



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 08:57 PM UTC

PDB ID : 6ENG / pdb_00006eng
Title : Crystal structure of the 43K ATPase domain of Escherichia coli gyrase B in complex with an aminocoumarin
Authors : Vanden Broeck, A.; McEwen, A.G.; Lamour, V.
Deposited on : 2017-10-04
Resolution : 2.30 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

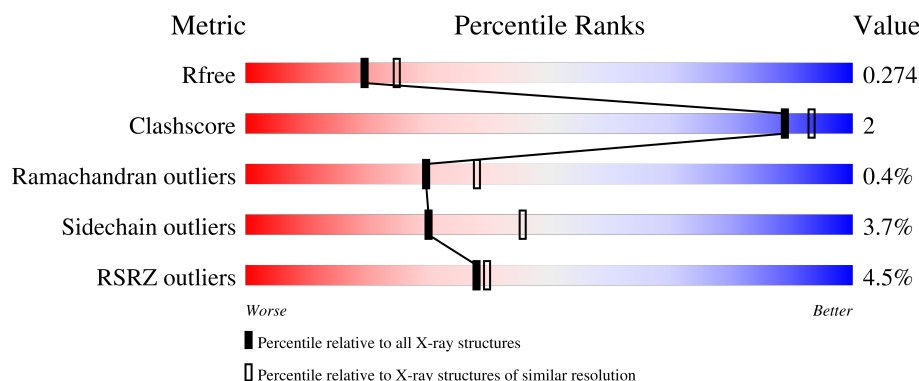
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	396	
1	B	396	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 6407 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.

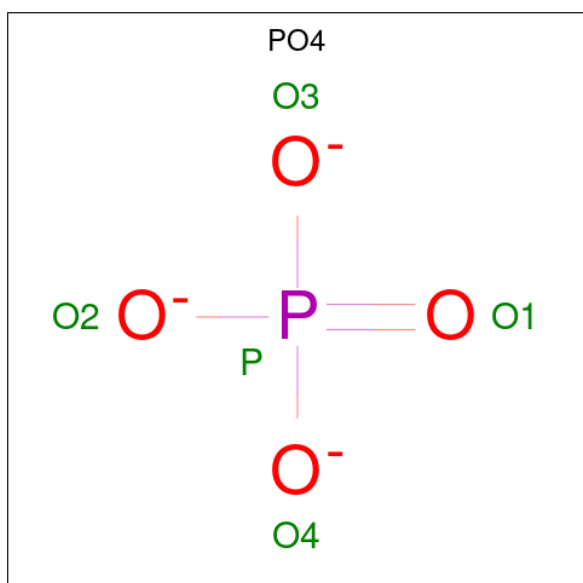
- Molecule 1 is a protein called DNA gyrase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	371	Total	C	N	O	S	0	6	0
			2921	1838	516	556	11			
1	B	379	Total	C	N	O	S	0	5	0
			2972	1862	529	571	10			

There are 6 discrepancies between the modelled and reference sequences:

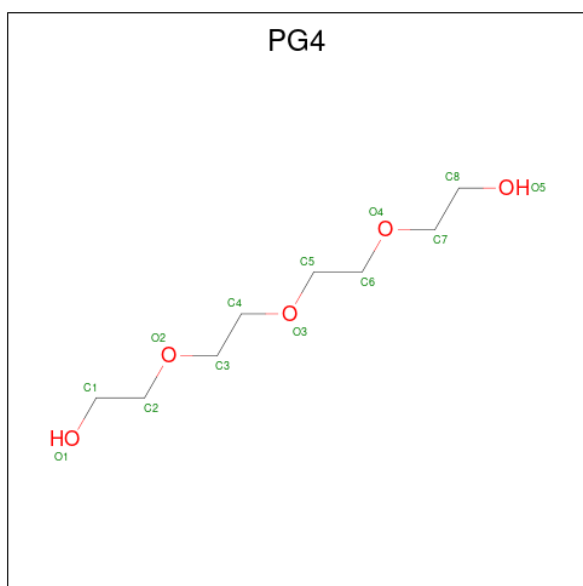
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P0AES6
A	-1	PRO	-	expression tag	UNP P0AES6
A	0	HIS	-	expression tag	UNP P0AES6
B	-2	GLY	-	expression tag	UNP P0AES6
B	-1	PRO	-	expression tag	UNP P0AES6
B	0	HIS	-	expression tag	UNP P0AES6

