



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:40 PM GMT

PDB ID : 4PLB  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

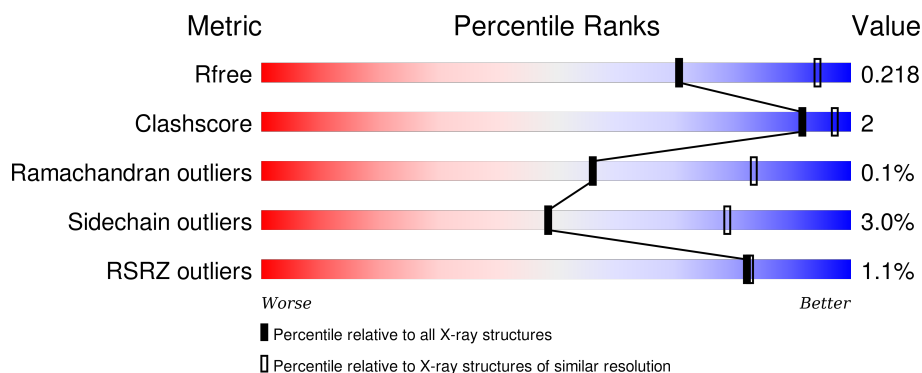
# 1 Overall quality at a glance

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))
$R_{free}$	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>25%</div> <div>70%</div> <div>5%</div> </div>
1	F	20	<div> <div>5%</div> <div>10%</div> <div>75%</div> <div>10%</div> <div>5%</div> </div>
2	B	692	<div> <div>%</div> <div>87%</div> <div>9%</div> <div>••</div> </div>
2	D	692	<div> <div>%</div> <div>89%</div> <div>7%</div> <div>•</div> </div>

## 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			

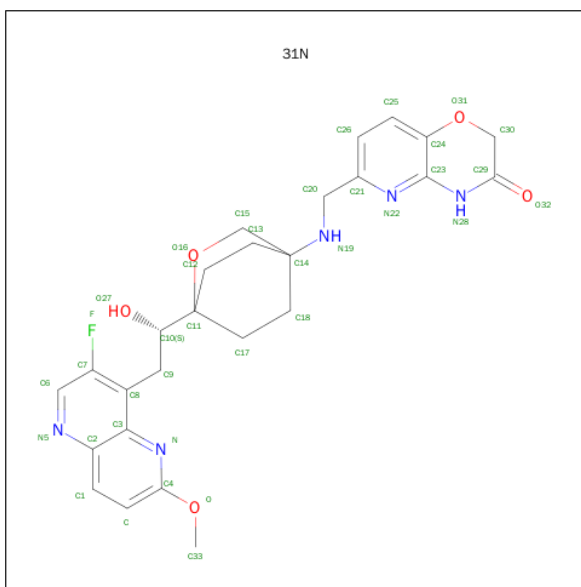
- Molecule 2 is a protein called Chimera protein of DNA gyrase subunits B and A.

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:

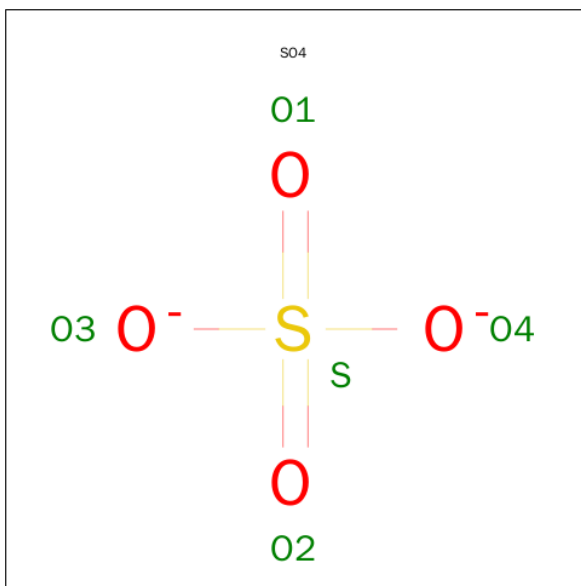
Chain	Residue	Modelled	Actual	Comment	Reference
B	409	PRO	-	expression tag	UNP P0A0K8
B	544	THR	-	linker	UNP P0A0K8
B	545	GLY	-	linker	UNP P0A0K8
B	1123	PHE	TYR	engineered mutation	UNP P20831
B	1457	THR	ALA	engineered mutation	UNP P20831
D	409	PRO	-	expression tag	UNP P0A0K8
D	544	THR	-	linker	UNP P0A0K8
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 (three-letter code: 31N) (formula: C<sub>26</sub>H<sub>28</sub>FN<sub>5</sub>O<sub>5</sub>).



