



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:14 AM UTC

PDB ID : 9N39 / pdb_00009n39
Title : DNA gyrase complexed with uncleaved DNA and Compound 185 to 2.25 Å resolution
Authors : Bell, C.E.; McElroy, C.A.; Ratigan, S.C.
Deposited on : 2025-01-30
Resolution : 2.25 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

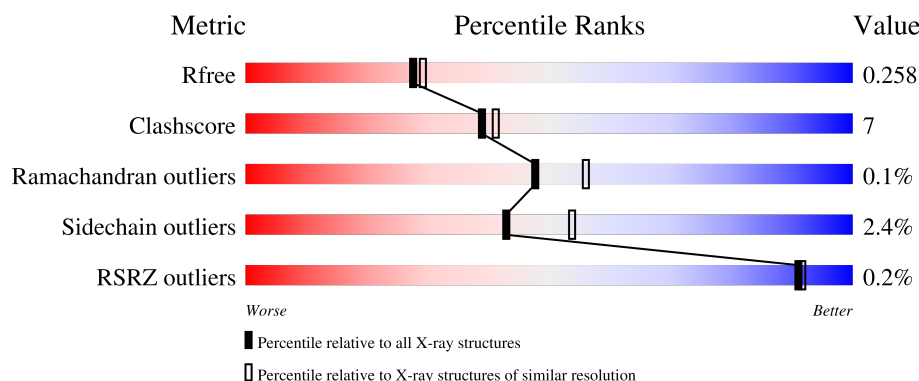
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

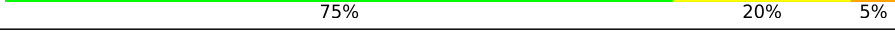
The reported resolution of this entry is 2.25 Å.

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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	693	
1	B	693	
2	C	20	
2	D	20	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	A1BVQ	D	101[A]	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11795 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 DNA gyrase subunit B fusion with DNA gyrase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	672	Total	C	N	O	S	0	0	0
			5318	3316	958	1019	25			
1	B	673	Total	C	N	O	S	0	0	0
			5317	3315	956	1021	25			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	408	GLY	-	expression tag	UNP P0A0K8
A	409	MET	-	expression tag	UNP P0A0K8
A	?	-	LEU	deletion	UNP P0A0K8
A	?	-	TYR	deletion	UNP P0A0K8
A	?	-	LYS	deletion	UNP P0A0K8
A	?	-	LEU	deletion	UNP P0A0K8
A	?	-	THR	deletion	UNP P0A0K8
A	?	-	GLN	deletion	UNP P0A0K8
A	?	-	GLY	deletion	UNP P0A0K8
A	?	-	LYS	deletion	UNP P0A0K8
A	?	-	GLN	deletion	UNP P0A0K8
A	?	-	LYS	deletion	UNP P0A0K8
A	?	-	TYR	deletion	UNP P0A0K8
A	?	-	TYR	deletion	UNP P0A0K8
A	?	-	VAL	deletion	UNP P0A0K8
A	?	-	TYR	deletion	UNP P0A0K8
A	?	-	ASN	deletion	UNP P0A0K8
A	?	-	ASP	deletion	UNP P0A0K8
A	?	-	ARG	deletion	UNP P0A0K8
A	?	-	GLU	deletion	UNP P0A0K8
A	?	-	LEU	deletion	UNP P0A0K8
A	?	-	ASP	deletion	UNP P0A0K8
A	?	-	LYS	deletion	UNP P0A0K8
A	?	-	LEU	deletion	UNP P0A0K8
A	?	-	LYS	deletion	UNP P0A0K8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	SER	deletion	UNP P0A0K8
A	?	-	GLU	deletion	UNP P0A0K8
A	?	-	LEU	deletion	UNP P0A0K8
A	?	-	ASN	deletion	UNP P0A0K8
A	?	-	PRO	deletion	UNP P0A0K8
A	?	-	THR	deletion	UNP P0A0K8
A	?	-	PRO	deletion	UNP P0A0K8
A	?	-	LYS	deletion	UNP P0A0K8
A	?	-	TRP	deletion	UNP P0A0K8
A	?	-	SER	deletion	UNP P0A0K8
A	?	-	ILE	deletion	UNP P0A0K8
A	544	THR	ALA	conflict	UNP P0A0K8
A	545	GLY	ARG	conflict	UNP P0A0K8
A	1123	PHE	TYR	conflict	UNP P20831
A	1457	THR	ALA	conflict	UNP P20831
B	408	GLY	-	expression tag	UNP P0A0K8
B	409	MET	-	expression tag	UNP P0A0K8
B	?	-	LEU	deletion	UNP P0A0K8
B	?	-	TYR	deletion	UNP P0A0K8
B	?	-	LYS	deletion	UNP P0A0K8
B	?	-	LEU	deletion	UNP P0A0K8
B	?	-	THR	deletion	UNP P0A0K8
B	?	-	GLN	deletion	UNP P0A0K8
B	?	-	GLY	deletion	UNP P0A0K8
B	?	-	LYS	deletion	UNP P0A0K8
B	?	-	GLN	deletion	UNP P0A0K8
B	?	-	LYS	deletion	UNP P0A0K8
B	?	-	TYR	deletion	UNP P0A0K8
B	?	-	TYR	deletion	UNP P0A0K8
B	?	-	VAL	deletion	UNP P0A0K8
B	?	-	TYR	deletion	UNP P0A0K8
B	?	-	ASN	deletion	UNP P0A0K8
B	?	-	ASP	deletion	UNP P0A0K8
B	?	-	ARG	deletion	UNP P0A0K8
B	?	-	GLU	deletion	UNP P0A0K8
B	?	-	LEU	deletion	UNP P0A0K8
B	?	-	ASP	deletion	UNP P0A0K8
B	?	-	LYS	deletion	UNP P0A0K8
B	?	-	LEU	deletion	UNP P0A0K8
B	?	-	LYS	deletion	UNP P0A0K8
B	?	-	SER	deletion	UNP P0A0K8
B	?	-	GLU	deletion	UNP P0A0K8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	LEU	deletion	UNP P0A0K8
B	?	-	ASN	deletion	UNP P0A0K8
B	?	-	PRO	deletion	UNP P0A0K8
B	?	-	THR	deletion	UNP P0A0K8
B	?	-	PRO	deletion	UNP P0A0K8
B	?	-	LYS	deletion	UNP P0A0K8
B	?	-	TRP	deletion	UNP P0A0K8
B	?	-	SER	deletion	UNP P0A0K8
B	?	-	ILE	deletion	UNP P0A0K8
B	544	THR	ALA	conflict	UNP P0A0K8
B	545	GLY	ARG	conflict	UNP P0A0K8
B	1123	PHE	TYR	conflict	UNP P20831
B	1457	THR	ALA	conflict	UNP P20831