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	B	1	Total	Cl	0	0
			1	1		

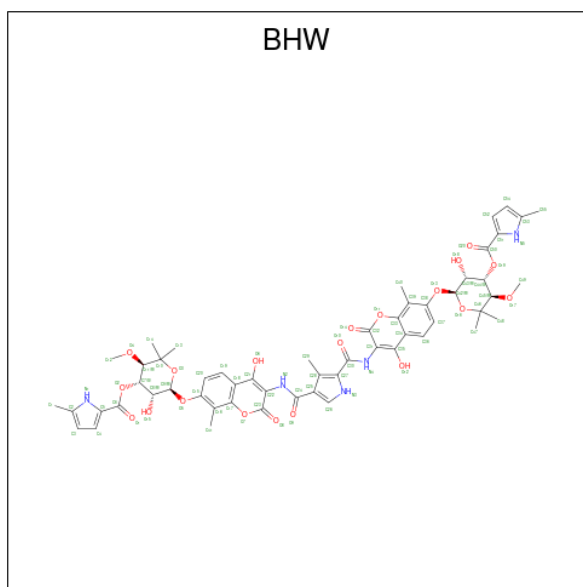
- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Na	0	0
			1	1		

- Molecule 6 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total	K	0	0
			3	3		

- Molecule 7 is Coumermycin A1 (CCD ID: BHW) (formula: C₅₅H₅₉N₅O₂₀).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			80	55	5	20		

- Molecule 8 is water.

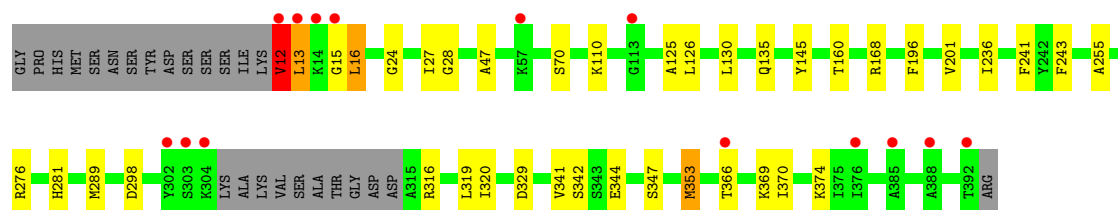
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	209	Total	O	0	3
			209	209		
8	B	181	Total	O	0	0
			181	181		

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 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.

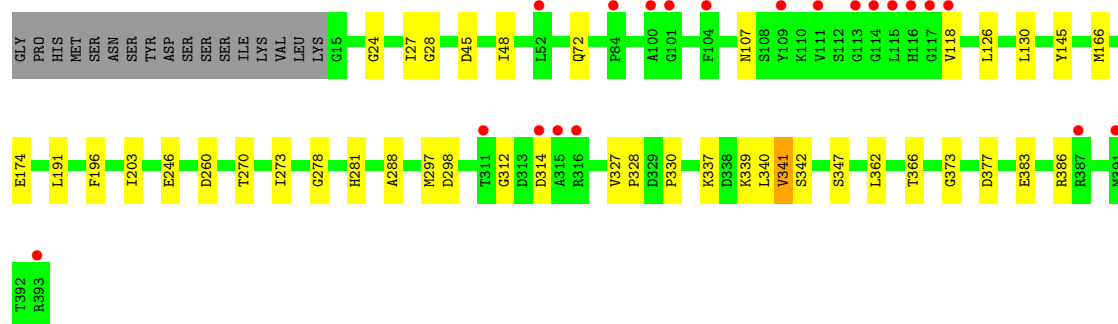
• Molecule 1: DNA gyrase subunit B

Chain A: 



