Full wwPDB EM Validation Report ⓘ

Mar 8, 2025 – 12:07 pm GMT

PDB ID	:	8S7O
EMDB ID	:	EMD-19782
Title	:	M. tuberculosis gyrase holocomplex with 150 bp DNA and BDM71403
Authors	:	Gedeon, A.; Yab, E.; Dinut, A.; Sadowski, E.; Capton, E.; Dreneau, A.; Gioia, B.; Piveteau, C.; Djaout, K.; Lecat, E.; Wehenkel, A.M.; Gubellini, F.; Mechaly, A.; Alzari, P.M.; Deprez, B.; Baulard, A.; Aubry, A.; Willand, N.; Petrella, S.
Deposited on	:	2024-03-04
Resolution	:	2.80 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp
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:

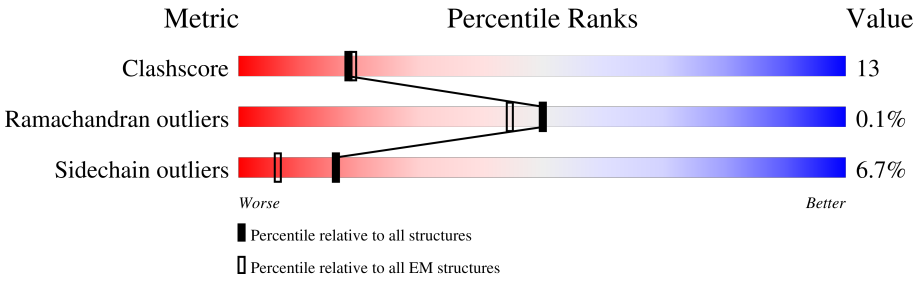
EMDB validation analysis	:	FAILED
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	837	40% 17% • 42%
1	C	837	39% 18% • 42%
2	B	678	18% 8% • 72%
2	D	678	18% 8% • 73%
3	E	150	5% 5% • 89%
4	F	150	• 8% • 89%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11253 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA gyrase subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	487	Total	C	N	O	S	0	0
			3826	2383	701	729	13		
1	C	487	Total	C	N	O	S	0	0
			3826	2383	701	729	13		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	501	ILE	ALA	conflict	UNP P9WG47
C	501	ILE	ALA	conflict	UNP P9WG47

- Molecule 2 is a protein called DNA gyrase subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	187	Total	C	N	O	S	0	0
			1446	908	257	274	7		
2	D	186	Total	C	N	O	S	0	0
			1437	902	255	273	7		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP P9WG45
B	-1	ALA	-	expression tag	UNP P9WG45
B	0	MET	-	expression tag	UNP P9WG45
B	1	VAL	-	expression tag	UNP P9WG45
B	2	ALA	-	expression tag	UNP P9WG45
B	3	ALA	-	expression tag	UNP P9WG45
B	4	GLN	-	expression tag	UNP P9WG45
D	-2	GLY	-	expression tag	UNP P9WG45
D	-1	ALA	-	expression tag	UNP P9WG45
D	0	MET	-	expression tag	UNP P9WG45
D	1	VAL	-	expression tag	UNP P9WG45

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Chain	Residue	Modelled	Actual	Comment	Reference
D	2	ALA	-	expression tag	UNP P9WG45
D	3	ALA	-	expression tag	UNP P9WG45
D	4	GLN	-	expression tag	UNP P9WG45

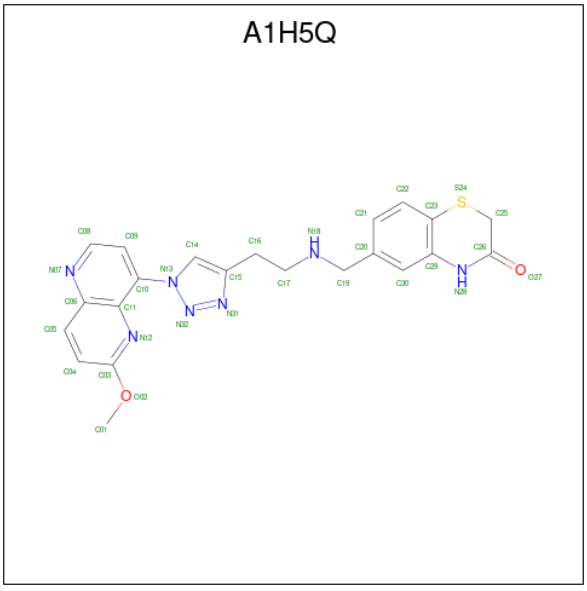
- Molecule 3 is a DNA chain called DNA (5'-D(*CP*CP*GP*GP*AP*AP*GP*GP*GP*GP*TP*AP*AP*TP*AP*CP*T)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	17	Total	C	N	O	P	0	0
			337	163	58	100	16		

- Molecule 4 is a DNA chain called DNA (5'-D(*CP*CP*GP*GP*AP*AP*GP*GP*GP*GP*TP*AP*AP*TP*AP*CP*T)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	17	Total	C	N	O	P	0	0
			349	166	70	97	16		

- Molecule 5 is 6-[[2-[1-(6-methoxy-1,5-naphthyridin-4-yl)-1,2,3-triazol-4-yl]ethylamino]methyl]-4H-1,4-benzothiazin-3-one (three-letter code: A1H5Q) (formula: $C_{22}H_{21}N_7O_2S$) (labeled as "Ligand of Interest" by depositor).



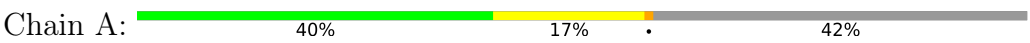
Mol	Chain	Residues	Atoms					AltConf
5	E	1	Total	C	N	O	S	0
			32	22	7	2	1	