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 (three-letter code: SO4) (formula: O<sub>4</sub>S).



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 (three-letter code: 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

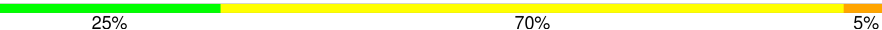
- Molecule 6 is water.

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 [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

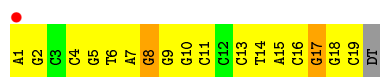
- Molecule 1: DNA (5'-D(P\*AP\*GP\*CP\*CP\*GP\*TP\*AP\*GP\*GP\*GP\*CP\*CP\*CP\*TP\*AP\*C P\*GP\*GP\*CP\*T)-3')

Chain E: 




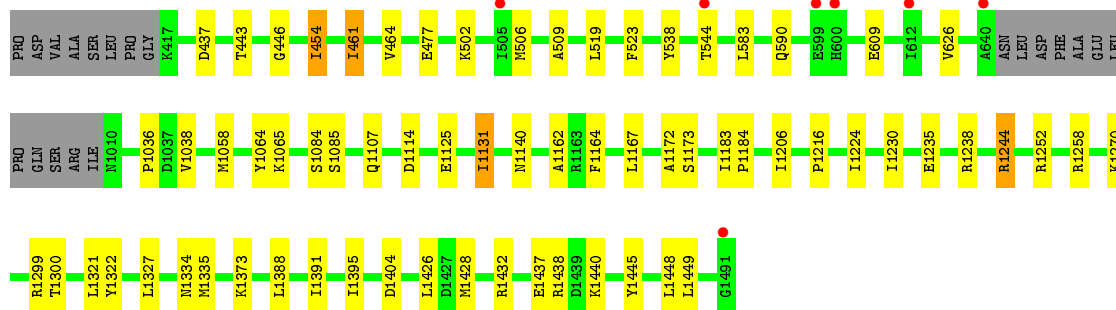
- Molecule 1: DNA (5'-D(P\*AP\*GP\*CP\*CP\*GP\*TP\*AP\*GP\*GP\*GP\*CP\*CP\*CP\*TP\*AP\*C P\*GP\*GP\*CP\*T)-3')

Chain F: 




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

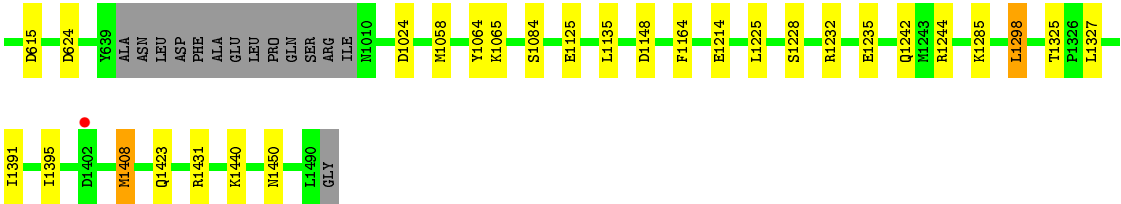
Chain B: 



- 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, $\alpha$ , $\beta$ , $\gamma$	93.31Å 93.31Å 410.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	27.12 – 2.69 27.08 – 2.69	Depositor EDS
% Data completeness (in resolution range)	99.6 (27.12-2.69) 100.0 (27.08-2.69)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	49.3	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 40.0	EDS
Estimated twinning fraction	0.064 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 55447 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11503	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 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, SO4, 31N

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	1.17	0/459	2.13	26/706 (3.7%)
1	F	1.16	0/437	2.13	28/672 (4.2%)
2	B	0.53	0/5351	0.72	0/7218
2	D	0.52	0/5369	0.73	0/7241
All	All	0.60	0/11616	0.93	54/15837 (0.3%)

There are no bond length outliers.