• Molecule 1: DNA gyrase subunit B

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	47.83Å 128.07Å 159.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.67 – 2.30 33.67 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.7 (33.67-2.30) 97.7 (33.67-2.30)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 2.29Å)	Xtriage
Refinement program	BUSTER	Depositor
R, R_{free}	0.200 , 0.257 0.213 , 0.274	Depositor DCC
R_{free} test set	2184 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	48.5	Xtriage
Anisotropy	0.719	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 67.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6407	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.37 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.7263e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: PG4, NA, CL, K, PO4, BHW

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	0.90	1/2992 (0.0%)	1.41	15/4037 (0.4%)
1	B	0.87	1/3040 (0.0%)	1.38	16/4102 (0.4%)
All	All	0.88	2/6032 (0.0%)	1.40	31/8139 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	329	ASP	CA-CB	6.30	1.57	1.52
1	B	297	MET	SD-CE	-5.51	1.65	1.79

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	196	PHE	CA-CB-CG	6.89	120.69	113.80
1	A	370	ILE	CA-C-N	6.22	128.39	120.56
1	A	370	ILE	C-N-CA	6.22	128.39	120.56
1	A	12	VAL	CA-C-N	6.12	128.39	120.44
1	A	12	VAL	C-N-CA	6.12	128.39	120.44
1	B	298	ASP	CA-CB-CG	6.09	118.69	112.60
1	B	341	VAL	CB-CA-C	5.95	117.04	110.62
1	A	344	GLU	CB-CG-CD	5.87	122.58	112.60
1	A	298	ASP	CA-C-N	5.85	128.12	120.28
1	A	298	ASP	C-N-CA	5.85	128.12	120.28
1	B	366	THR	N-CA-C	-5.84	104.83	111.14
1	B	314	ASP	CA-CB-CG	5.67	118.27	112.60
1	B	107	ASN	CA-CB-CG	5.60	118.20	112.60
1	B	373	GLY	CA-C-N	5.59	127.70	120.44
1	B	373	GLY	C-N-CA	5.59	127.70	120.44
1	A	196	PHE	CA-CB-CG	5.44	119.24	113.80
1	B	288	ALA	CA-C-N	5.30	127.33	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	288	ALA	C-N-CA	5.30	127.33	120.44
1	A	369	LYS	CA-C-N	5.22	127.14	120.56
1	A	369	LYS	C-N-CA	5.22	127.14	120.56
1	B	362	LEU	CA-C-N	5.22	127.28	120.28
1	B	362	LEU	C-N-CA	5.22	127.28	120.28
1	A	366	THR	CB-CA-C	5.15	119.03	110.90
1	A	47	ALA	CA-C-N	5.13	128.57	120.47
1	A	47	ALA	C-N-CA	5.13	128.57	120.47
1	A	201	VAL	N-CA-CB	5.13	116.31	110.72
1	B	260	ASP	CA-CB-CG	5.09	117.69	112.60
1	B	341	VAL	N-CA-CB	-5.06	106.31	112.33
1	B	366	THR	CA-C-N	5.03	127.01	120.28
1	B	366	THR	C-N-CA	5.03	127.01	120.28
1	A	298	ASP	CA-CB-CG	5.01	117.61	112.60