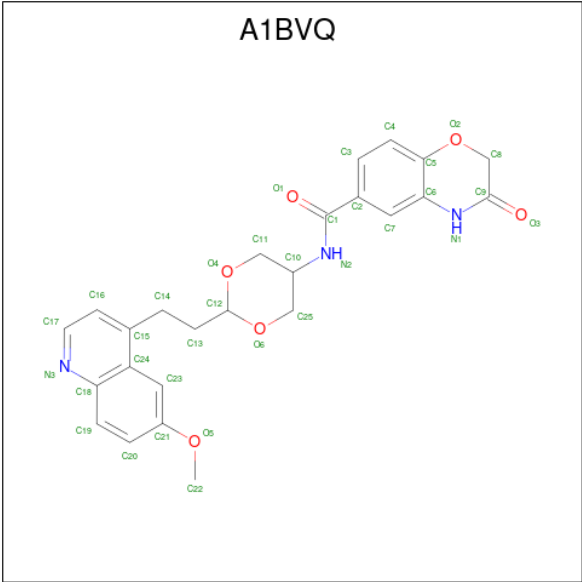
- Molecule 2 is a DNA chain called DNA (5'-D(P*AP*GP*CP*CP*GP*TP*AP*GP*GP*G P*CP*CP*CP*TP*AP*CP*GP*GP*CP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	20	Total	C	N	O	P	0	0	0
			410	193	77	120	20			
2	D	20	Total	C	N	O	P	0	0	0
			390	183	75	113	19			

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		
3	B	1	Total	Mn	0	0
			1	1		

- Molecule 4 is N-{(2r,5r)-2-[2-(6-methoxyquinolin-4-yl)ethyl]-1,3-dioxan-5-yl}-3-oxo-3,4-dihydro-2H-1,4-benzoxazine-6-carboxamide (CCD ID: A1BVQ) (formula: C₂₅H₂₅N₃O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	N	O	0	1
			68	50	6	12		

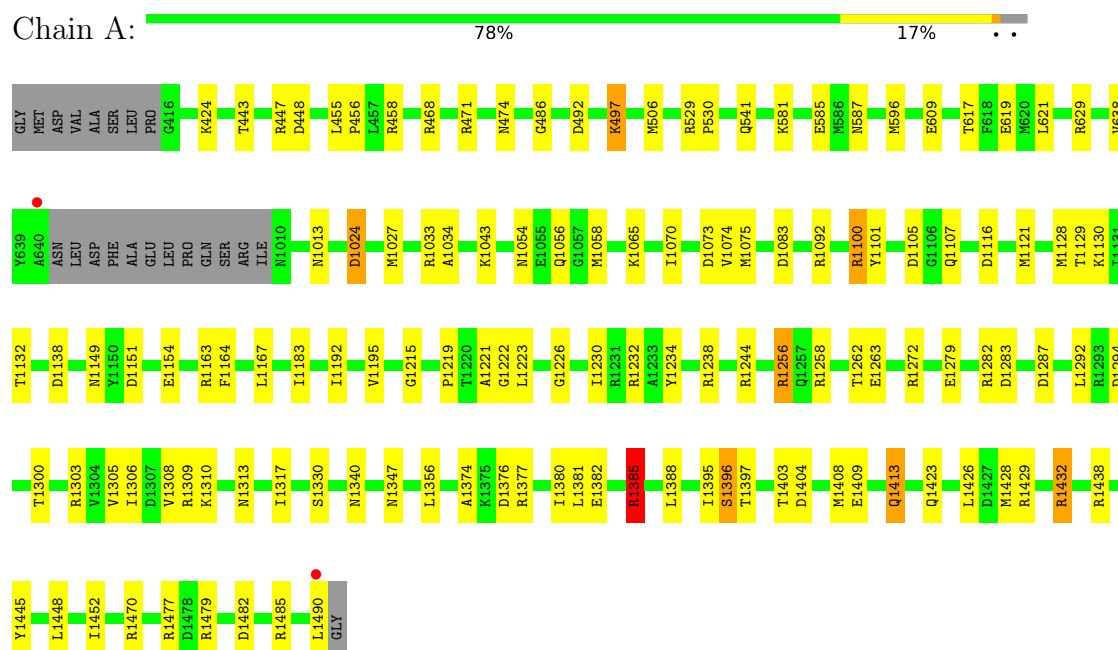
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	124	Total	O	0	0
			124	124		
5	B	128	Total	O	0	0
			128	128		
5	C	19	Total	O	0	0
			19	19		
5	D	19	Total	O	0	0
			19	19		

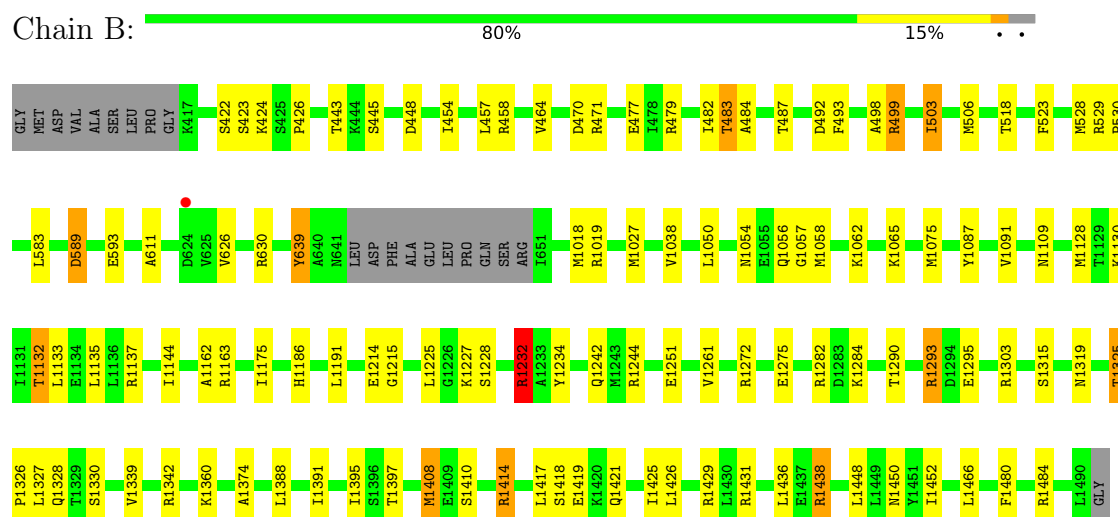
3 Residue-property plots

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 gyrase subunit B fusion with DNA gyrase subunit A