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	10	DG	P-O3'-C3'	10.03	131.73	119.70
1	E	6	DT	O4'-C1'-N1	9.96	114.97	108.00
1	F	16	DC	O4'-C4'-C3'	-9.75	100.15	106.00
1	E	13	DC	O4'-C1'-N1	8.99	114.29	108.00
1	E	9	DG	O4'-C4'-C3'	-8.89	100.67	106.00
1	F	9	DG	O4'-C4'-C3'	-8.89	100.67	106.00
1	E	14	DT	O4'-C4'-C3'	-8.70	100.78	106.00
1	E	19	DC	O4'-C1'-N1	8.38	113.87	108.00
1	F	19	DC	O4'-C1'-N1	8.37	113.86	108.00
1	F	18	DG	P-O3'-C3'	8.27	129.62	119.70
1	F	10	DG	O4'-C1'-N9	8.17	113.72	108.00
1	E	13	DC	C4'-C3'-C2'	-8.11	95.80	103.10
1	F	4	DC	O4'-C4'-C3'	-7.56	101.47	106.00
1	F	14	DT	C4'-C3'-C2'	-7.51	96.34	103.10
1	F	11	DC	P-O3'-C3'	7.24	128.39	119.70
1	E	10	DG	O4'-C1'-N9	7.24	113.07	108.00
1	F	6	DT	O4'-C1'-N1	7.04	112.93	108.00
1	F	14	DT	O4'-C1'-N1	6.86	112.80	108.00
1	E	19	DC	C4'-C3'-C2'	-6.74	97.03	103.10
1	F	13	DC	C4'-C3'-C2'	-6.60	97.16	103.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	2	DG	O4'-C1'-N9	6.57	112.60	108.00
1	E	8	DG	P-O3'-C3'	6.49	127.49	119.70
1	F	13	DC	O4'-C1'-N1	6.47	112.53	108.00
1	E	20	DT	O4'-C1'-N1	6.42	112.49	108.00
1	E	9	DG	O4'-C1'-N9	6.40	112.48	108.00
1	F	17	DG	P-O3'-C3'	6.13	127.06	119.70
1	E	10	DG	P-O3'-C3'	6.04	126.95	119.70
1	E	19	DC	C1'-O4'-C4'	-6.04	104.06	110.10
1	E	7	DA	O4'-C4'-C3'	-5.99	102.11	104.50
1	E	1	DA	O4'-C1'-N9	5.99	112.19	108.00
1	F	1	DA	OP1-P-OP2	-5.89	110.76	119.60
1	E	2	DG	P-O3'-C3'	5.87	126.74	119.70
1	F	16	DC	C1'-O4'-C4'	-5.83	104.27	110.10
1	E	19	DC	P-O3'-C3'	5.78	126.64	119.70
1	E	1	DA	O4'-C4'-C3'	-5.70	102.22	104.50
1	F	6	DT	N3-C4-O4	-5.68	116.49	119.90
1	F	4	DC	O4'-C1'-N1	5.67	111.97	108.00
1	E	14	DT	O4'-C1'-N1	5.66	111.96	108.00
1	E	19	DC	O4'-C4'-C3'	-5.58	102.27	104.50
1	F	14	DT	N3-C4-O4	-5.56	116.57	119.90
1	E	20	DT	N3-C2-O2	-5.49	119.01	122.30
1	E	12	DC	O4'-C1'-N1	5.42	111.80	108.00
1	F	17	DG	O4'-C1'-N9	-5.40	104.22	108.00
1	F	6	DT	C4-C5-C7	5.35	122.21	119.00
1	F	16	DC	P-O3'-C3'	5.30	126.06	119.70
1	F	11	DC	P-O5'-C5'	5.27	129.33	120.90
1	E	17	DG	O4'-C1'-N9	-5.26	104.32	108.00
1	F	7	DA	C6-N1-C2	5.12	121.67	118.60
1	E	18	DG	P-O3'-C3'	5.11	125.83	119.70
1	E	5	DG	C3'-C2'-C1'	-5.10	96.38	102.50
1	F	5	DG	O4'-C1'-N9	5.07	111.55	108.00
1	E	7	DA	N1-C2-N3	-5.05	126.77	129.30
1	F	8	DG	P-O3'-C3'	5.04	125.75	119.70
1	F	15	DA	N1-C2-N3	-5.03	126.78	129.30

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	19	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
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	48	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 (48) 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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:464:VAL:HG21	2:B:523:PHE:HA	2.00	0.44
1:F:8:DG:H1'	2:D:460:LYS:HG3	1.99	0.44
1:E:10:DG:H5''	2:B:437:ASP:HB2	1.99	0.44
2:D:487:THR:O	2:D:493:PHE:HA	2.17	0.43
2:B:1391:ILE:O	2:B:1395:ILE:HG12	2.18	0.43
2:B:446:GLY:HA2	2:D:1298:LEU:HD22	2.00	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:B:1064:TYR:HB3	2:B:1125:GLU:HB3	2.00	0.43
2:B:1428:MET:HG2	2:B:1432:ARG:HG3	2.01	0.43
2:B:1388:LEU:HB2	2:B:1438:ARG:HD3	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%)	56	83
2	D	668/692 (96%)	650 (97%)	18 (3%)	0	100	100
All	All	1337/1384 (97%)	1298 (97%)	38 (3%)	1 (0%)	56	83

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%)	52	82
2	D	567/591 (96%)	548 (97%)	19 (3%)	44	75
All	All	1128/1182 (95%)	1094 (97%)	34 (3%)	48	79

