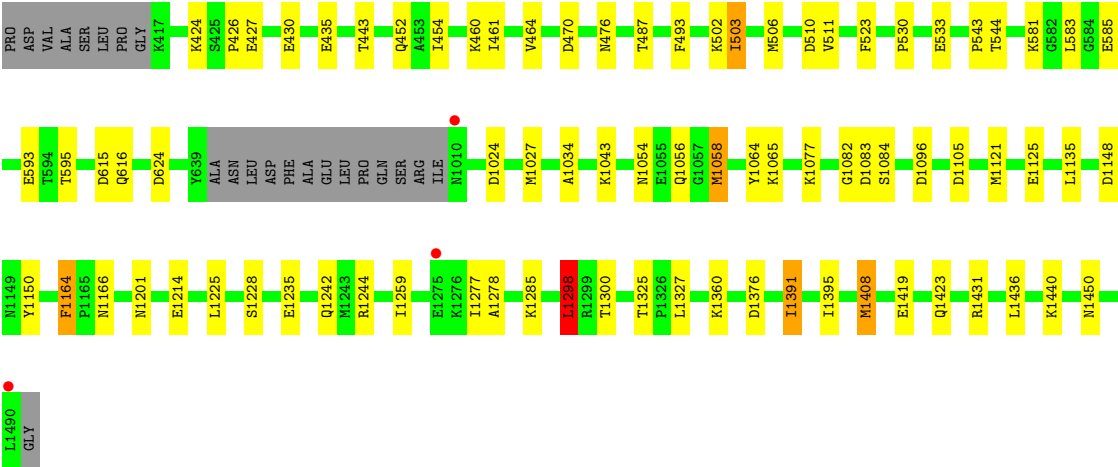
- Molecule 2: Chimera protein of DNA gyrase subunits B and A

Chain B: 



- Molecule 2: Chimera protein of DNA gyrase subunits B and A

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	93.31Å 93.31Å 410.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	27.12 – 2.69 27.12 – 2.69	Depositor EDS
% Data completeness (in resolution range)	99.6 (27.12-2.69) 99.9 (27.12-2.69)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.49 (at 2.68Å)	Xtriage
Refinement program	BUSTER 2.9.7	Depositor
R, R_{free}	0.176 , 0.220 0.179 , 0.218	Depositor DCC
R_{free} test set	2812 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	49.3	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 32.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.064 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11503	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.22% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MN, 31N, SO4

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	E	0.52	0/459	1.36	3/706 (0.4%)
1	F	0.51	0/437	1.46	6/672 (0.9%)
2	B	0.87	0/5351	1.41	32/7218 (0.4%)
2	D	0.86	2/5369 (0.0%)	1.45	37/7241 (0.5%)
All	All	0.84	2/11616 (0.0%)	1.43	78/15837 (0.5%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1164	PHE	CA-C	5.90	1.58	1.52
2	D	543	PRO	C-N	-5.67	1.26	1.33