- Molecule 1: DNA gyrase subunit B fusion with DNA gyrase subunit A



- Molecule 2: 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')

Chain C:  60% 40%



- Molecule 2: 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')

Chain D:  75% 20% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	93.48Å 93.48Å 410.38Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	23.89 – 2.25 23.89 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.7 (23.89-2.25) 98.7 (23.89-2.25)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 2.26Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.202 , 0.256 0.207 , 0.258	Depositor DCC
R_{free} test set	4774 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	43.9	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 16.8	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	0.96	EDS
Total number of atoms	11795	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% 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, A1BVQ

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	0.62	0/5390	1.25	25/7262 (0.3%)
1	B	0.62	0/5389	1.23	13/7266 (0.2%)
2	C	0.50	0/459	1.20	2/706 (0.3%)
2	D	0.45	0/437	1.39	3/674 (0.4%)
All	All	0.61	0/11675	1.25	43/15908 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
1	B	0	7
All	All	0	14

There are no bond length outliers.

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1450	ASN	CB-CA-C	7.78	123.26	110.81
1	A	1024	ASP	CB-CA-C	-7.67	98.53	110.81
2	D	1	DA	O3'-P-O5'	7.55	115.33	104.00
2	D	5	DG	O3'-P-O5'	-7.22	93.17	104.00
1	A	581	LYS	N-CA-CB	6.84	120.21	109.82
1	B	470	ASP	CA-CB-CG	6.65	119.25	112.60
1	A	458	ARG	CB-CA-C	-6.62	102.35	111.95
1	B	448	ASP	CA-CB-CG	6.59	119.19	112.60
1	A	1279	GLU	CB-CA-C	-6.54	100.34	110.81
1	A	1073	ASP	CA-CB-CG	6.51	119.11	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1340	ASN	CB-CA-C	-6.26	102.56	111.95
1	A	617	THR	CA-CB-OG1	-6.14	100.39	109.60
1	A	1083	ASP	CA-CB-CG	6.13	118.73	112.60
1	B	1132	THR	CA-CB-OG1	-6.13	100.41	109.60
1	B	630	ARG	CB-CA-C	-6.06	100.38	110.68
1	A	1151	ASP	CA-CB-CG	6.02	118.62	112.60
1	A	1138	ASP	CA-CB-CG	6.00	118.60	112.60
1	A	619	GLU	CB-CG-CD	5.99	122.78	112.60
1	A	1132	THR	CA-CB-OG1	-5.92	100.72	109.60
1	B	639	TYR	N-CA-CB	-5.89	101.94	110.36
1	A	1300	THR	CA-CB-OG1	-5.86	100.81	109.60
1	B	1227	LYS	N-CA-C	-5.78	105.81	112.92
1	A	638	VAL	N-CA-CB	-5.75	106.90	112.65
1	B	1175	ILE	CA-C-N	-5.75	116.83	123.04
1	B	1175	ILE	C-N-CA	-5.75	116.83	123.04
1	A	1116	ASP	CA-CB-CG	5.68	118.28	112.60
1	A	1164	PHE	CB-CA-C	5.49	117.56	109.22
1	A	1262	THR	CA-CB-OG1	-5.48	101.38	109.60
1	B	589	ASP	CA-CB-CG	5.48	118.08	112.60
1	A	1138	ASP	CB-CA-C	-5.41	101.16	111.06
1	A	581	LYS	CB-CA-C	-5.40	102.33	110.92
1	A	1244	ARG	N-CA-CB	-5.39	101.51	111.53
1	B	1480	PHE	CA-CB-CG	-5.38	108.42	113.80
1	A	1107	GLN	N-CA-CB	-5.30	102.45	110.77
2	C	9	DG	O3'-P-O5'	5.17	111.76	104.00
1	A	1482	ASP	CA-CB-CG	5.17	117.77	112.60
1	A	1263	GLU	CB-CG-CD	5.16	121.38	112.60
2	D	14	DT	C2'-C3'-O3'	5.12	119.18	111.50
1	B	483	THR	CA-CB-OG1	-5.11	101.94	109.60
1	A	448	ASP	CA-CB-CG	5.10	117.70	112.60
2	C	16	DC	O3'-P-O5'	-5.06	96.41	104.00
1	B	479	ARG	CB-CA-C	5.03	118.77	110.88
1	A	1376	ASP	CA-CB-CG	5.02	117.62	112.60

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1100	ARG	Sidechain
1	A	1163	ARG	Sidechain
1	A	1256	ARG	Sidechain
1	A	1287	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	A	1385	ARG	Sidechain
1	A	1432	ARG	Sidechain
1	A	1470	ARG	Sidechain
1	B	1019	ARG	Sidechain
1	B	1163	ARG	Sidechain
1	B	1232	ARG	Sidechain
1	B	1293	ARG	Sidechain
1	B	1414	ARG	Sidechain
1	B	1429	ARG	Sidechain
1	B	499	ARG	Sidechain

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	5318	0	5363	71	0
1	B	5317	0	5339	71	0
2	C	410	0	224	7	0
2	D	390	0	209	12	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	D	68	0	0	20	0
5	A	124	0	0	8	0
5	B	128	0	0	1	0
5	C	19	0	0	0	0
5	D	19	0	0	0	0
All	All	11795	0	11135	154	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 7.