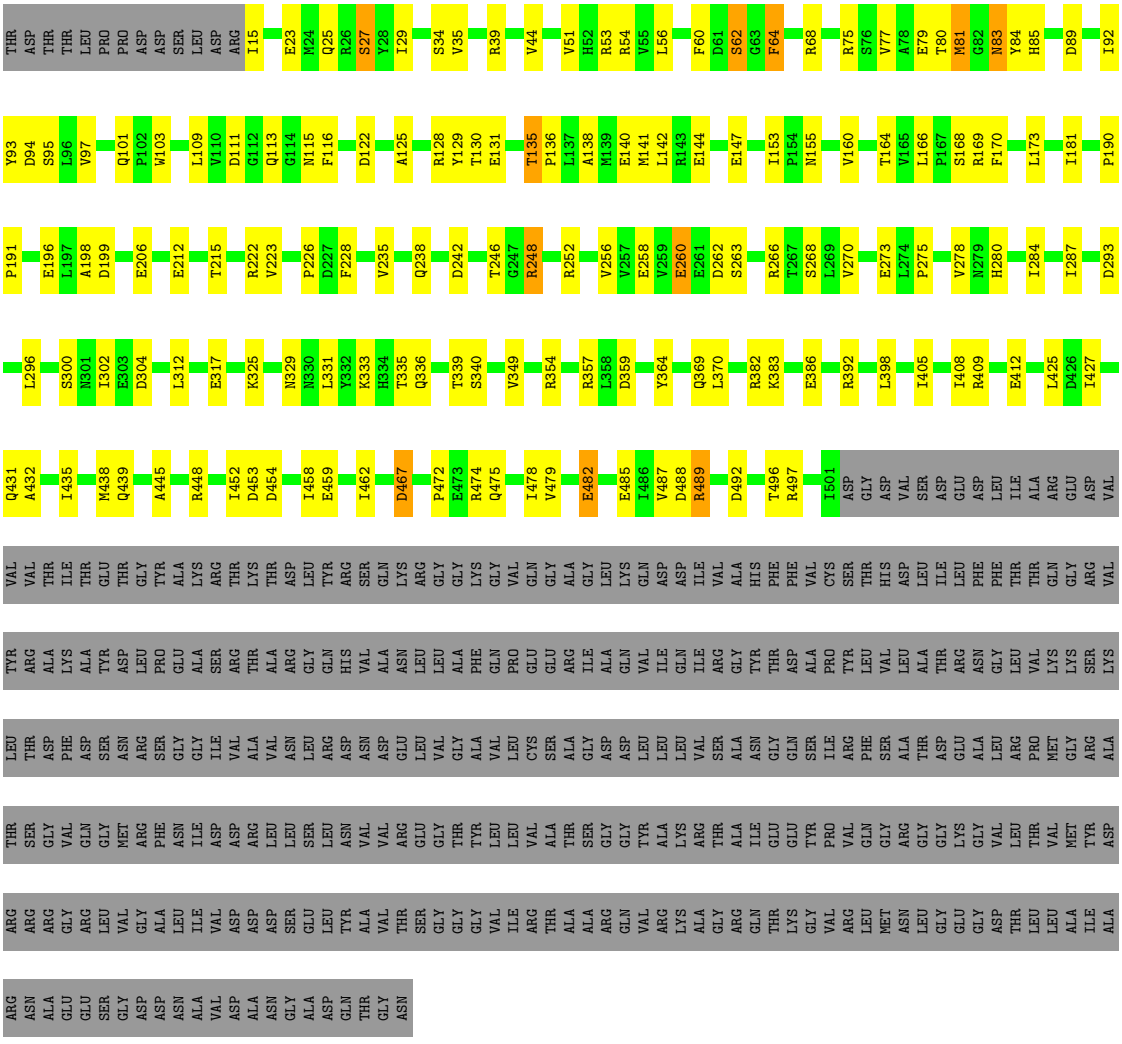
3 Residue-property plots (i)

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

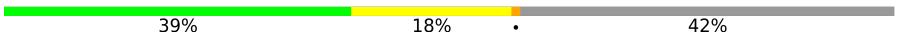
Chain A:

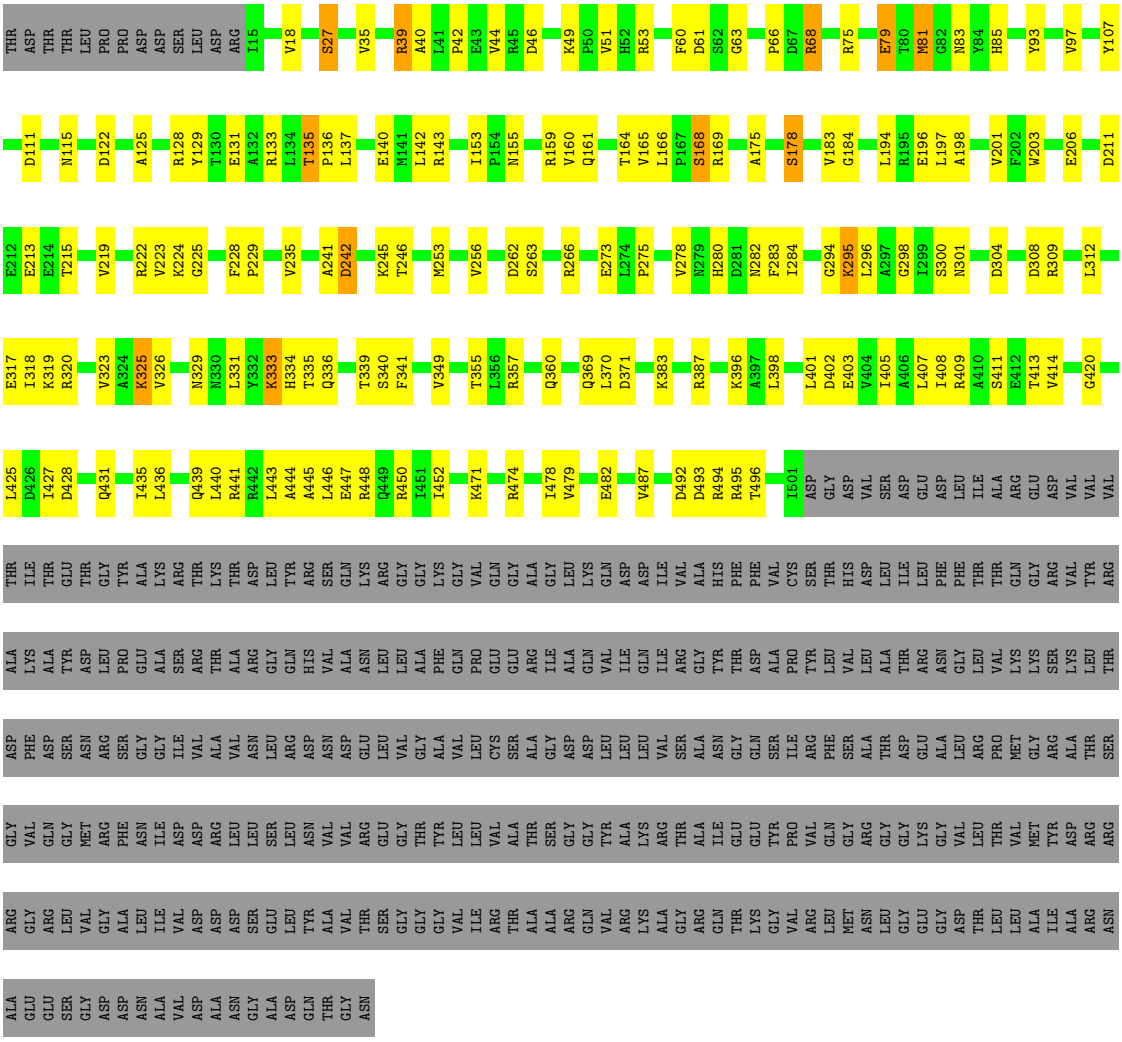




• Molecule 1: DNA gyrase subunit A

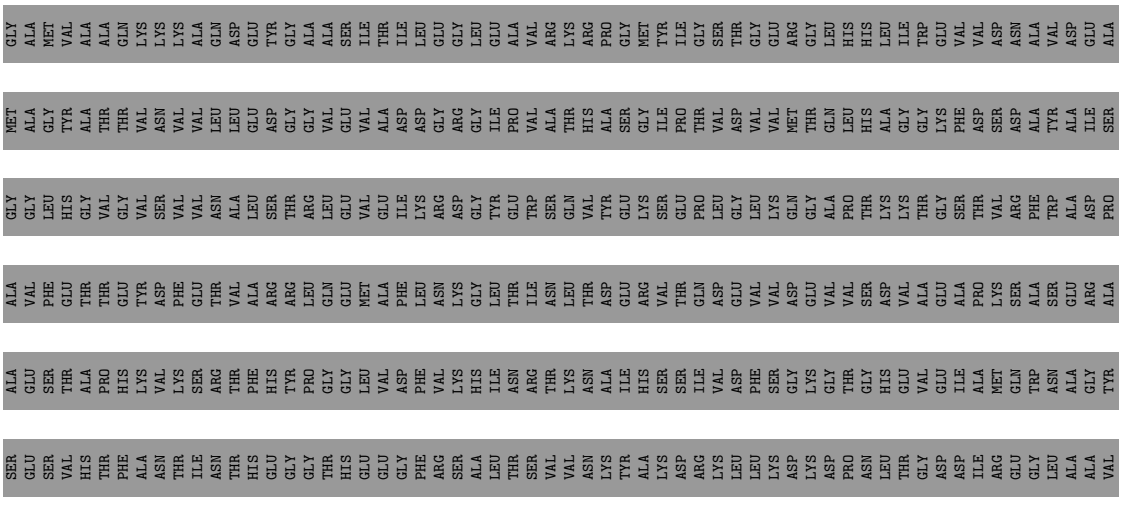
Chain C:

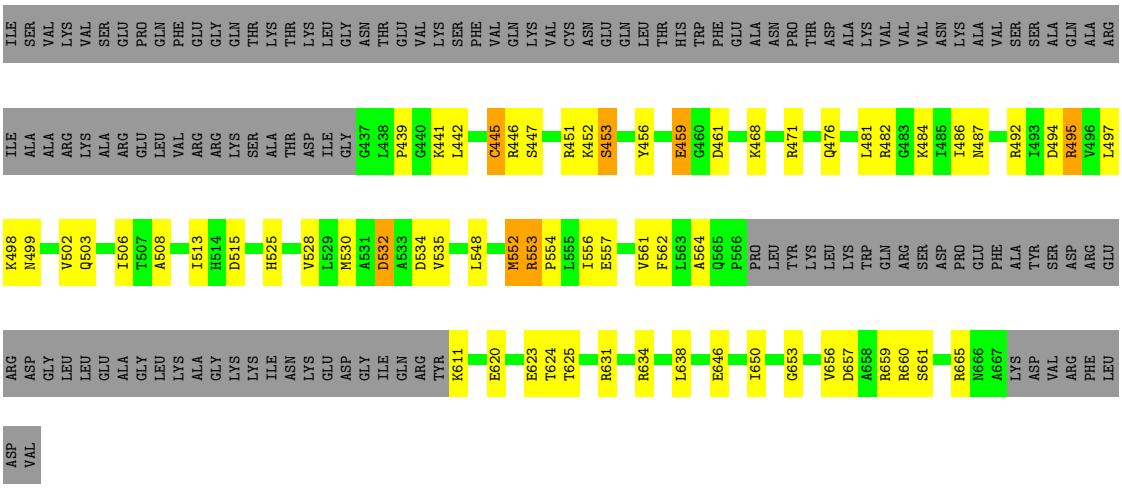




• Molecule 2: DNA gyrase subunit B

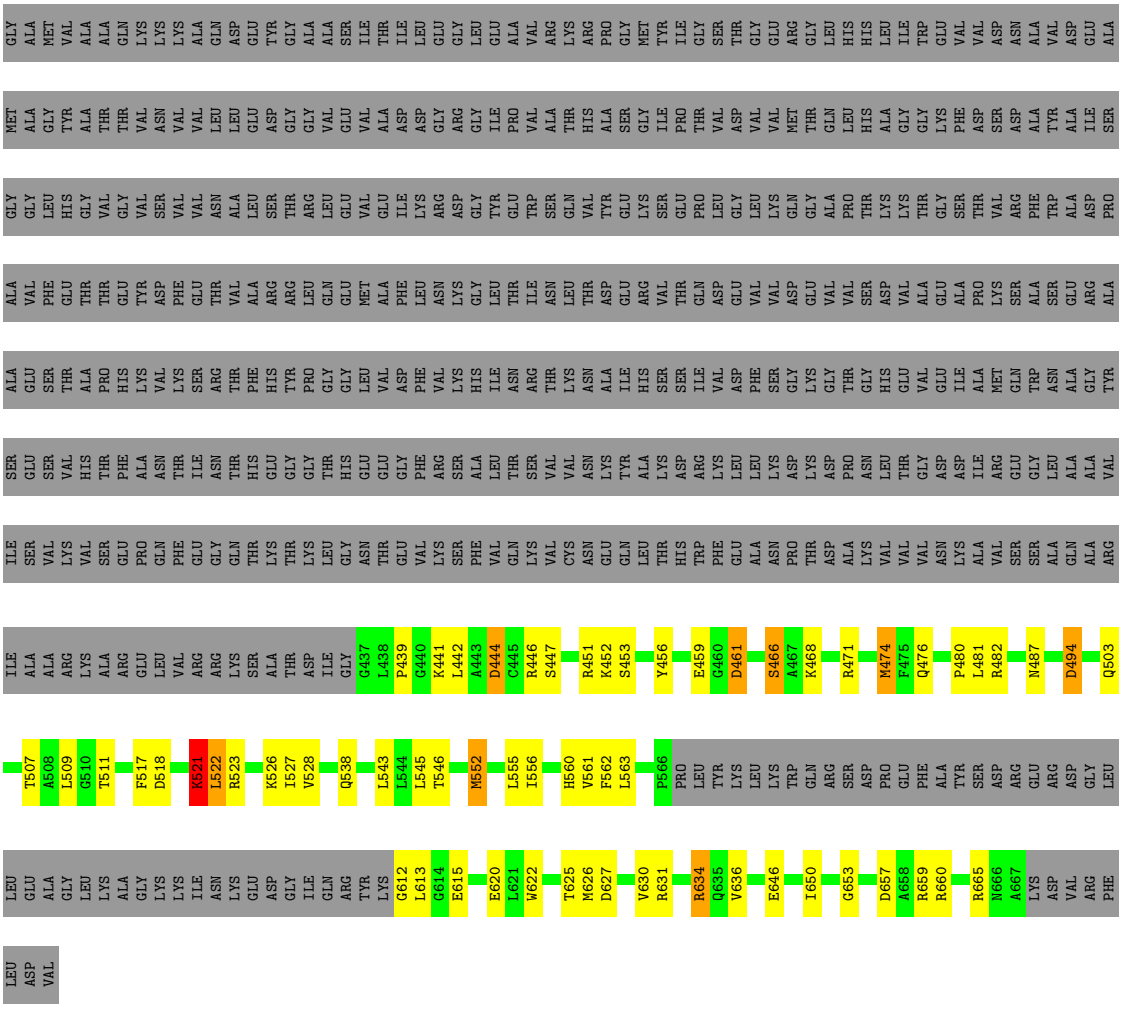
Chain B: 18% 8% • 72%





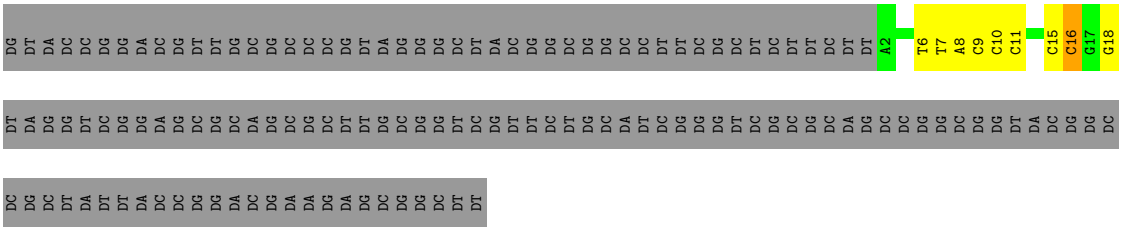
• Molecule 2: DNA gyrase subunit B

Chain D: 18% 8% 73%



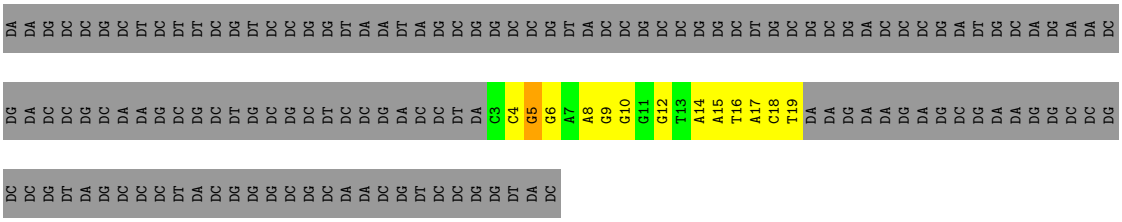
• Molecule 3: DNA (5'-D(*CP*CP*GP*GP*AP*AP*GP*GP*GP*GP*TP*AP*AP*TP*AP*CP*T)-3')

Chain E: 5% 5% 89%



• Molecule 4: DNA (5’-D(*CP*CP*GP*GP*AP*AP*GP*GP*GP*GP*TP*AP*AP*TP*AP*CP *T)-3’)

Chain F: 8% 89%



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	987000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1H5Q

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	0.28	0/3885	0.55	0/5263
1	C	0.26	0/3885	0.54	0/5263
2	B	0.27	0/1465	0.53	0/1973
2	D	0.25	0/1456	0.53	0/1962
3	E	0.63	0/376	1.08	1/577 (0.2%)
4	F	0.66	0/393	1.07	2/606 (0.3%)
All	All	0.31	0/11460	0.60	3/15644 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	4	DC	P-O3'-C3'	-8.22	109.84	119.70
3	E	16	DC	P-O3'-C3'	-7.81	110.33	119.70
4	F	5	DG	P-O3'-C3'	-7.68	110.48	119.70

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	3826	0	3842	98	0
1	C	3826	0	3842	102	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1446	0	1471	48	0
2	D	1437	0	1458	41	0
3	E	337	0	188	13	0
4	F	349	0	188	20	0
5	E	32	0	0	0	0
All	All	11253	0	10989	288	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 13.