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1437	GLU	N-CA-C	8.12	119.91	111.14
1	F	10	DG	P-O3'-C3'	7.69	131.73	120.20
2	D	1278	ALA	CA-C-N	7.38	130.03	120.44
2	D	1278	ALA	C-N-CA	7.38	130.03	120.44
2	D	544	THR	N-CA-C	-7.13	101.64	110.41
2	D	1105	ASP	CA-CB-CG	7.09	119.69	112.60
2	D	1077	LYS	N-CA-C	7.01	120.32	111.69
2	D	1298	LEU	CA-C-N	6.72	131.93	120.71
2	D	1298	LEU	C-N-CA	6.72	131.93	120.71
2	D	1166	ASN	N-CA-C	6.71	118.60	111.28
2	B	1083	ASP	N-CA-C	6.56	118.43	111.28
2	B	1129	THR	N-CA-C	-6.47	101.20	110.59
2	D	1391	ILE	N-CA-C	6.45	117.13	110.36
2	B	610	ASP	CA-CB-CG	6.44	119.04	112.60
2	D	1034	ALA	N-CA-C	6.37	120.26	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	18	DG	P-O3'-C3'	6.28	129.62	120.20
2	B	1078	TYR	N-CA-C	6.27	121.33	113.43
1	F	11	DC	P-O5'-C5'	6.22	129.33	120.00
2	D	1376	ASP	CA-CB-CG	6.22	118.82	112.60
2	B	510	ASP	CA-CB-CG	6.15	118.75	112.60
2	B	1166	ASN	N-CA-C	6.14	117.97	111.28
2	B	485	PHE	CA-CB-CG	6.09	119.89	113.80
2	B	627	GLU	N-CA-C	5.80	117.28	111.07
2	B	1043	LYS	N-CA-C	-5.78	102.83	110.40
2	D	435	GLU	N-CA-C	5.75	118.32	111.71
2	B	1077	LYS	N-CA-C	5.72	118.72	111.69
2	B	1299	ARG	CA-C-N	5.53	128.72	120.31
2	B	1299	ARG	C-N-CA	5.53	128.72	120.31
2	B	1164	PHE	CA-CB-CG	5.46	119.26	113.80
1	F	11	DC	P-O3'-C3'	5.46	128.39	120.20
2	D	503	ILE	N-CA-C	-5.45	99.12	106.85
2	D	1201	ASN	CA-CB-CG	5.42	118.02	112.60
2	D	511	VAL	N-CA-C	5.38	116.11	110.62
2	B	1034	ALA	N-CA-C	5.37	119.93	112.90
2	B	478	ILE	N-CA-C	-5.36	105.10	110.30
2	D	1043	LYS	N-CA-C	-5.33	103.46	110.39
2	D	1259	ILE	N-CA-C	-5.33	100.72	108.17
2	D	1027	MET	CA-C-N	5.32	127.40	120.28
2	D	1027	MET	C-N-CA	5.32	127.40	120.28
2	D	1082	GLY	CA-C-N	5.27	127.60	120.38
2	D	1082	GLY	C-N-CA	5.27	127.60	120.38
2	D	1096	ASP	CA-CB-CG	5.26	117.86	112.60
2	D	1360	LYS	CA-C-N	5.26	127.28	120.44
2	D	1360	LYS	C-N-CA	5.26	127.28	120.44
2	B	1391	ILE	N-CA-C	5.26	116.62	110.62
1	E	14	DT	P-O5'-C5'	5.23	127.85	120.00
2	D	470	ASP	CA-C-N	5.23	127.29	120.28
2	D	470	ASP	C-N-CA	5.23	127.29	120.28
2	B	435	GLU	N-CA-C	5.22	117.88	111.82
2	B	1228	SER	N-CA-C	5.22	117.37	111.11
2	B	447	ARG	N-CA-C	5.22	117.06	110.33
2	D	510	ASP	CA-CB-CG	5.21	117.81	112.60
1	E	15	DA	P-O5'-C5'	5.21	127.82	120.00
2	B	1482	ASP	CA-CB-CG	5.20	117.80	112.60
2	B	635	ASP	CA-CB-CG	5.19	117.79	112.60
2	D	1150	TYR	N-CA-C	5.19	117.68	111.71
2	B	469	LEU	N-CA-C	5.18	117.60	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	5	DG	P-O5'-C5'	5.15	127.73	120.00
2	D	616	GLN	CA-C-N	5.14	127.44	120.65
2	D	616	GLN	C-N-CA	5.14	127.44	120.65
2	B	1300	THR	N-CA-C	5.13	117.77	111.82
2	B	1347	ASN	CA-CB-CG	5.13	117.73	112.60
2	D	1277	ILE	CA-C-N	5.13	127.11	120.44
2	D	1277	ILE	C-N-CA	5.13	127.11	120.44
2	B	1142	ASP	N-CA-C	5.12	118.50	111.54
2	B	1454	GLU	CB-CG-CD	5.12	121.30	112.60
2	D	1058	MET	CA-C-N	5.11	129.21	121.03
2	D	1058	MET	C-N-CA	5.11	129.21	121.03
1	F	19	DC	C2'-C3'-O3'	5.10	119.15	111.50
2	B	1201	ASN	CA-CB-CG	5.09	117.69	112.60
2	D	1054	ASN	CA-C-N	5.08	127.08	120.28
2	D	1054	ASN	C-N-CA	5.08	127.08	120.28
2	D	452	GLN	N-CA-C	5.06	116.87	108.02
2	B	1391	ILE	N-CA-CB	5.06	116.79	110.47
1	E	10	DG	P-O5'-C5'	5.03	127.55	120.00
2	B	1228	SER	CA-C-N	5.03	125.53	120.00
2	B	1228	SER	C-N-CA	5.03	125.53	120.00
2	B	1211	GLU	N-CA-C	-5.00	105.93	112.23

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	E	410	0	224	1	0
1	F	390	0	212	2	0
2	B	5279	0	5266	31	0
2	D	5297	0	5293	21	0
3	F	37	0	28	0	0
4	B	5	0	0	0	0
4	D	10	0	0	0	0
5	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	1	0	0	0	0
6	B	32	0	0	0	0
6	D	27	0	0	0	0
6	E	9	0	0	0	0
6	F	5	0	0	0	0
All	All	11503	0	11023	50	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 2.

