



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:43 PM UTC

PDB ID : 3O3J / pdb_00003o3j
Title : Crystal structure of Arabidopsis thaliana peptide deformylase 1B (AtPDF1B) in complex with inhibitor 6b
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Deposited on : 2010-07-24
Resolution : 3.00 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

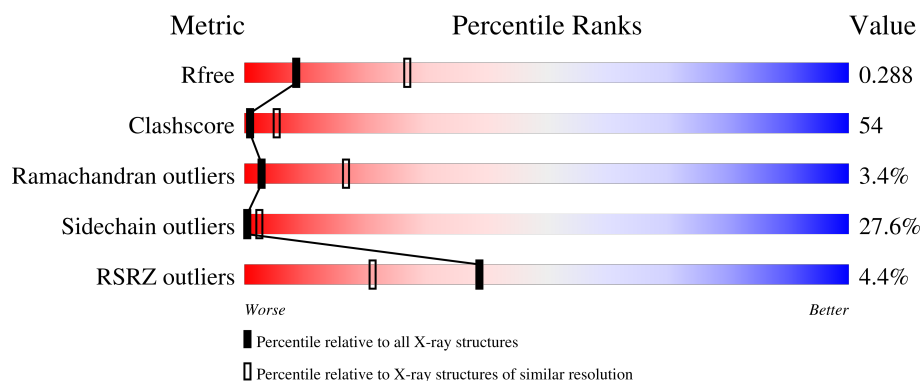
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	193	

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
3	BB4	A	300	-	X	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1482 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 Peptide deformylase 1B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	180	Total	C	N	O	S	0	0	0
			1377	880	221	270	6			

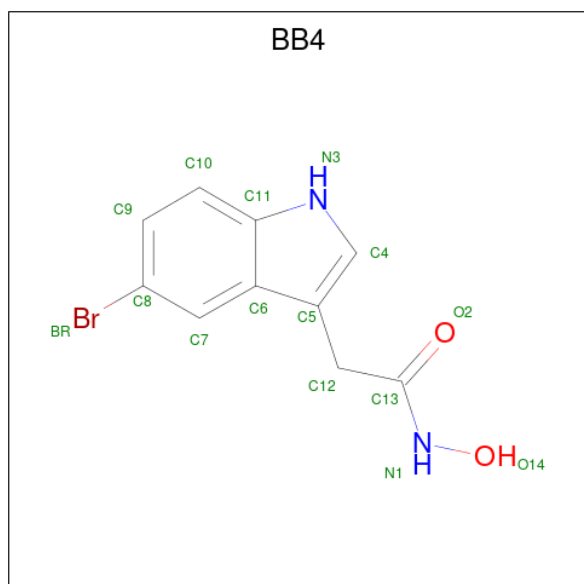
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q9FUZ2
A	2	GLU	-	expression tag	UNP Q9FUZ2

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	6	Total	Zn	0	0
			6	6		

- Molecule 3 is 2-(5-bromo-1H-indol-3-yl)-N-hydroxyacetamide (CCD ID: BB4) (formula: C₁₀H₉BrN₂O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	Br	C	N	O	0	0
			15	1	10	2	2		

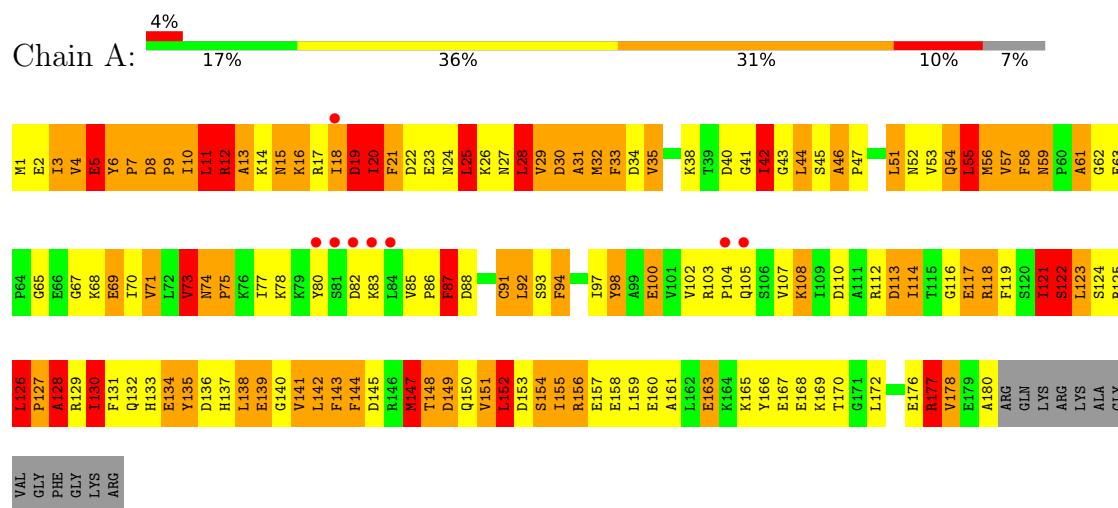
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	84	Total	O	0	0
			84	84		

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: Peptide deformylase 1B



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	57.50Å 57.50Å 144.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.75 – 3.00 28.75 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (28.75-3.00) 99.1 (28.75-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.88 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.200 , 0.285 0.228 , 0.288	Depositor DCC
R_{free} test set	263 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	65.8	Xtriage
Anisotropy	0.689	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 84.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	1482	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.13% 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: BB4, ZN