All (288) 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)
3:E:9:DC:O2	4:F:12:DG:N2	2.10	0.84
1:A:427:ILE:HG23	1:A:431:GLN:HG2	1.65	0.78
2:B:659:ARG:NH1	4:F:17:DA:OP2	2.16	0.78
2:B:487:ASN:HB2	4:F:15:DA:H5"	1.67	0.75
1:A:398:LEU:HD11	1:A:448:ARG:HG2	1.70	0.73
2:B:556:ILE:HD13	2:B:561:VAL:HG21	1.71	0.73
1:C:198:ALA:HB2	1:C:487:VAL:HG21	1.72	0.72
2:B:660:ARG:NH2	4:F:18:DC:OP1	2.21	0.71
1:A:485:GLU:HG3	1:A:489:ARG:HH12	1.53	0.71
2:D:456:TYR:OH	2:D:631:ARG:NH1	2.24	0.71
1:C:51:VAL:HG11	4:F:6:DG:H5'	1.72	0.70
1:C:425:LEU:HB2	1:C:427:ILE:HG12	1.74	0.70
1:A:198:ALA:HB2	1:A:487:VAL:HG21	1.73	0.70
1:A:304:ASP:O	2:D:446:ARG:NH1	2.25	0.70
1:A:445:ALA:HA	1:A:448:ARG:HE	1.56	0.69
2:D:521:LYS:HD2	2:D:523:ARG:HG2	1.74	0.69
1:C:471:LYS:HB2	1:C:474:ARG:HG3	1.74	0.69
2:B:661:SER:O	2:B:665:ARG:HG2	1.92	0.69
1:C:407:LEU:HD21	1:C:420:GLY:HA3	1.73	0.69
2:B:456:TYR:OH	2:B:631:ARG:NH1	2.25	0.69
1:C:213:GLU:OE1	1:C:213:GLU:N	2.26	0.68
2:B:484:LYS:NZ	3:E:7:DT:O2	2.27	0.67
2:D:471:ARG:NH1	2:D:476:GLN:O	2.26	0.67
1:C:300:SER:HB3	1:C:319:LYS:HG3	1.77	0.67
1:C:296:LEU:HD21	1:C:334:HIS:HB2	1.75	0.66
1:C:474:ARG:O	1:C:478:ILE:HG13	1.95	0.66
2:B:548:LEU:HB3	2:B:556:ILE:HD11	1.76	0.66
2:B:446:ARG:NH1	1:C:304:ASP:O	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:627:ASP:HB3	2:D:630:VAL:HG22	1.78	0.66
1:C:241:ALA:O	1:C:245:LYS:HG2	1.96	0.65
2:B:653:GLY:O	2:B:659:ARG:NH2	2.26	0.65
1:C:46:ASP:HB2	1:C:165:VAL:HG23	1.79	0.65
1:A:392:ARG:NH1	1:A:459:GLU:OE2	2.30	0.64
1:C:27:SER:HB3	2:D:538:GLN:HB3	1.80	0.64
2:B:471:ARG:NH1	2:B:476:GLN:O	2.30	0.63
1:C:83:ASN:OD1	1:C:159:ARG:NH2	2.31	0.63
2:D:528:VAL:HG22	2:D:562:PHE:HB2	1.79	0.63
1:A:25:GLN:HG2	1:A:29:ILE:HD13	1.79	0.63
2:B:553:ARG:HH11	2:B:553:ARG:HB3	1.64	0.63
1:C:301:ASN:HB3	1:C:317:GLU:HG2	1.81	0.63
1:A:335:THR:HG22	1:A:336:GLN:H	1.64	0.63
1:A:448:ARG:O	1:A:452:ILE:HG12	1.99	0.63
1:C:63:GLY:O	1:C:68:ARG:NH1	2.32	0.62
2:B:461:ASP:N	3:E:10:DC:OP1	2.32	0.62
1:A:190:PRO:HB2	1:A:226:PRO:HB3	1.80	0.62
1:A:23:GLU:O	1:A:27:SER:OG	2.19	0.61
2:B:459:GLU:HA	2:B:481:LEU:HB2	1.83	0.61
2:B:528:VAL:HG22	2:B:562:PHE:HB2	1.83	0.61
2:B:656:VAL:HG21	4:F:17:DA:H3'	1.81	0.61
1:C:445:ALA:HA	1:C:448:ARG:HE	1.66	0.60
1:C:403:GLU:OE2	1:C:403:GLU:N	2.31	0.60
1:A:39:ARG:HD2	3:E:6:DT:H2"	1.82	0.59
2:D:509:LEU:HD21	2:D:527:ILE:HG12	1.83	0.59
2:D:494:ASP:OD1	2:D:494:ASP:N	2.35	0.59
1:C:222:ARG:O	1:C:224:LYS:NZ	2.35	0.59
1:C:447:GLU:OE1	1:C:450:ARG:NH1	2.36	0.59
1:C:83:ASN:O	1:C:155:ASN:ND2	2.36	0.58
1:C:275:PRO:HG2	1:C:278:VAL:HG21	1.84	0.58
1:C:398:LEU:HD12	1:C:401:LEU:HD13	1.85	0.58
2:D:517:PHE:HZ	2:D:555:LEU:HD13	1.68	0.58
2:D:563:LEU:HB2	2:D:634:ARG:HB2	1.86	0.57
2:D:612:GLY:N	2:D:615:GLU:OE2	2.38	0.57
1:C:115:ASN:HB3	1:C:125:ALA:HB2	1.87	0.57
1:C:294:GLY:C	1:C:295:LYS:HD2	2.25	0.57
1:C:183:VAL:HG22	3:E:16:DC:H4'	1.87	0.57
1:A:128:ARG:NH1	4:F:9:DG:OP2	2.37	0.56
1:A:287:ILE:HG13	1:A:302:ILE:HD13	1.86	0.56
1:C:131:GLU:OE1	1:C:131:GLU:N	2.38	0.56
2:D:665:ARG:O	2:D:665:ARG:NE	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:VAL:HG11	1:A:349:VAL:HG12	1.87	0.56
1:C:398:LEU:HD21	1:C:448:ARG:HB3	1.88	0.56
1:A:212:GLU:OE1	1:A:357:ARG:NH2	2.39	0.56
2:B:620:GLU:O	2:B:624:THR:HG22	2.06	0.56
1:A:129:TYR:OH	4:F:9:DG:OP1	2.23	0.56
1:A:474:ARG:O	1:A:478:ILE:HG13	2.06	0.56
1:C:203:TRP:HZ3	1:C:215:THR:HG22	1.71	0.55
1:C:183:VAL:HA	3:E:16:DC:O3'	2.07	0.55
1:A:256:VAL:HB	1:A:273:GLU:HB2	1.88	0.55
2:B:486:ILE:HD12	4:F:14:DA:H5"	1.88	0.55
2:D:653:GLY:O	2:D:659:ARG:NH2	2.39	0.55
2:B:487:ASN:ND2	4:F:16:DT:OP2	2.40	0.55
1:C:431:GLN:O	1:C:435:ILE:HG12	2.06	0.55
1:A:169:ARG:NH1	1:A:369:GLN:OE1	2.40	0.54
1:A:62:SER:HB3	1:A:64:PHE:CE2	2.42	0.54
1:C:42:PRO:HG3	1:C:178:SER:HB3	1.89	0.54
2:D:646:GLU:O	2:D:650:ILE:HG23	2.07	0.54
1:A:458:ILE:O	1:A:462:ILE:HG13	2.08	0.54
1:A:409:ARG:HE	1:C:401:LEU:HD23	1.73	0.54
2:D:556:ILE:HD13	2:D:561:VAL:HG21	1.90	0.54
1:C:266:ARG:HE	1:C:320:ARG:HD2	1.72	0.54
1:C:242:ASP:O	1:C:246:THR:OG1	2.22	0.53
2:D:561:VAL:HG23	2:D:636:VAL:HB	1.90	0.53
2:D:622:TRP:HA	2:D:626:MET:HB2	1.89	0.53
1:A:60:PHE:HB2	1:A:142:LEU:HD13	1.91	0.53
1:A:354:ARG:NH2	1:A:364:TYR:OH	2.41	0.53
2:B:445:CYS:SG	2:B:453:SER:OG	2.67	0.53