All (154) 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:1121:MET:HE2	4:D:101[A]:A1BVQ:C7	1.93	0.99
1:A:1121:MET:HE2	4:D:101[A]:A1BVQ:C6	1.91	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:11:DC:C2	4:D:101[A]:A1BVQ:N3	2.34	0.96
1:A:1121:MET:CE	4:D:101[A]:A1BVQ:C6	2.55	0.84
2:D:11:DC:C6	4:D:101[A]:A1BVQ:C17	2.70	0.74
2:C:10:DG:C2	4:D:101[A]:A1BVQ:C19	2.70	0.74
1:A:1423:GLN:OE1	1:B:1431:ARG:NH1	2.20	0.74
1:B:1087:TYR:O	1:B:1091:VAL:HG23	1.91	0.71
1:A:1388:LEU:HD21	1:A:1428:MET:HE1	1.75	0.69
1:A:471:ARG:HG2	1:A:471:ARG:NH1	2.12	0.65
2:D:11:DC:C5	4:D:101[A]:A1BVQ:C17	2.80	0.64
1:A:1294:ASP:OD2	5:A:1601:HOH:O	2.15	0.63
1:A:1056:GLN:HB2	1:A:1058:MET:HE3	1.82	0.60
1:B:1388:LEU:HD13	1:B:1438:ARG:HG2	1.83	0.60
1:B:1391:ILE:O	1:B:1395:ILE:HG12	2.01	0.60
2:C:10:DG:C2	4:D:101[B]:A1BVQ:C17	2.84	0.60
1:A:1413:GLN:HE21	1:A:1413:GLN:HA	1.67	0.59
1:B:1315:SER:O	1:B:1319:ASN:ND2	2.35	0.59
2:C:1:DA:H5'	2:C:1:DA:N3	2.17	0.59
1:A:1382:GLU:OE2	1:A:1445:TYR:OH	2.18	0.59
1:B:1135:LEU:HD23	1:B:1162:ALA:HA	1.85	0.59
2:C:10:DG:N2	4:D:101[A]:A1BVQ:C19	2.66	0.58
1:B:1232:ARG:HG2	1:B:1232:ARG:HH11	1.67	0.57
1:A:1429:ARG:HG2	1:A:1429:ARG:HH11	1.70	0.57
1:B:1225:LEU:HD11	1:B:1244:ARG:NE	2.21	0.56
2:D:11:DC:N3	4:D:101[A]:A1BVQ:N3	2.54	0.55
1:B:1293:ARG:HG3	1:B:1293:ARG:HH11	1.71	0.55
1:A:1056:GLN:CB	1:A:1058:MET:HE3	2.36	0.55
1:A:1121:MET:CE	4:D:101[A]:A1BVQ:N1	2.70	0.54
1:A:1192:ILE:HG21	1:A:1477:ARG:HB2	1.88	0.54
1:A:1230:ILE:HG13	5:A:1618:HOH:O	2.06	0.53
1:B:1137:ARG:HD2	5:B:1662:HOH:O	2.07	0.53
1:A:471:ARG:HG2	1:A:471:ARG:HH11	1.72	0.53
1:B:529:ARG:NH2	1:B:611:ALA:HB1	2.23	0.53
1:A:1222:GLY:C	1:A:1223:LEU:HD12	2.33	0.53
1:B:589:ASP:O	1:B:593:GLU:HG2	2.09	0.53
2:D:11:DC:N3	4:D:101[A]:A1BVQ:C18	2.72	0.52
1:A:1385:ARG:HH11	1:A:1385:ARG:CB	2.22	0.52
1:B:1186:HIS:HB2	1:B:1191:LEU:HD11	1.92	0.52
1:B:1360:LYS:HD2	1:B:1466:LEU:HD13	1.92	0.52
1:A:1404:ASP:CG	1:B:1431:ARG:HH21	2.17	0.51
1:A:1121:MET:HE3	4:D:101[A]:A1BVQ:C6	2.40	0.51
1:A:1272:ARG:NH1	5:A:1610:HOH:O	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1121:MET:HE2	4:D:101[A]:A1BVQ:N1	2.24	0.51
1:A:1034:ALA:O	1:A:1043:LYS:HE2	2.10	0.51
1:B:626:VAL:HG11	2:C:17:DG:H3'	1.93	0.50
1:B:1054:ASN:HA	1:B:1128:MET:CE	2.40	0.50
1:A:1149:ASN:CG	1:A:1154:GLU:HB2	2.36	0.50
1:B:1417:LEU:HD13	1:B:1425:ILE:HD12	1.93	0.50
2:D:11:DC:C4	4:D:101[A]:A1BVQ:C17	2.95	0.50
1:B:493:PHE:CE1	1:B:530:PRO:HB2	2.46	0.50
1:B:464:VAL:HG21	1:B:523:PHE:HA	1.93	0.49
1:B:1050:LEU:HD22	1:B:1132:THR:HG21	1.94	0.49
1:B:1225:LEU:HD11	1:B:1244:ARG:HD2	1.94	0.49
1:B:518:THR:HB	1:B:1018:MET:HE1	1.94	0.49
1:B:1215:GLY:HA2	1:B:1234:TYR:OH	2.12	0.49
1:B:1272:ARG:NH2	2:D:3:DC:H5''	2.28	0.49
1:A:1070:ILE:O	1:A:1074:VAL:HG23	2.11	0.49
1:A:1292:LEU:CD1	1:A:1306:ILE:HG12	2.43	0.49
1:B:487:THR:HG22	1:B:498:ALA:HA	1.93	0.49
1:A:1408:MET:SD	1:A:1426:LEU:HD12	2.53	0.49
1:A:1377:ARG:HG3	1:A:1448:LEU:HD11	1.94	0.49
1:B:1038:VAL:HG11	1:B:1339:VAL:HG22	1.94	0.49
1:B:1418:SER:OG	1:B:1421:GLN:HG3	2.13	0.49
1:A:1303:ARG:HG3	1:A:1303:ARG:NH1	2.28	0.48
1:B:493:PHE:CD1	1:B:493:PHE:O	2.66	0.48
1:B:1448:LEU:O	1:B:1452:ILE:HG13	2.13	0.48
1:A:1054:ASN:HA	1:A:1128:MET:HE1	1.95	0.48
1:B:503:ILE:HD12	1:B:503:ILE:N	2.27	0.48
1:A:1377:ARG:CG	1:A:1448:LEU:HD11	2.44	0.48
1:B:506:MET:HG2	1:B:583:LEU:HD11	1.94	0.48
1:B:1272:ARG:NH2	2:D:3:DC:OP1	2.46	0.48
1:A:486:GLY:O	1:A:497:LYS:HB3	2.14	0.48
2:C:18:DG:H2''	2:C:19:DC:C6	2.49	0.48
2:D:11:DC:N1	4:D:101[A]:A1BVQ:C17	2.76	0.48
1:A:1374:ALA:HB1	1:A:1448:LEU:HD22	1.94	0.48
1:A:1092:ARG:NH1	5:A:1608:HOH:O	2.40	0.47
1:B:471:ARG:NH2	2:C:14:DT:OP1	2.47	0.47