All (50) 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)
2:B:461:ILE:HD11	2:B:477:GLU:HB3	1.73	0.71
2:B:1058:MET:HG2	2:B:1065:LYS:HG3	1.72	0.69
2:B:461:ILE:HG22	2:B:519:LEU:HB3	1.78	0.66
2:B:1238[B]:ARG:HE	2:B:1334:ASN:ND2	1.99	0.60
2:B:443:THR:HG22	2:B:454:ILE:HG12	1.87	0.56
2:D:1058:MET:HG2	2:D:1065:LYS:HG3	1.86	0.56
2:B:1426:LEU:HB3	2:D:1431:ARG:HB3	1.87	0.55
2:D:464:VAL:HG21	2:D:523:PHE:HA	1.88	0.55
2:D:1391:ILE:O	2:D:1395:ILE:HG12	2.06	0.55
2:B:1183:ILE:HG12	2:B:1335:MET:HG2	1.89	0.55
2:B:1224:ILE:HG21	2:B:1230:ILE:HD11	1.90	0.54
2:D:530:PRO:HA	2:D:533:GLU:HB2	1.90	0.52
2:B:502:LYS:HG2	2:B:538:TYR:CE1	2.45	0.52
2:D:1225:LEU:HD21	2:D:1244:ARG:HD2	1.91	0.52
1:F:17:DG:H3'	2:B:626:VAL:HG11	1.95	0.49
2:B:506:MET:HG2	2:B:583:LEU:HD11	1.95	0.49
2:B:1445:TYR:CE2	2:B:1449:LEU:HD11	2.47	0.49
2:B:1038:VAL:HA	2:B:1167:LEU:HD22	1.95	0.48
2:B:1252:ARG:HD3	2:B:1258:ARG:HB3	1.96	0.48
2:D:593:GLU:HA	2:D:593:GLU:OE1	2.14	0.48
2:B:509:ALA:HB1	2:B:544:THR:HG22	1.96	0.48
2:D:424:LYS:O	2:D:426:PRO:HD3	2.15	0.46
2:B:1036:PRO:HG3	2:B:1172:ALA:CB	2.46	0.45
2:D:1064:TYR:HB3	2:D:1125:GLU:HB3	1.99	0.45
2:D:1083:ASP:HB2	2:D:1121:MET:HE1	1.98	0.44
1:F:8:DG:H1'	2:D:460:LYS:HG3	1.99	0.44
2:B:464:VAL:HG21	2:B:523:PHE:HA	2.00	0.44
1:E:10:DG:H5''	2:B:437:ASP:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:446:GLY:HA2	2:D:1298:LEU:HD22	2.00	0.43
2:B:1391:ILE:O	2:B:1395:ILE:HG12	2.18	0.43
2:D:487:THR:O	2:D:493:PHE:HA	2.17	0.43
2:B:1206:ILE:HG21	2:B:1235:GLU:HG3	2.00	0.43
2:B:1244:ARG:HG2	2:B:1322:TYR:CE1	2.53	0.43
2:D:1408:MET:SD	2:D:1423:GLN:HG2	2.57	0.43
2:D:1056:GLN:HB3	2:D:1058:MET:HE3	2.01	0.43
2:B:1064:TYR:HB3	2:B:1125:GLU:HB3	2.00	0.43
2:B:1388:LEU:HB2	2:B:1438:ARG:HD3	2.01	0.43
2:B:1428:MET:HG2	2:B:1432:ARG:HG3	2.01	0.43
2:B:1107:GLN:HB3	2:B:1125:GLU:HB2	2.00	0.42
2:D:1135:LEU:HG	2:D:1164:PHE:CE2	2.55	0.42
2:D:1325:THR:OG1	2:D:1327:LEU:HB2	2.20	0.42
2:B:1321:LEU:HB3	2:B:1327:LEU:HD22	2.02	0.41
2:D:443:THR:HG22	2:D:454:ILE:HG12	2.02	0.41
2:B:1131:ILE:HD12	2:B:1164:PHE:CE1	2.56	0.41
2:D:430:GLU:HG2	2:D:502:LYS:HB2	2.03	0.41
2:B:1114:ASP:OD1	2:B:1270:LYS:HB3	2.20	0.40
2:B:1437:GLU:HA	2:B:1440:LYS:HB2	2.04	0.40
2:D:506:MET:HG2	2:D:583:LEU:HD11	2.02	0.40
2:B:1184:PRO:HB2	2:B:1216:PRO:HB3	2.04	0.40
2:D:581:LYS:HG2	2:D:585:GLU:OE2	2.21	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	
2	B	669/692 (97%)	648 (97%)	20 (3%)	1 (0%)	48	73
2	D	668/692 (96%)	650 (97%)	18 (3%)	0	100	100
All	All	1337/1384 (97%)	1298 (97%)	38 (3%)	1 (0%)	48	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1162	ALA