1:A:115:ASN:HB3	1:A:125:ALA:HB2	1.90	0.53
1:C:478:ILE:O	1:C:482:GLU:HG3	2.09	0.53
1:A:113:GLN:HB3	1:A:131:GLU:HG3	1.91	0.52
1:A:94:ASP:OD1	1:A:95:SER:N	2.42	0.52
2:B:646:GLU:O	2:B:650:ILE:HG23	2.10	0.52
1:C:325:LYS:O	1:C:329:ASN:ND2	2.31	0.52
1:C:262:ASP:OD1	1:C:263:SER:N	2.43	0.52
1:C:308:ASP:OD1	1:C:309:ARG:NH1	2.42	0.52
1:C:339:THR:HG22	1:C:340:SER:H	1.75	0.52
1:A:242:ASP:O	1:A:246:THR:OG1	2.25	0.52
1:A:427:ILE:HD12	1:A:431:GLN:HG3	1.91	0.52
1:A:56:LEU:HD11	1:A:109:LEU:HD13	1.91	0.52
4:F:17:DA:C8	4:F:17:DA:H5"	2.45	0.52
2:D:461:ASP:N	4:F:10:DG:OP1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:LEU:O	1:C:201:VAL:HG23	2.11	0.51
2:D:459:GLU:HA	2:D:481:LEU:HB2	1.91	0.51
1:C:129:TYR:OH	3:E:9:DC:OP1	2.28	0.51
1:A:136:PRO:O	1:A:140:GLU:HG2	2.11	0.51
1:A:339:THR:OG1	1:A:340:SER:N	2.44	0.51
1:C:81:MET:HA	1:C:85:HIS:O	2.10	0.51
1:C:401:LEU:HD21	1:C:443:LEU:HD13	1.92	0.51
1:C:427:ILE:HG22	1:C:428:ASP:O	2.10	0.51
1:A:262:ASP:OD1	1:A:263:SER:N	2.40	0.50
1:A:258:GLU:HG2	1:A:270:VAL:HB	1.94	0.50
1:A:181:ILE:HG12	4:F:17:DA:C2	2.46	0.50
1:A:81:MET:HA	1:A:85:HIS:O	2.12	0.50
1:A:425:LEU:HB2	1:A:427:ILE:HG12	1.93	0.50
4:F:17:DA:H5"	4:F:17:DA:H8	1.77	0.50
1:A:296:LEU:HD21	1:A:331:LEU:HD23	1.93	0.50
1:C:75:ARG:O	1:C:79:GLU:HG2	2.11	0.50
1:A:113:GLN:NE2	1:A:131:GLU:OE2	2.45	0.50
1:C:35:VAL:HA	1:C:39:ARG:HB3	1.93	0.50
1:C:448:ARG:O	1:C:452:ILE:HG13	2.11	0.50
1:C:493:ASP:OD2	1:C:493:ASP:N	2.35	0.50
1:A:472:PRO:O	1:A:475:GLN:HG2	2.12	0.49
2:B:499:ASN:O	2:B:503:GLN:HG2	2.12	0.49
1:A:35:VAL:O	1:A:39:ARG:HB3	2.12	0.49
3:E:8:DA:H2'	3:E:9:DC:O4'	2.11	0.49
1:A:325:LYS:O	1:A:329:ASN:ND2	2.29	0.49
1:C:169:ARG:NH2	1:C:482:GLU:OE1	2.46	0.49
1:C:441:ARG:O	1:C:447:GLU:HG3	2.13	0.49
2:B:656:VAL:O	2:B:659:ARG:HG2	2.11	0.49
1:C:294:GLY:O	1:C:295:LYS:HD2	2.13	0.49
1:A:467:ASP:OD2	1:A:474:ARG:NH1	2.36	0.49
1:C:44:VAL:HG11	1:C:349:VAL:HG12	1.94	0.49
2:B:503:GLN:NE2	2:B:506:ILE:HD11	2.27	0.49
2:D:444:ASP:OD2	2:D:523:ARG:NH2	2.46	0.49
2:D:441:LYS:HB3	2:D:480:PRO:HG2	1.95	0.48
2:D:487:ASN:HB2	3:E:15:DC:H5"	1.95	0.48
1:A:248:ARG:NH2	4:F:19:DT:OP1	2.46	0.48
1:C:153:ILE:HG12	1:C:164:THR:HG22	1.94	0.48
1:C:370:LEU:HD23	1:C:479:VAL:HG21	1.95	0.48
1:A:83:ASN:O	1:A:155:ASN:ND2	2.29	0.48
1:C:60:PHE:HB2	1:C:142:LEU:HD13	1.95	0.48
2:B:494:ASP:OD1	2:B:495:ARG:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:ILE:HD12	1:A:15:ILE:HA	1.75	0.47
1:A:300:SER:OG	1:A:317:GLU:OE1	2.32	0.47
1:C:128:ARG:NH1	3:E:9:DC:OP2	2.46	0.47
1:C:228:PHE:H	1:C:496:THR:CG2	2.28	0.47
1:A:275:PRO:HG2	1:A:278:VAL:HG21	1.96	0.47
1:A:280:HIS:CE1	1:A:312:LEU:HD22	2.49	0.47
2:B:502:VAL:O	2:B:506:ILE:HG23	2.14	0.47
1:C:53:ARG:HG3	1:C:166:LEU:HG	1.96	0.47
1:A:111:ASP:HB2	1:A:135:THR:HG23	1.97	0.47
1:A:329:ASN:O	1:A:333:LYS:HG2	2.14	0.47
2:B:534:ASP:OD1	2:B:534:ASP:N	2.48	0.47
1:A:479:VAL:O	1:A:482:GLU:HG3	2.15	0.46
1:C:440:LEU:O	1:C:443:LEU:HB2	2.15	0.46
2:B:554:PRO:HA	2:B:557:GLU:CG	2.45	0.46
1:C:168:SER:O	1:C:369:GLN:NE2	2.48	0.46
2:D:503:GLN:O	2:D:507:THR:HG23	2.16	0.46
1:C:107:TYR:OH	1:C:194:LEU:N	2.47	0.46
1:C:136:PRO:O	1:C:140:GLU:HG2	2.14	0.46
1:A:199:ASP:HB3	1:A:222:ARG:HD2	1.98	0.46
1:C:93:TYR:O	1:C:97:VAL:HG23	2.16	0.46
1:C:283:PHE:HD1	1:C:336:GLN:HB2	1.80	0.46
1:A:168:SER:O	1:A:369:GLN:NE2	2.49	0.46
1:A:435:ILE:O	1:A:438:MET:HB2	2.15	0.46
2:D:660:ARG:NH2	3:E:18:DG:OP1	2.48	0.46
1:A:62:SER:HB3	1:A:64:PHE:CZ	2.51	0.46
2:D:468:LYS:O	2:D:471:ARG:HG2	2.16	0.46
2:D:552:MET:HB3	2:D:555:LEU:HB2	1.98	0.46
1:C:256:VAL:HB	1:C:273:GLU:HB2	1.98	0.45
1:A:260:GLU:OE1	1:A:268:SER:OG	2.34	0.45
1:A:485:GLU:HA	1:A:488:ASP:OD1	2.16	0.45
1:C:107:TYR:HB3	1:C:137:LEU:HD13	1.98	0.45
2:D:439:PRO:HG2	2:D:442:LEU:HB2	1.98	0.45
2:D:522:LEU:HD11	2:D:527:ILE:HD11	1.97	0.45
2:D:522:LEU:HD21	2:D:560:HIS:ND1	2.32	0.45
1:A:284:ILE:HG12	1:A:304:ASP:OD1	2.16	0.45
1:A:453:ASP:OD1	1:A:454:ASP:N	2.50	0.45
3:E:11:DC:C6	3:E:11:DC:H5'	2.52	0.45
1:C:253:MET:HB2	1:C:275:PRO:HB3	1.97	0.45
1:C:206:GLU:N	1:C:206:GLU:OE1	2.50	0.45
1:A:454:ASP:O	1:A:458:ILE:HG12	2.17	0.44
1:A:432:ALA:HA	1:A:435:ILE:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:ILE:O	1:A:408:ILE:HG22	2.18	0.44