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	2921	0	2910	12	0
1	B	2972	0	2948	10	0
2	A	10	0	0	0	0
2	B	15	0	0	0	0
3	A	13	0	18	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	1	0	0	0	0
6	A	3	0	0	0	0
7	B	80	0	0	0	0
8	A	209	0	0	2	0
8	B	181	0	0	0	0
All	All	6407	0	5876	22	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 (22) 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:110:LYS:HE2	8:A:658:HOH:O	1.96	0.66
1:A:24:GLY:HA2	1:A:28:GLY:O	2.03	0.57
1:A:130:LEU:HB3	1:A:145:TYR:HB2	1.91	0.52
1:B:72[B]:GLN:HB3	1:B:166:MET:HG2	1.91	0.51
1:B:278:GLY:O	1:B:339:LYS:HA	2.11	0.50
1:B:383:GLU:HG2	1:B:386[A]:ARG:HH11	1.77	0.49
1:A:236:ILE:HD13	1:A:374:LYS:HD3	1.95	0.48
1:B:24:GLY:HA2	1:B:28:GLY:O	2.13	0.48
1:B:270:THR:HG21	1:B:340:LEU:HD13	1.95	0.47
1:B:273:ILE:HD13	1:B:337:LYS:HD3	1.99	0.45
1:B:130:LEU:HB3	1:B:145:TYR:HB2	1.98	0.44
1:A:15:GLY:HA3	8:A:587:HOH:O	2.17	0.44
1:A:241:PHE:O	1:A:255:ALA:HA	2.17	0.44
1:B:191:LEU:HD22	1:B:203:ILE:HG21	2.01	0.42
1:B:327:VAL:HA	1:B:328:PRO:HD3	1.97	0.41
1:A:16:LEU:HB3	1:A:125:ALA:HB2	2.03	0.41
1:A:70:SER:HB3	1:A:168:ARG:HD2	2.03	0.41
1:A:135:GLN:HB3	1:A:160:THR:HG21	2.01	0.41
1:A:12:VAL:HB	1:A:13:LEU:H	1.68	0.41
1:B:327:VAL:HG13	1:B:330:PRO:HB3	2.03	0.41
1:A:289[A]:MET:HE1	1:A:319:LEU:HD22	2.02	0.41
1:A:243:PHE:HE2	1:A:353:MET:HG3	1.86	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 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	373/396 (94%)	364 (98%)	8 (2%)	1 (0%)	36 46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	382/396 (96%)	368 (96%)	12 (3%)	2 (0%)	24	31
All	All	755/792 (95%)	732 (97%)	20 (3%)	3 (0%)	30	38

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	312	GLY
1	B	342	SER
1	A	342	SER

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 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	314/330 (95%)	302 (96%)	12 (4%)	29	44
1	B	317/330 (96%)	306 (96%)	11 (4%)	32	48
All	All	631/660 (96%)	608 (96%)	23 (4%)	30	47

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	VAL
1	A	13	LEU
1	A	16	LEU
1	A	27	ILE
1	A	126	LEU
1	A	276	ARG
1	A	281	HIS
1	A	316	ARG
1	A	320	ILE
1	A	341	VAL
1	A	347	SER
1	A	353	MET
1	B	27	ILE

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Mol	Chain	Res	Type
1	B	45	ASP
1	B	48	ILE
1	B	118	VAL
1	B	126	LEU
1	B	174	GLU
1	B	246	GLU
1	B	281	HIS
1	B	341	VAL
1	B	347	SER
1	B	377	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	HIS
1	A	72	GLN
1	A	217	HIS
1	A	351	GLN
1	B	141	HIS
1	B	151	GLN
1	B	294	ASN
1	B	351	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 13 ligands modelled in this entry, 6 are monoatomic - leaving 7 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$
2	PO4	B	402	-	4,4,4	2.61	3 (75%)	6,6,6	0.57	0
2	PO4	A	401	-	4,4,4	2.18	3 (75%)	6,6,6	0.29	0
2	PO4	B	403	-	4,4,4	2.55	3 (75%)	6,6,6	0.64	0
7	BHW	B	401	-	88,88,88	1.56	11 (12%)	117,135,135	2.10	21 (17%)
2	PO4	B	404	-	4,4,4	2.60	3 (75%)	6,6,6	0.52	0
3	PG4	A	403	-	12,12,12	0.24	0	11,11,11	0.19	0
2	PO4	A	402	-	4,4,4	2.11	2 (50%)	6,6,6	0.59	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
7	BHW	B	401	-	-	5/44/90/90	0/9/9/9
3	PG4	A	403	-	-	4/10/10/10	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	401	BHW	C5-N1	-6.75	1.26	1.37
7	B	401	BHW	C52-C51	4.96	1.54	1.41
7	B	401	BHW	C27-C28	4.94	1.52	1.40
7	B	401	BHW	C4-C5	4.88	1.54	1.41
7	B	401	BHW	C10-C11	4.46	1.60	1.53
7	B	401	BHW	C51-N5	-4.45	1.30	1.37
2	B	404	PO4	P-O1	4.31	1.60	1.50
2	B	402	PO4	P-O1	4.30	1.60	1.50
2	B	403	PO4	P-O1	4.18	1.60	1.50
7	B	401	BHW	C53-N5	4.00	1.45	1.36
7	B	401	BHW	C46-C45	3.60	1.58	1.53
7	B	401	BHW	C2-N1	3.40	1.44	1.36
2	A	401	PO4	P-O1	2.61	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	402	PO4	P-O1	2.40	1.56	1.50
7	B	401	BHW	C22-C23	2.18	1.52	1.45
7	B	401	BHW	C31-C32	2.13	1.51	1.45
2	A	402	PO4	P-O3	2.06	1.60	1.54
2	A	401	PO4	P-O2	2.04	1.60	1.54
2	B	402	PO4	P-O4	2.03	1.60	1.54
2	A	401	PO4	P-O4	2.03	1.60	1.54
2	B	403	PO4	P-O2	2.03	1.60	1.54
2	B	404	PO4	P-O3	2.01	1.60	1.54
2	B	404	PO4	P-O4	2.01	1.60	1.54
2	B	402	PO4	P-O3	2.01	1.60	1.54
2	B	403	PO4	P-O4	2.00	1.60	1.54