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	454	ILE
2	B	461	ILE
2	B	590	GLN
2	B	609	GLU
2	B	1084	SER
2	B	1085	SER
2	B	1131	ILE
2	B	1140	ASN
2	B	1173	SER
2	B	1244	ARG
2	B	1299	ARG
2	B	1300	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	1373	LYS
2	B	1404	ASP
2	B	1448	LEU
2	D	442	SER
2	D	461	ILE
2	D	476	ASN
2	D	595	THR
2	D	615	ASP
2	D	624	ASP
2	D	1024	ASP
2	D	1084	SER
2	D	1148	ASP
2	D	1214	GLU
2	D	1228	SER
2	D	1232	ARG
2	D	1235	GLU
2	D	1242	GLN
2	D	1285	LYS
2	D	1298	LEU
2	D	1408	MET
2	D	1440	LYS
2	D	1450	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	590	GLN
2	B	605	GLN
2	B	1054	ASN
2	B	1324	GLN
2	B	1334	ASN
2	D	590	GLN
2	D	605	GLN
2	D	1242	GLN
2	D	1368	GLN
2	D	1370	ASN

### 5.3.3 RNA ⓘ

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 carbohydrates 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	B	1501	-	4,4,4	0.40	0	6,6,6	0.12	0
4	SO4	D	1501	-	4,4,4	0.51	0	6,6,6	0.17	0
4	SO4	D	1502	-	4,4,4	0.80	0	6,6,6	0.28	0
3	31N	F	101	-	38,42,42	1.23	5 (13%)	37,63,63	1.79	11 (29%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	B	1501	-	-	0/0/0/0	0/0/0/0
4	SO4	D	1501	-	-	0/0/0/0	0/0/0/0
4	SO4	D	1502	-	-	0/0/0/0	0/0/0/0
3	31N	F	101	-	-	0/16/48/48	0/4/6/6

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	101	31N	C3-C2	-2.48	1.39	1.42
3	F	101	31N	C9-C8	-2.27	1.48	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	101	31N	C1-C2	-2.02	1.38	1.41
3	F	101	31N	C4-N	2.49	1.34	1.30
3	F	101	31N	O-C4	3.11	1.40	1.35

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	101	31N	C33-O-C4	-4.24	111.62	117.38
3	F	101	31N	C6-C7-C8	-2.80	118.06	123.45
3	F	101	31N	C1-C2-C3	-2.53	116.85	119.48
3	F	101	31N	C-C4-N	-2.40	122.62	125.39
3	F	101	31N	O27-C10-C9	-2.26	103.68	109.19
3	F	101	31N	O32-C29-N28	-2.03	119.64	121.53
3	F	101	31N	C3-C2-N5	2.08	123.80	121.58
3	F	101	31N	C4-N-C3	2.31	118.39	116.17
3	F	101	31N	C30-C29-N28	2.80	120.61	116.86
3	F	101	31N	C13-C14-C18	2.96	111.31	108.95
3	F	101	31N	F-C7-C8	3.96	122.31	117.45

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	E	20/20 (100%)	-0.76	0 100 100	31, 43, 52, 61	0
1	F	19/20 (95%)	-0.37	1 (5%) 30 28	33, 41, 67, 93	0
2	B	672/692 (97%)	-0.21	7 (1%) 84 85	32, 48, 67, 87	0
2	D	670/692 (96%)	-0.22	7 (1%) 84 85	33, 49, 68, 83	0
All	All	1381/1424 (96%)	-0.22	15 (1%) 82 83	31, 48, 67, 93	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1491	GLY	3.9
2	D	491	GLY	3.2
2	B	612	ILE	3.0
2	B	640	ALA	3.0
2	D	518	THR	2.8
2	D	1402	ASP	2.7
1	F	1	DA	2.7
2	D	544	THR	2.6
2	B	599	GLU	2.5
2	D	522	THR	2.4
2	B	600	HIS	2.4
2	B	505	ILE	2.3
2	B	544	THR	2.3
2	D	521	LEU	2.2
2	D	519	LEU	2.2

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	31N	F	101	37/37	0.91	0.18	1.39	42,57,66,66	0
4	SO4	D	1502	5/5	0.91	0.31	1.04	107,111,112,113	0
5	MN	B	1502	1/1	0.99	0.14	-0.27	50,50,50,50	0
5	MN	D	1503	1/1	0.99	0.10	-0.97	47,47,47,47	0
4	SO4	D	1501	5/5	0.94	0.12	-	88,93,93,94	0
4	SO4	B	1501	5/5	0.89	0.18	-	107,111,112,112	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.