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	
2	B	561/591 (95%)	546 (97%)	15 (3%)	39	69
2	D	567/591 (96%)	545 (96%)	22 (4%)	28	57
All	All	1128/1182 (95%)	1091 (97%)	37 (3%)	33	63

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	450	ARG
2	B	454	ILE
2	B	461	ILE
2	B	590	GLN
2	B	595	THR
2	B	609	GLU
2	B	1062	LYS
2	B	1084	SER
2	B	1085	SER
2	B	1131	ILE
2	B	1140	ASN
2	B	1300	THR
2	B	1373	LYS
2	B	1442	GLU
2	B	1448	LEU
2	D	427	GLU
2	D	461	ILE
2	D	476	ASN
2	D	503	ILE
2	D	595	THR
2	D	615	ASP
2	D	624	ASP

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Mol	Chain	Res	Type
2	D	1024	ASP
2	D	1084	SER
2	D	1148	ASP
2	D	1214	GLU
2	D	1228	SER
2	D	1235	GLU
2	D	1242	GLN
2	D	1285	LYS
2	D	1298	LEU
2	D	1300	THR
2	D	1408	MET
2	D	1419	GLU
2	D	1436	LEU
2	D	1440	LYS
2	D	1450	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	480	GLN
2	B	541	GLN
2	B	597	ASN
2	B	600	HIS
2	B	605	GLN
2	B	631	GLN
2	B	1054	ASN
2	B	1140	ASN
2	B	1324	GLN
2	B	1334	ASN
2	B	1358	HIS
2	B	1413	GLN
2	D	476	ASN
2	D	480	GLN
2	D	541	GLN
2	D	590	GLN
2	D	605	GLN
2	D	631	GLN
2	D	1107	GLN
2	D	1242	GLN
2	D	1358	HIS
2	D	1368	GLN
2	D	1370	ASN

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Mol	Chain	Res	Type
2	D	1412	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	SO4	D	1501	-	4,4,4	0.41	0	6,6,6	0.15	0
4	SO4	D	1502	-	4,4,4	0.54	0	6,6,6	0.27	0
3	31N	F	101	-	40,42,42	1.27	5 (12%)	51,63,63	1.67	11 (21%)
4	SO4	B	1501	-	4,4,4	0.46	0	6,6,6	0.12	0

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
3	31N	F	101	-	-	0/18/48/48	0/7/6/6

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	101	31N	C9-C10	-3.27	1.50	1.53
3	F	101	31N	O-C4	3.22	1.40	1.35
3	F	101	31N	C9-C8	-2.26	1.48	1.51
3	F	101	31N	C1-C2	-2.22	1.38	1.41
3	F	101	31N	C3-C2	-2.03	1.39	1.42

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	101	31N	C33-O-C4	-3.84	111.62	117.33
3	F	101	31N	F-C7-C8	3.71	122.31	117.66
3	F	101	31N	C23-N28-C29	-3.63	118.76	124.50
3	F	101	31N	C12-C13-C14	-3.59	108.43	113.56
3	F	101	31N	C6-C7-C8	-2.99	118.06	122.65
3	F	101	31N	C18-C14-C13	2.63	111.31	108.84
3	F	101	31N	C17-C18-C14	-2.62	109.82	113.56
3	F	101	31N	O27-C10-C9	-2.47	103.68	108.51
3	F	101	31N	C8-C3-N	2.28	120.67	118.23
3	F	101	31N	C1-C2-C3	-2.15	116.85	119.55
3	F	101	31N	C17-C11-C12	-2.14	107.96	110.07