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	401	BHW	C30-C27-N3	7.28	126.67	117.70
7	B	401	BHW	C3-C2-N1	6.83	111.30	107.00
7	B	401	BHW	C28-C27-N3	-6.81	104.24	107.53
7	B	401	BHW	C5-N1-C2	-6.80	106.13	110.05
7	B	401	BHW	C54-C53-N5	6.67	111.20	107.00
7	B	401	BHW	C51-N5-C53	-6.42	106.35	110.05
7	B	401	BHW	C3-C4-C5	-5.57	101.73	107.95
7	B	401	BHW	C55-C53-N5	-4.46	114.99	121.56
7	B	401	BHW	C10-O3-C9	4.34	125.08	115.44
7	B	401	BHW	C54-C52-C51	-4.01	103.48	107.95
7	B	401	BHW	C25-C26-N3	3.97	112.38	108.66
7	B	401	BHW	C46-O16-C42	3.81	123.90	115.44
7	B	401	BHW	C4-C5-N1	3.75	112.46	107.04
7	B	401	BHW	C1-C2-N1	-3.55	116.33	121.56
7	B	401	BHW	O16-C46-C45	3.32	113.00	107.67
7	B	401	BHW	O16-C42-C43	2.98	116.41	110.42
7	B	401	BHW	O19-C44-C43	2.71	113.99	107.76
7	B	401	BHW	C4-C5-C6	-2.57	123.78	130.40
7	B	401	BHW	C52-C51-N5	2.42	110.54	107.04
7	B	401	BHW	O2-C7-C8	2.23	112.88	107.76
7	B	401	BHW	C14-C10-C11	2.01	115.41	111.91

There are no chirality outliers.