1:A:1121:MET:CE	4:D:101[A]:A1BVQ:C9	2.92	0.47
1:B:1282:ARG:C	1:B:1284:LYS:H	2.22	0.47
1:A:587:ASN:HA	5:A:1678:HOH:O	2.13	0.47
1:A:1226:GLY:HA2	1:A:1490:LEU:HG	1.97	0.47
1:A:529:ARG:N	1:A:530:PRO:CD	2.78	0.47
1:B:1225:LEU:HD11	1:B:1244:ARG:CD	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1242:GLN:HE22	1:B:1330:SER:HB3	1.80	0.47
1:B:529:ARG:N	1:B:530:PRO:CD	2.78	0.47
1:B:443:THR:HG22	1:B:454:ILE:CD1	2.45	0.47
1:A:585:GLU:O	1:A:585:GLU:HG2	2.15	0.46
1:A:1479:ARG:HD2	5:A:1713:HOH:O	2.15	0.46
1:A:1282:ARG:HG2	1:A:1283:ASP:OD1	2.15	0.46
1:B:1397:THR:HG23	1:B:1414:ARG:NH2	2.30	0.46
2:D:11:DC:C2	4:D:101[A]:A1BVQ:C17	2.97	0.46
1:A:443:THR:HG23	1:A:506:MET:HE1	1.96	0.46
1:B:424:LYS:O	1:B:426:PRO:HD3	2.15	0.46
1:B:1058:MET:HE2	1:B:1065:LYS:HG3	1.98	0.46
1:B:1027:MET:HE2	1:B:1027:MET:HB3	1.89	0.45
1:A:1256:ARG:NH1	5:A:1615:HOH:O	2.49	0.45
1:B:1109:ASN:OD1	1:B:1109:ASN:C	2.58	0.45
1:B:1144:ILE:C	1:B:1144:ILE:HD12	2.42	0.45
1:B:1075:MET:HE1	4:D:101[A]:A1BVQ:C4	2.47	0.45
1:A:1195:VAL:CG1	1:A:1356:LEU:HD13	2.47	0.44
1:A:609:GLU:HG3	1:A:1013:ASN:HD22	1.82	0.44
1:A:1234:TYR:O	1:A:1347:ASN:HB2	2.16	0.44
1:B:1058:MET:CE	1:B:1065:LYS:HG3	2.48	0.44
2:D:1:DA:H2'	2:D:1:DA:N3	2.32	0.44
1:A:1100:ARG:HG3	1:A:1101:TYR:CE2	2.53	0.44
1:B:529:ARG:HH22	1:B:611:ALA:HB1	1.81	0.44
1:A:1219:PRO:HA	1:A:1485:ARG:HH11	1.82	0.44
1:A:1238:ARG:HG2	1:A:1238:ARG:HH11	1.83	0.44
1:A:1448:LEU:O	1:A:1452:ILE:HG13	2.18	0.44
1:A:541:GLN:NE2	5:A:1607:HOH:O	2.38	0.43
1:B:484:ALA:O	1:B:499:ARG:HD3	2.18	0.43
1:B:1261:VAL:HG21	1:B:1327:LEU:HD11	2.00	0.43
1:B:1374:ALA:HB1	1:B:1448:LEU:HD11	1.99	0.43
1:B:1056:GLN:CB	1:B:1058:MET:HE3	2.48	0.43
1:A:621:LEU:O	1:A:629:ARG:HD3	2.17	0.43
1:B:493:PHE:CD1	1:B:493:PHE:C	2.97	0.43
1:B:1242:GLN:NE2	1:B:1330:SER:HB3	2.34	0.43
1:A:1105:ASP:HB2	1:A:1129:THR:HG22	2.01	0.43
1:A:1313:ASN:OD1	1:A:1313:ASN:C	2.61	0.43
1:A:1385:ARG:HH11	1:A:1385:ARG:HB3	1.83	0.43
1:A:1215:GLY:HA2	1:A:1234:TYR:OH	2.19	0.42
1:B:639:TYR:CD2	1:B:1342:ARG:HG2	2.54	0.42
1:A:1380:ILE:HD13	1:A:1380:ILE:HA	1.87	0.42
1:B:1058:MET:SD	1:B:1065:LYS:CG	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1075:MET:HE1	4:D:101[B]:A1BVQ:C4	2.49	0.42
1:B:422:SER:O	1:B:423:SER:C	2.61	0.42
1:A:1167:LEU:HD11	1:A:1183:ILE:HD12	2.02	0.42
1:B:1326:PRO:C	1:B:1328:GLN:N	2.77	0.42
1:A:1303:ARG:HG3	1:A:1303:ARG:HH11	1.85	0.42
1:A:1396:SER:O	1:A:1397:THR:C	2.63	0.42
1:B:477:GLU:OE1	1:B:477:GLU:N	2.52	0.42
1:B:1408:MET:HG2	1:B:1426:LEU:HD12	2.01	0.42
1:A:1058:MET:HE2	1:A:1065:LYS:HG2	2.02	0.41
1:A:1309:ARG:O	1:A:1310:LYS:C	2.63	0.41
1:A:468:ARG:HG2	1:A:468:ARG:HH21	1.83	0.41
1:B:482:ILE:O	1:B:483:THR:C	2.63	0.41
1:A:1258:ARG:HD2	1:A:1305:VAL:HG13	2.02	0.41
1:B:1325:THR:OG1	1:B:1327:LEU:HB2	2.20	0.41
1:B:1057:GLY:O	1:B:1062:LYS:HD2	2.21	0.41
1:B:1295:GLU:HB2	1:B:1303:ARG:HD3	2.02	0.41
1:A:447:ARG:HB3	1:A:596:MET:HE1	2.03	0.41
1:A:1027:MET:HE2	1:A:1027:MET:HB3	1.95	0.41
1:A:1308:VAL:HG22	1:A:1317:ILE:HD12	2.02	0.41
1:A:424:LYS:HD3	1:A:424:LYS:HA	1.90	0.40
1:A:455:LEU:HA	1:A:456:PRO:HD2	1.97	0.40
1:B:1215:GLY:O	1:B:1484:ARG:NH2	2.50	0.40
1:B:1408:MET:HE1	1:B:1419:GLU:CG	2.52	0.40
1:B:457:LEU:O	1:B:458:ARG:HD3	2.21	0.40
1:B:528:MET:O	1:B:529:ARG:C	2.65	0.40
1:B:1130:LYS:O	1:B:1133:LEU:HB2	2.21	0.40
1:B:1272:ARG:NH2	2:D:3:DC:C5'	2.84	0.40
1:A:1377:ARG:O	1:A:1381:LEU:HG	2.21	0.40
1:B:1397:THR:CG2	1:B:1410:SER:HB3	2.51	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	668/693 (96%)	637 (95%)	29 (4%)	2 (0%)	36	40
1	B	669/693 (96%)	634 (95%)	35 (5%)	0	100	100
All	All	1337/1386 (96%)	1271 (95%)	64 (5%)	2 (0%)	48	56