1:A:53:ARG:HG3	1:A:166:LEU:HG	1.98	0.44
1:A:77:VAL:HG22	1:A:92:ILE:HG22	2.00	0.44
1:A:138:ALA:HA	1:A:141:MET:HB2	1.98	0.44
1:A:409:ARG:HH21	1:C:401:LEU:HG	1.83	0.44
1:C:211:ASP:OD1	1:C:211:ASP:N	2.51	0.44
1:C:298:GLY:O	1:C:318:ILE:HG23	2.18	0.44
1:A:54:ARG:HH11	1:A:85:HIS:CD2	2.35	0.44
1:C:225:GLY:O	1:C:494:ARG:NH2	2.45	0.44
1:C:253:MET:CE	1:C:341:PHE:HB2	2.48	0.44
1:C:331:LEU:O	1:C:335:THR:OG1	2.31	0.44
2:D:543:LEU:O	2:D:546:THR:HG22	2.17	0.44
1:C:184:GLY:O	2:D:660:ARG:NE	2.51	0.43
2:D:526:LYS:HB2	2:D:526:LYS:HE3	1.62	0.43
1:A:235:VAL:CG2	1:A:252:ARG:HE	2.31	0.43
4:F:5:DG:H8	4:F:5:DG:OP2	2.01	0.43
4:F:16:DT:H4'	4:F:17:DA:OP1	2.17	0.43
1:A:75:ARG:O	1:A:79:GLU:HG3	2.18	0.43
2:D:518:ASP:OD1	2:D:518:ASP:N	2.51	0.43
2:B:506:ILE:HG22	2:B:552:MET:CE	2.48	0.43
2:B:611:LYS:HA	2:B:611:LYS:HD3	1.77	0.43
1:C:253:MET:HE2	1:C:341:PHE:HB2	2.01	0.43
1:C:436:LEU:HD23	1:C:436:LEU:HA	1.87	0.43
1:C:441:ARG:HH11	1:C:441:ARG:HB2	1.84	0.43
3:E:7:DT:H2'	3:E:8:DA:C8	2.54	0.43
4:F:8:DA:H2'	4:F:9:DG:O4'	2.18	0.43
2:B:445:CYS:HG	2:B:453:SER:HG	1.65	0.43
1:C:111:ASP:HB2	1:C:135:THR:HG23	2.01	0.43
1:C:284:ILE:HG12	1:C:304:ASP:OD1	2.18	0.43
2:D:446:ARG:NH2	2:D:474:MET:HB2	2.34	0.43
1:A:382:ARG:O	1:A:386:GLU:HG3	2.19	0.43
2:B:623:GLU:HA	2:B:623:GLU:OE1	2.18	0.43
1:A:215:THR:HG23	1:A:359:ASP:HB2	1.99	0.43
1:A:115:ASN:HB2	2:D:466:SER:OG	2.19	0.43
1:A:228:PHE:H	1:A:496:THR:HG21	1.83	0.43
2:B:553:ARG:HH11	2:B:553:ARG:CB	2.30	0.42
2:D:482:ARG:HD2	4:F:10:DG:H1'	2.01	0.42
1:A:198:ALA:CB	1:A:487:VAL:HG21	2.45	0.42
1:C:219:VAL:O	1:C:223:VAL:HG22	2.19	0.42
1:C:411:SER:OG	1:C:413:THR:O	2.35	0.42
2:D:545:LEU:HD23	2:D:545:LEU:HA	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:498:LYS:O	2:B:498:LYS:NZ	2.33	0.42
1:A:228:PHE:H	1:A:496:THR:CG2	2.33	0.42
1:C:357:ARG:HG2	1:C:360:GLN:HE21	1.85	0.42
1:A:191:PRO:HG2	1:A:228:PHE:HA	2.00	0.42
1:A:412:GLU:O	1:C:446:LEU:HB2	2.19	0.42
1:A:492:ASP:N	1:A:492:ASP:OD1	2.53	0.42
2:B:532:ASP:OD1	2:B:532:ASP:N	2.50	0.42
1:A:409:ARG:HH22	1:C:402:ASP:HA	1.85	0.42
2:B:439:PRO:HG2	2:B:442:LEU:HB2	2.01	0.42
1:A:101:GLN:HG2	1:A:103:TRP:CZ2	2.55	0.42
2:B:439:PRO:HG3	2:B:508:ALA:HB2	2.00	0.42
1:C:229:PRO:HA	1:C:495:ARG:HH11	1.83	0.42
1:A:153:ILE:HG12	1:A:164:THR:HG22	2.02	0.42
1:A:206:GLU:OE2	1:A:206:GLU:N	2.52	0.42
1:A:196:GLU:HB3	1:A:223:VAL:HG12	2.02	0.41
2:B:441:LYS:HD2	2:B:441:LYS:HA	1.95	0.41
2:B:468:LYS:O	2:B:471:ARG:HG2	2.20	0.41
1:C:280:HIS:CE1	1:C:312:LEU:HD22	2.55	0.41
2:D:613:LEU:O	2:D:613:LEU:HD13	2.20	0.41
1:A:155:ASN:ND2	1:A:160:VAL:HG12	2.35	0.41
4:F:16:DT:H2"	4:F:17:DA:O5'	2.20	0.41
1:A:34:SER:OG	2:B:535:VAL:HG11	2.20	0.41
1:A:54:ARG:HG2	1:A:84:TYR:HB3	2.02	0.41
1:A:80:THR:HG22	1:A:85:HIS:HB2	2.01	0.41
1:A:427:ILE:HG23	1:A:431:GLN:CG	2.44	0.41
2:B:492:ARG:H	2:B:492:ARG:HG2	1.63	0.41
2:B:497:LEU:HD11	2:B:513:ILE:HD13	2.01	0.41
2:B:506:ILE:HG22	2:B:552:MET:HE3	2.02	0.41
1:A:122:ASP:OD1	2:D:468:LYS:NZ	2.53	0.41
2:B:553:ARG:HE	2:B:638:LEU:HD21	1.85	0.41
1:A:144:GLU:HG2	1:A:147:GLU:OE2	2.21	0.41
1:C:66:PRO:HA	1:C:133:ARG:HD2	2.02	0.41
1:C:107:TYR:CE2	1:C:175:ALA:HB1	2.55	0.41
1:C:196:GLU:HB3	1:C:223:VAL:HG12	2.02	0.41
1:A:370:LEU:HD23	1:A:479:VAL:HG21	2.03	0.41
1:C:40:ALA:HA	1:C:49:LYS:HD3	2.03	0.41
1:C:79:GLU:HG2	1:C:79:GLU:H	1.59	0.41
1:C:396:LYS:NZ	1:C:396:LYS:HB3	2.36	0.41
1:C:444:ALA:O	1:C:448:ARG:HG3	2.21	0.41
1:C:492:ASP:OD1	1:C:492:ASP:N	2.54	0.41
1:C:160:VAL:HG22	1:C:161:GLN:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:308:ASP:OD1	1:C:308:ASP:N	2.53	0.40
1:C:333:LYS:HD3	1:C:333:LYS:HA	1.88	0.40
1:C:405:ILE:O	1:C:408:ILE:HG22	2.21	0.40
2:D:521:LYS:O	2:D:522:LEU:C	2.58	0.40
1:A:116:PHE:CE1	1:A:130:THR:HB	2.57	0.40
2:B:451:ARG:HE	2:B:525:HIS:CE1	2.39	0.40
1:A:93:TYR:O	1:A:97:VAL:HG23	2.21	0.40
1:A:235:VAL:HG21	1:A:252:ARG:HE	1.87	0.40
2:B:530:MET:HG3	2:B:564:ALA:HB3	2.02	0.40
2:B:532:ASP:HB2	2:B:534:ASP:OD1	2.20	0.40
1:C:323:VAL:O	1:C:326:VAL:HG22	2.21	0.40
1:A:44:VAL:HA	1:A:173:LEU:HD22	2.03	0.40
2:B:503:GLN:HE22	2:B:506:ILE:HD11	1.87	0.40
1:C:280:HIS:C	1:C:282:ASN:H	2.25	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 PDB entries followed by that with respect to all EM entries.