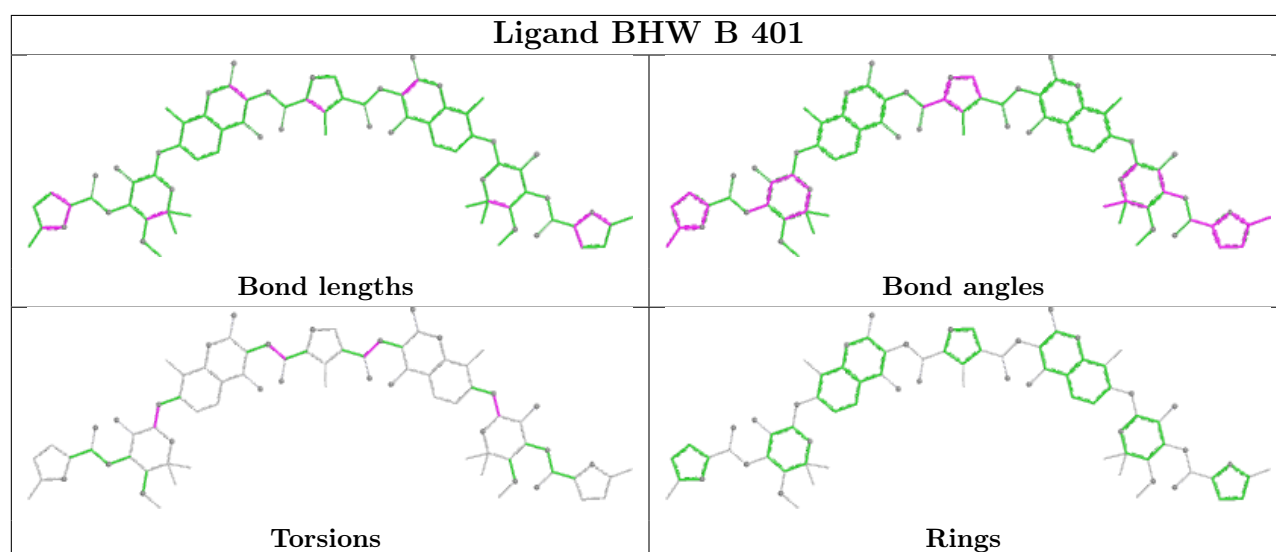
All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	401	BHW	O9-C24-N2-C22
7	B	401	BHW	C27-C30-N4-C31
7	B	401	BHW	O10-C30-N4-C31
3	A	403	PG4	O2-C3-C4-O3
7	B	401	BHW	O16-C42-O13-C38
7	B	401	BHW	O3-C9-O5-C15
3	A	403	PG4	C1-C2-O2-C3
3	A	403	PG4	C6-C5-O3-C4
3	A	403	PG4	C3-C4-O3-C5

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	371/396 (93%)	0.33	14 (3%)	44 46	26, 57, 97, 171	6 (1%)
1	B	379/396 (95%)	0.45	20 (5%)	32 34	31, 64, 100, 117	5 (1%)
All	All	750/792 (94%)	0.39	34 (4%)	38 40	26, 61, 99, 171	11 (1%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	12	VAL	4.8
1	A	13	LEU	4.4
1	B	116	HIS	3.7
1	B	115	LEU	3.7
1	A	392	THR	3.7
1	A	304	LYS	2.9
1	B	315	ALA	2.9
1	B	113	GLY	2.8
1	A	366	THR	2.8
1	B	114	GLY	2.8
1	A	302	TYR	2.7
1	A	15	GLY	2.7
1	B	100	ALA	2.6
1	B	387[A]	ARG	2.6
1	B	117	GLY	2.6
1	A	57[A]	LYS	2.6
1	A	14	LYS	2.5
1	B	111	VAL	2.5
1	B	104	PHE	2.4
1	A	388	ALA	2.4
1	A	113	GLY	2.3
1	B	391	MET	2.3
1	A	385	ALA	2.3
1	B	101	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	303	SER	2.2
1	B	84	PRO	2.2
1	B	52	LEU	2.2
1	B	316	ARG	2.1
1	B	109	TYR	2.1
1	B	393	ARG	2.1
1	A	376	ILE	2.1
1	B	314	ASP	2.1
1	B	118	VAL	2.1
1	B	311	THR	2.0