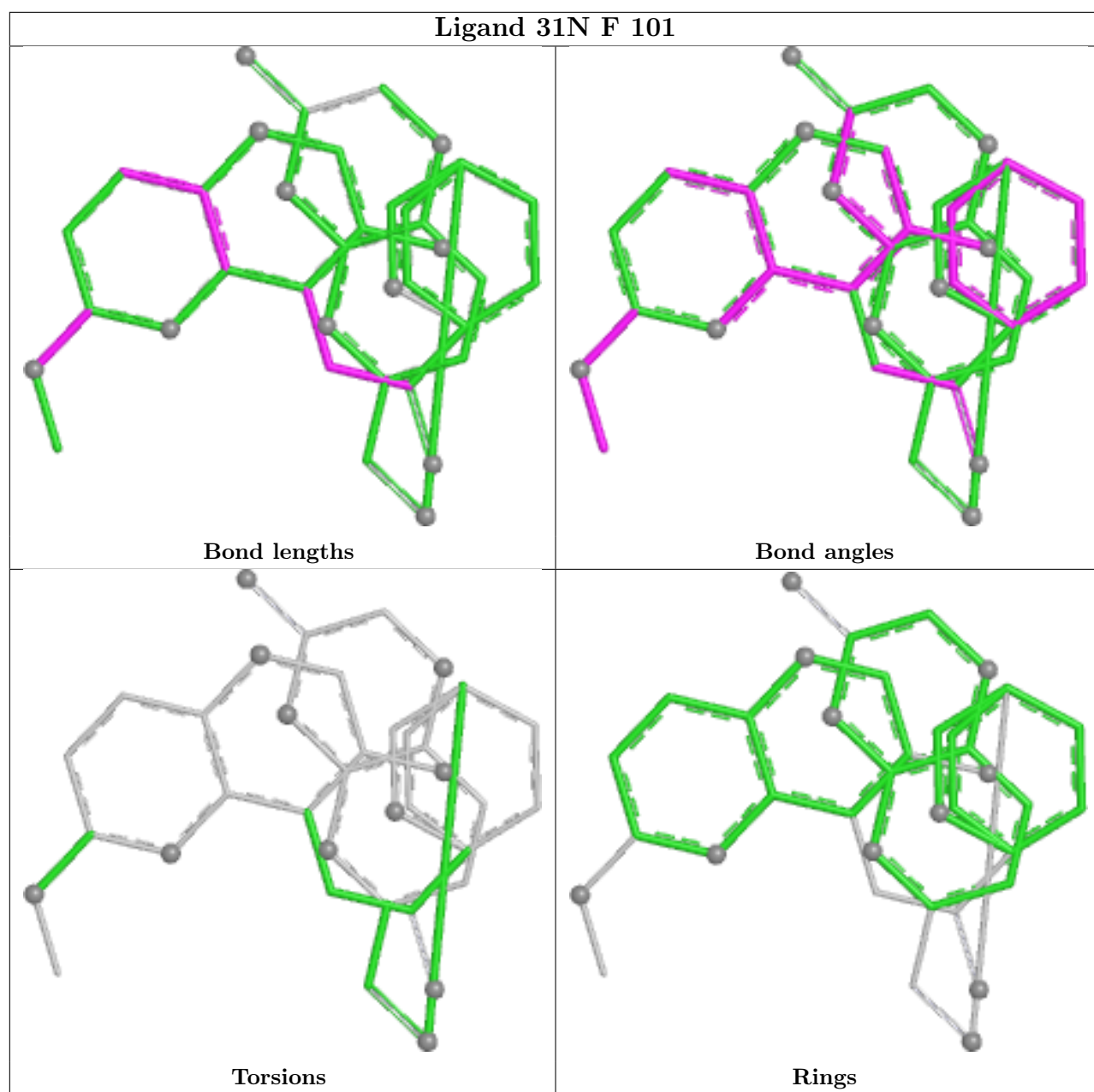
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

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	E	20/20 (100%)	-0.91	0 100 100	31, 43, 52, 61	0
1	F	19/20 (95%)	-0.59	1 (5%) 32 28	33, 41, 67, 93	0
2	B	672/692 (97%)	-0.24	6 (0%) 81 80	19, 48, 67, 87	1 (0%)
2	D	670/692 (96%)	-0.29	3 (0%) 88 87	17, 49, 68, 83	2 (0%)
All	All	1381/1424 (96%)	-0.28	10 (0%) 84 83	17, 48, 67, 93	3 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	1010	ASN	3.8
1	F	1	DA	3.4
2	B	1439	ASP	2.9
2	B	590	GLN	2.7
2	B	640	ALA	2.7
2	B	1436	LEU	2.5
2	B	1073	ASP	2.3
2	D	1490	LEU	2.1
2	D	1275[A]	GLU	2.1
2	B	1010	ASN	2.1