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	485/837 (58%)	470 (97%)	14 (3%)	1 (0%)	44 73
1	C	485/837 (58%)	472 (97%)	13 (3%)	0	100 100
2	B	183/678 (27%)	179 (98%)	4 (2%)	0	100 100
2	D	182/678 (27%)	176 (97%)	5 (3%)	1 (0%)	25 56
All	All	1335/3030 (44%)	1297 (97%)	36 (3%)	2 (0%)	50 77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	521	LYS

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Mol	Chain	Res	Type
1	A	64	PHE

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 PDB entries followed by that with respect to all EM entries.

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	407/685 (59%)	387 (95%)	20 (5%)	21 52
1	C	407/685 (59%)	383 (94%)	24 (6%)	16 44
2	B	155/555 (28%)	141 (91%)	14 (9%)	8 25
2	D	154/555 (28%)	137 (89%)	17 (11%)	5 17
All	All	1123/2480 (45%)	1048 (93%)	75 (7%)	16 38

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	SER
1	A	51	VAL
1	A	62	SER
1	A	68	ARG
1	A	81	MET
1	A	83	ASN
1	A	89	ASP
1	A	135	THR
1	A	170	PHE
1	A	238	GLN
1	A	248	ARG
1	A	260	GLU
1	A	266	ARG
1	A	293	ASP
1	A	383	LYS
1	A	439	GLN
1	A	467	ASP
1	A	482	GLU
1	A	489	ARG
1	A	497	ARG

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Mol	Chain	Res	Type
2	B	445	CYS
2	B	447	SER
2	B	452	LYS
2	B	453	SER
2	B	459	GLU
2	B	482	ARG
2	B	495	ARG
2	B	515	ASP
2	B	532	ASP
2	B	552	MET
2	B	553	ARG
2	B	625	THR
2	B	634	ARG
2	B	657	ASP
1	C	18	VAL
1	C	27	SER
1	C	39	ARG
1	C	61	ASP
1	C	68	ARG
1	C	79	GLU
1	C	81	MET
1	C	122	ASP
1	C	135	THR
1	C	143	ARG
1	C	168	SER
1	C	178	SER
1	C	235	VAL
1	C	242	ASP
1	C	295	LYS
1	C	325	LYS
1	C	333	LYS
1	C	355	THR
1	C	371	ASP
1	C	383	LYS
1	C	387	ARG
1	C	409	ARG
1	C	414	VAL
1	C	439	GLN
2	D	444	ASP
2	D	447	SER
2	D	451	ARG
2	D	452	LYS

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Mol	Chain	Res	Type
2	D	453	SER
2	D	461	ASP
2	D	466	SER
2	D	474	MET
2	D	494	ASP
2	D	511	THR
2	D	521	LYS
2	D	522	LEU
2	D	552	MET
2	D	620	GLU
2	D	625	THR
2	D	634	ARG
2	D	657	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	HIS
1	A	193	ASN
1	A	280	HIS
1	A	334	HIS
2	B	476	GLN
1	C	25	GLN
1	C	172	ASN
1	C	280	HIS
1	C	360	GLN
1	C	433	GLN
2	D	525	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	$\#\|Z\| > 2$
5	A1H5Q	E	201	-	34,36,36	3.90	8 (23%)	36,50,50	2.46	8 (22%)

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
5	A1H5Q	E	201	-	-	4/11/22/22	0/5/5/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	201	A1H5Q	C26-N28	17.77	1.54	1.35
5	E	201	A1H5Q	C29-N28	11.20	1.59	1.39
5	E	201	A1H5Q	C11-C06	-4.17	1.36	1.42
5	E	201	A1H5Q	C25-S24	-3.77	1.70	1.80
5	E	201	A1H5Q	C25-C26	3.12	1.53	1.51
5	E	201	A1H5Q	O02-C03	2.87	1.39	1.35
5	E	201	A1H5Q	O27-C26	-2.27	1.18	1.23
5	E	201	A1H5Q	C23-S24	-2.07	1.73	1.76

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	201	A1H5Q	C03-N12-C11	9.23	121.84	117.09
5	E	201	A1H5Q	C25-S24-C23	8.36	112.47	97.37
5	E	201	A1H5Q	C04-C03-N12	-3.71	121.88	125.57
5	E	201	A1H5Q	C08-N07-C06	2.97	121.53	116.93
5	E	201	A1H5Q	C09-C08-N07	-2.70	120.39	124.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	201	A1H5Q	C01-O02-C03	-2.51	113.42	117.36
5	E	201	A1H5Q	C14-C15-N31	-2.21	108.05	111.34
5	E	201	A1H5Q	O02-C03-C04	2.00	120.19	116.71

There are no chirality outliers.

All (4) torsion outliers are listed below:

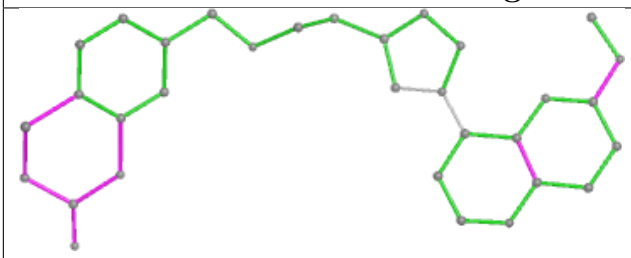
Mol	Chain	Res	Type	Atoms
5	E	201	A1H5Q	C11-C10-N13-N32
5	E	201	A1H5Q	C15-C16-C17-N18
5	E	201	A1H5Q	C16-C17-N18-C19
5	E	201	A1H5Q	C20-C19-N18-C17

There are no ring outliers.

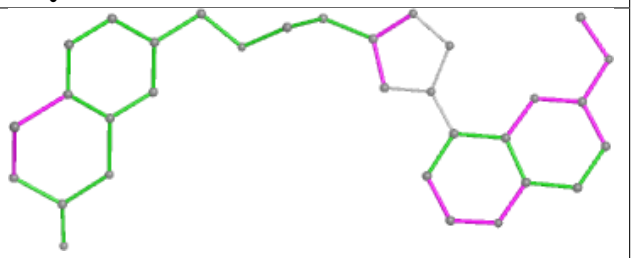
No monomer is involved in short contacts.

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

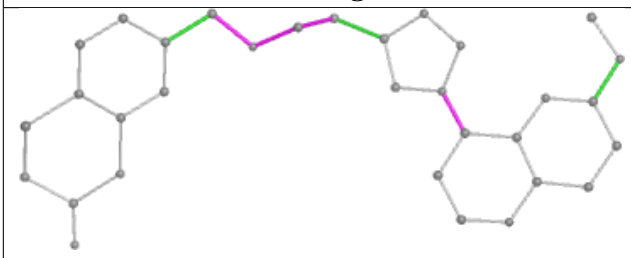
Ligand A1H5Q E 201



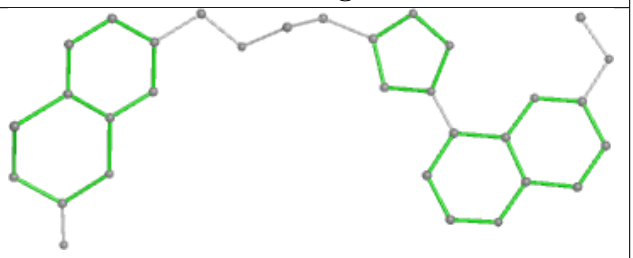
Bond lengths



Bond angles



Torsions



Rings

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.