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

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

6.3 Carbohydrates [i](#)

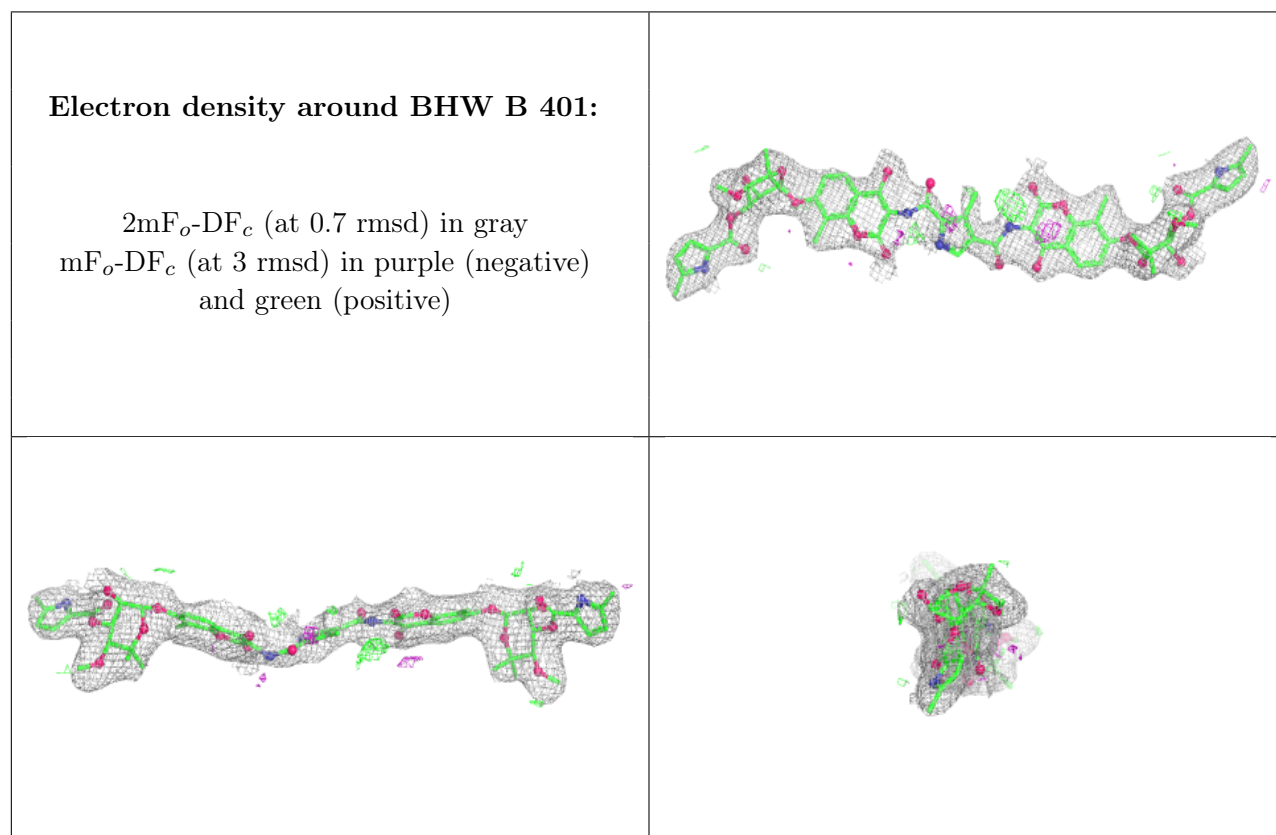
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PO4	B	404	5/5	0.64	0.12	136,136,137,137	0
2	PO4	B	402	5/5	0.77	0.11	95,95,97,98	0
3	PG4	A	403	13/13	0.78	0.20	80,92,98,98	0
2	PO4	A	401	5/5	0.79	0.11	100,102,104,104	0
2	PO4	A	402	5/5	0.88	0.09	79,81,81,86	0
2	PO4	B	403	5/5	0.91	0.09	83,85,87,90	0
4	CL	B	405	1/1	0.91	0.14	83,83,83,83	0
6	K	A	408	1/1	0.91	0.07	86,86,86,86	0
7	BHW	B	401	80/80	0.91	0.10	38,57,101,103	0
4	CL	A	404	1/1	0.92	0.16	88,88,88,88	0
5	NA	A	405	1/1	0.93	0.07	43,43,43,43	0
6	K	A	406	1/1	0.94	0.07	83,83,83,83	0
6	K	A	407	1/1	0.97	0.08	54,54,54,54	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.