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](#)

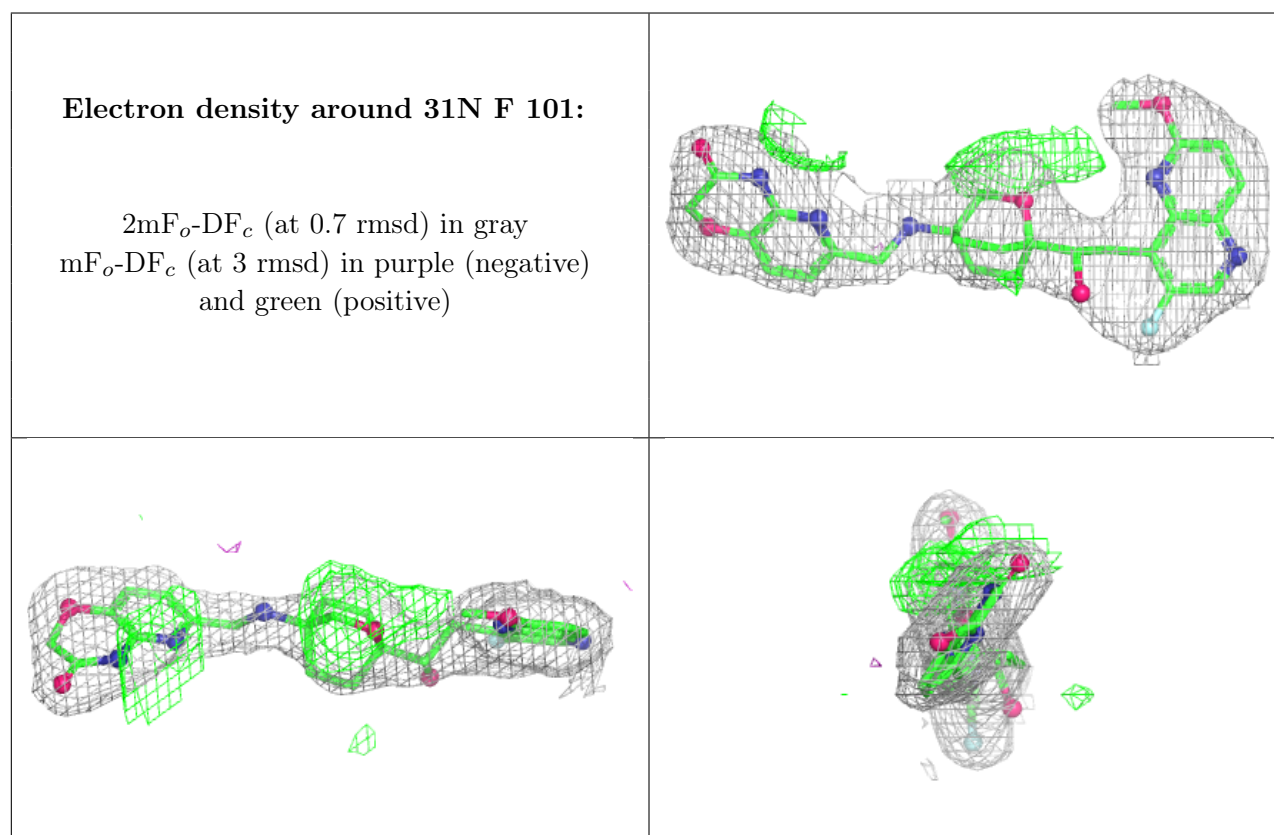
There are no oligosaccharides in this entry.

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
4	SO4	B	1501	5/5	0.76	0.12	107,111,112,112	0
4	SO4	D	1502	5/5	0.80	0.12	107,111,112,113	0
4	SO4	D	1501	5/5	0.85	0.09	88,93,93,94	0
3	31N	F	101	37/37	0.91	0.12	42,57,66,66	0
5	MN	D	1503	1/1	0.99	0.03	47,47,47,47	0
5	MN	B	1502	1/1	1.00	0.03	50,50,50,50	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.