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1033	ARG
1	A	1221	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	
1	A	573/591 (97%)	558 (97%)	15 (3%)	40	50
1	B	571/591 (97%)	558 (98%)	13 (2%)	44	55
All	All	1144/1182 (97%)	1116 (98%)	28 (2%)	43	54

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	474	ASN
1	A	492	ASP
1	A	497	LYS
1	A	1024	ASP
1	A	1130	LYS
1	A	1232	ARG
1	A	1330	SER
1	A	1385	ARG
1	A	1395	ILE
1	A	1396	SER
1	A	1403	THR
1	A	1409	GLU
1	A	1413	GLN
1	A	1432	ARG

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Mol	Chain	Res	Type
1	A	1438	ARG
1	B	445	SER
1	B	492	ASP
1	B	503	ILE
1	B	1214	GLU
1	B	1228	SER
1	B	1232	ARG
1	B	1251	GLU
1	B	1275	GLU
1	B	1290	THR
1	B	1325	THR
1	B	1408	MET
1	B	1436	LEU
1	B	1438	ARG

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

Mol	Chain	Res	Type
1	A	476	ASN
1	A	480	GLN
1	A	1354	HIS
1	A	1413	GLN
1	B	600	HIS
1	B	631	GLN
1	B	1095	GLN
1	B	1107	GLN
1	B	1319	ASN
1	B	1320	ASN

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

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	A1BVQ	D	101[A]	-	37,38,38	2.83	5 (13%)	45,53,53	2.47	16 (35%)
4	A1BVQ	D	101[B]	-	37,38,38	2.17	5 (13%)	45,53,53	2.65	6 (13%)

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	A1BVQ	D	101[A]	-	-	4/15/34/34	0/5/5/5
4	A1BVQ	D	101[B]	-	-	3/15/34/34	0/5/5/5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	101[A]	A1BVQ	C19-C20	12.72	1.64	1.36
4	D	101[B]	A1BVQ	C19-C18	-8.49	1.27	1.41
4	D	101[B]	A1BVQ	O5-C21	6.71	1.50	1.37
4	D	101[A]	A1BVQ	C23-C24	6.01	1.53	1.42
4	D	101[A]	A1BVQ	O5-C21	5.65	1.48	1.37
4	D	101[A]	A1BVQ	C20-C21	-5.64	1.28	1.38
4	D	101[B]	A1BVQ	C23-C24	5.44	1.52	1.42
4	D	101[A]	A1BVQ	C17-N3	2.63	1.37	1.32
4	D	101[B]	A1BVQ	C20-C21	-2.15	1.34	1.38
4	D	101[B]	A1BVQ	C11-C10	2.02	1.53	1.51

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	101[B]	A1BVQ	C19-C18-C24	-10.61	107.70	119.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	101[B]	A1BVQ	C20-C21-C23	-8.66	109.57	120.83
4	D	101[A]	A1BVQ	C20-C21-C23	-7.19	111.48	120.83
4	D	101[A]	A1BVQ	C20-C19-C18	-6.57	112.94	120.80
4	D	101[B]	A1BVQ	C20-C19-C18	6.39	128.45	120.80
4	D	101[B]	A1BVQ	C19-C18-N3	5.81	127.90	118.55
4	D	101[A]	A1BVQ	C19-C20-C21	5.75	127.59	120.13
4	D	101[A]	A1BVQ	C2-C1-N2	-4.30	109.08	117.04
4	D	101[A]	A1BVQ	C19-C18-C24	-3.67	115.18	119.13
4	D	101[A]	A1BVQ	C6-N1-C9	-3.53	120.22	124.45
4	D	101[A]	A1BVQ	C5-C6-N1	-3.32	115.76	118.56
4	D	101[A]	A1BVQ	O1-C1-N2	3.13	128.42	122.47
4	D	101[A]	A1BVQ	C22-O5-C21	3.09	124.13	117.50
4	D	101[A]	A1BVQ	C25-O6-C12	2.74	116.02	112.24
4	D	101[A]	A1BVQ	C10-N2-C1	2.52	127.33	122.56
4	D	101[A]	A1BVQ	C23-C24-C18	2.50	121.94	118.99
4	D	101[A]	A1BVQ	C21-C23-C24	2.46	123.22	120.09
4	D	101[B]	A1BVQ	C16-C17-N3	-2.40	121.04	124.60
4	D	101[A]	A1BVQ	C7-C6-N1	2.36	123.85	119.76
4	D	101[A]	A1BVQ	O2-C5-C4	2.30	120.55	116.89
4	D	101[A]	A1BVQ	O2-C8-C9	-2.28	108.99	114.81
4	D	101[B]	A1BVQ	O1-C1-N2	2.12	126.50	122.47

There are no chirality outliers.

All (7) torsion outliers are listed below:

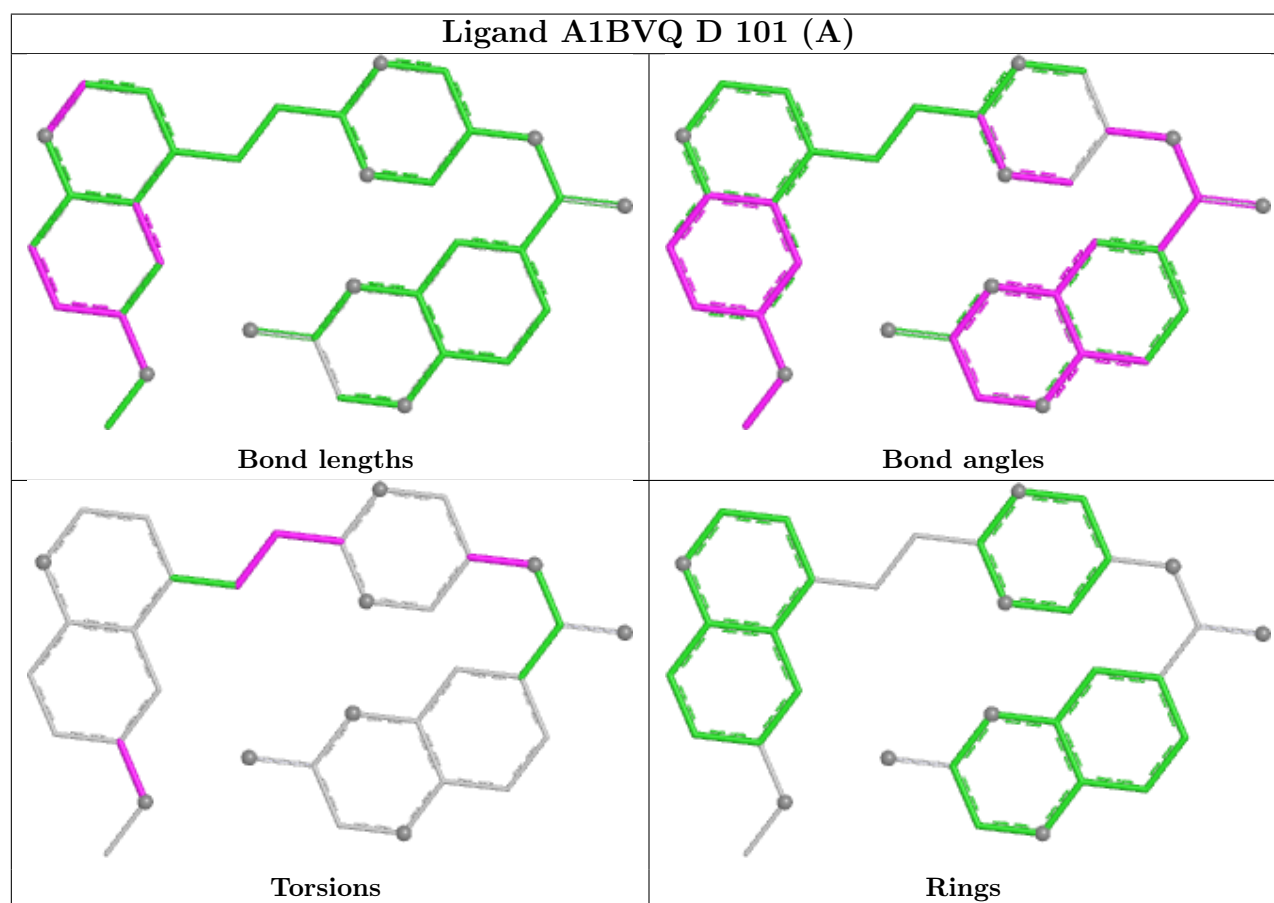
Mol	Chain	Res	Type	Atoms
4	D	101[A]	A1BVQ	C25-C10-N2-C1
4	D	101[A]	A1BVQ	C12-C13-C14-C15
4	D	101[B]	A1BVQ	C20-C21-O5-C22
4	D	101[B]	A1BVQ	C23-C21-O5-C22
4	D	101[A]	A1BVQ	O4-C12-C13-C14
4	D	101[A]	A1BVQ	C23-C21-O5-C22
4	D	101[B]	A1BVQ	C13-C14-C15-C24

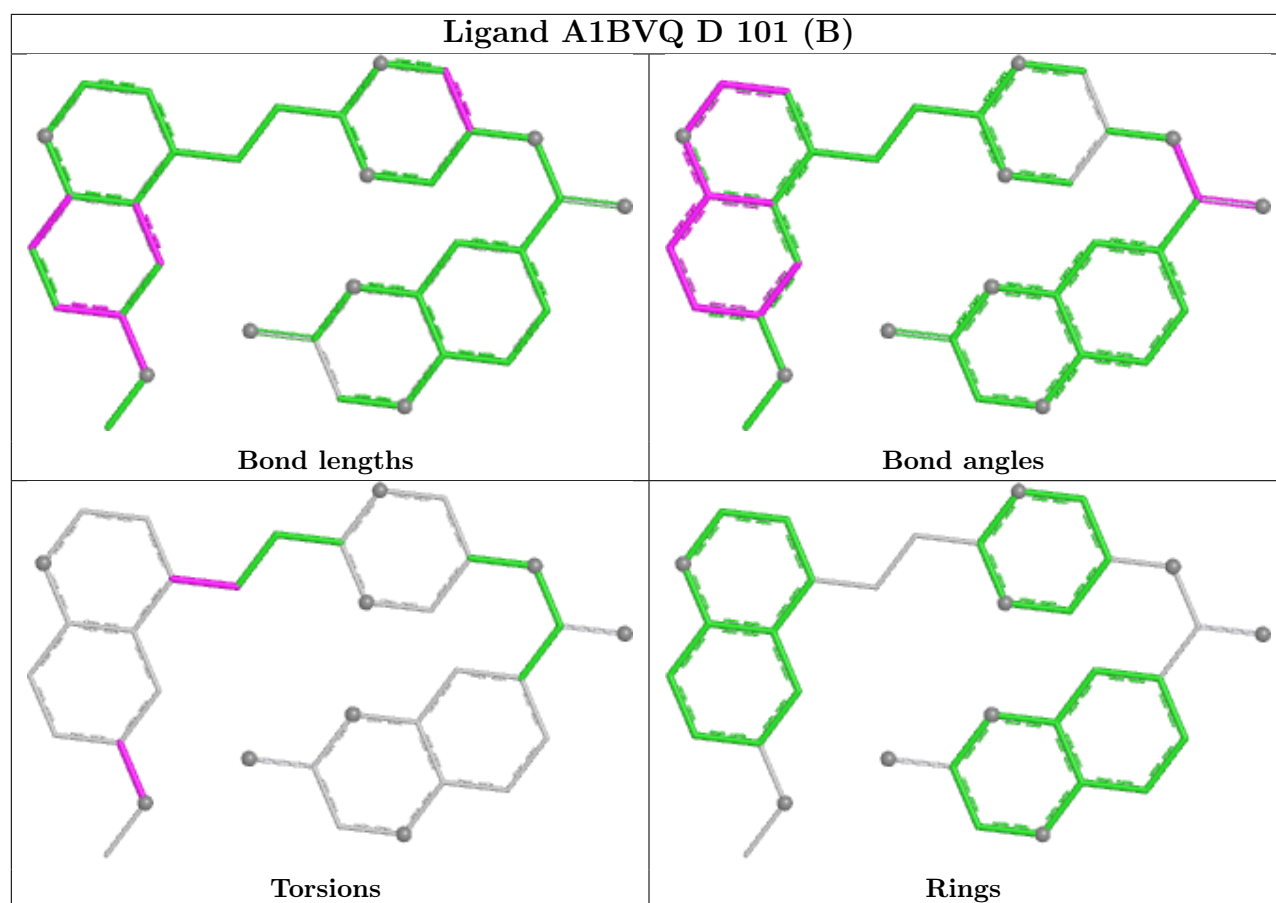
There are no ring outliers.

2 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	101[A]	A1BVQ	18	0
4	D	101[B]	A1BVQ	2	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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	672/693 (96%)	-0.32	2 (0%) 90 90	35, 54, 77, 96	0
1	B	673/693 (97%)	-0.29	1 (0%) 92 92	33, 54, 79, 104	0
2	C	20/20 (100%)	-0.97	0 100 100	38, 46, 61, 66	0
2	D	20/20 (100%)	-0.90	0 100 100	36, 49, 84, 108	0
All	All	1385/1426 (97%)	-0.33	3 (0%) 91 92	33, 54, 78, 108	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1490	LEU	3.1
1	B	624	ASP	2.3
1	A	640	ALA	2.3

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](#)

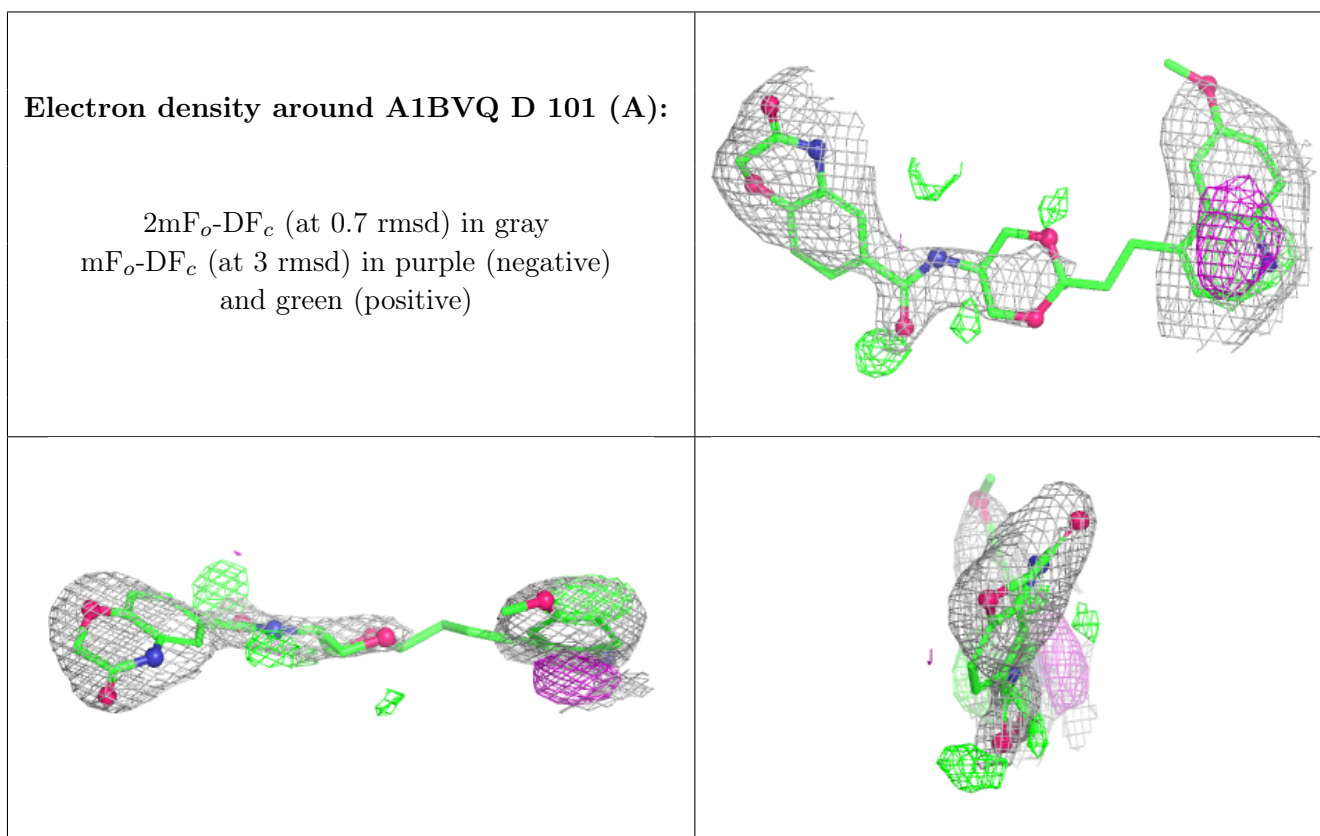
There are no oligosaccharides in this entry.

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.

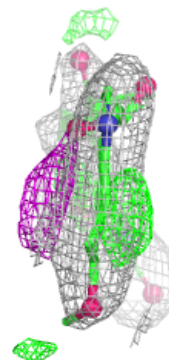
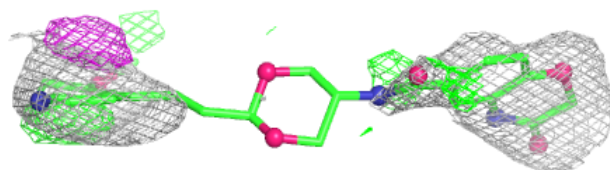
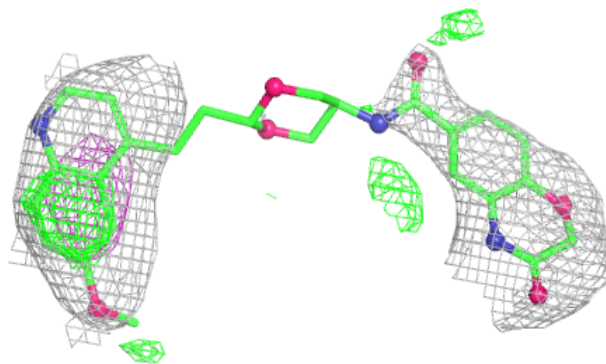
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	A1BVQ	D	101[A]	34/34	0.92	0.17	35,45,59,63	34
4	A1BVQ	D	101[B]	34/34	0.92	0.17	46,56,66,68	34
3	MN	A	1501	1/1	1.00	0.02	56,56,56,56	0
3	MN	B	1501	1/1	1.00	0.01	55,55,55,55	0

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 A1BVQ D 101 (B):

$2mF_o-DF_c$ (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.