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	2.64	91/1405 (6.5%)	2.35	77/1913 (4.0%)

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	1

All (91) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	141	VAL	CA-CB	-13.24	1.38	1.54
1	A	151	VAL	CA-CB	13.02	1.68	1.54
1	A	10	ILE	CA-CB	-11.63	1.40	1.54
1	A	34	ASP	CG-OD1	11.16	1.46	1.25
1	A	16	LYS	CD-CE	11.11	1.85	1.52
1	A	110	ASP	CG-OD1	10.91	1.46	1.25
1	A	18	ILE	CA-C	10.87	1.66	1.52
1	A	46	ALA	CA-CB	-10.27	1.39	1.53
1	A	83	LYS	CA-CB	9.64	1.69	1.53
1	A	69	GLU	N-CA	9.33	1.58	1.46
1	A	82	ASP	CA-CB	9.20	1.67	1.53
1	A	83	LYS	N-CA	8.71	1.57	1.46
1	A	152	LEU	CG-CD1	7.91	1.78	1.52
1	A	130	ILE	CA-CB	-7.71	1.44	1.54
1	A	20	ILE	CA-CB	7.55	1.64	1.54
1	A	70	ILE	N-CA	7.50	1.55	1.46
1	A	16	LYS	N-CA	7.37	1.55	1.45
1	A	57	VAL	CA-C	-7.29	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	68	LYS	CA-CB	7.27	1.69	1.53
1	A	57	VAL	CA-CB	-7.22	1.42	1.54
1	A	142	LEU	C-O	7.08	1.32	1.23
1	A	21	PHE	CA-C	-7.06	1.43	1.52
1	A	46	ALA	C-O	7.03	1.31	1.24
1	A	7	PRO	C-O	6.97	1.37	1.23
1	A	78	LYS	CA-CB	6.91	1.64	1.53
1	A	73	VAL	N-CA	-6.85	1.38	1.46
1	A	97	ILE	CA-C	6.82	1.61	1.52
1	A	144	PHE	N-CA	-6.81	1.37	1.46
1	A	30	ASP	CG-OD1	6.68	1.38	1.25
1	A	94	PHE	C-O	6.58	1.31	1.24
1	A	86	PRO	N-CA	6.56	1.52	1.46
1	A	143	PHE	C-O	-6.48	1.16	1.24
1	A	25	LEU	CA-C	6.44	1.61	1.52
1	A	108	LYS	CA-CB	6.33	1.63	1.53
1	A	34	ASP	CG-OD2	6.30	1.37	1.25
1	A	126	LEU	C-O	-6.21	1.18	1.24
1	A	70	ILE	CA-CB	6.17	1.61	1.54
1	A	92	LEU	C-O	-6.14	1.16	1.24
1	A	141	VAL	CA-C	-6.12	1.45	1.52
1	A	15	ASN	N-CA	-6.11	1.38	1.46
1	A	58	PHE	CA-C	6.09	1.59	1.52
1	A	52	ASN	C-O	6.04	1.30	1.23
1	A	161	ALA	CA-CB	5.97	1.62	1.53
1	A	121	ILE	CG1-CD1	5.88	1.74	1.51
1	A	128	ALA	CA-CB	-5.84	1.43	1.53
1	A	88	ASP	N-CA	-5.83	1.39	1.46
1	A	42	ILE	CA-C	-5.81	1.45	1.52
1	A	134	GLU	CD-OE2	5.79	1.36	1.25
1	A	139	GLU	N-CA	-5.75	1.39	1.46
1	A	29	VAL	N-CA	-5.66	1.39	1.46
1	A	87	PHE	CA-C	-5.66	1.45	1.52
1	A	85	VAL	N-CA	5.61	1.53	1.46
1	A	58	PHE	C-O	5.61	1.29	1.23
1	A	69	GLU	CG-CD	5.60	1.66	1.52
1	A	11	LEU	N-CA	5.58	1.53	1.46
1	A	40	ASP	CA-CB	5.53	1.61	1.53
1	A	20	ILE	CG1-CD1	5.53	1.73	1.51
1	A	19	ASP	CA-CB	5.52	1.62	1.53
1	A	94	PHE	CB-CG	5.46	1.63	1.50
1	A	27	ASN	N-CA	-5.45	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	165	LYS	CA-CB	5.44	1.61	1.53
1	A	14	LYS	CB-CG	5.43	1.68	1.52
1	A	21	PHE	C-O	-5.43	1.17	1.24
1	A	27	ASN	CA-C	-5.42	1.46	1.52
1	A	74	ASN	C-O	-5.42	1.17	1.24
1	A	12	ARG	C-O	5.40	1.30	1.24
1	A	19	ASP	CG-OD1	5.40	1.35	1.25
1	A	121	ILE	CA-CB	5.38	1.62	1.54
1	A	13	ALA	CA-C	5.36	1.59	1.52
1	A	105	GLN	C-O	5.33	1.30	1.24
1	A	100	GLU	C-O	5.32	1.30	1.24
1	A	29	VAL	CA-C	5.29	1.59	1.52
1	A	3	ILE	CA-CB	-5.28	1.47	1.54
1	A	178	VAL	CA-CB	-5.26	1.46	1.54
1	A	30	ASP	CB-CG	-5.21	1.39	1.52
1	A	135	TYR	CA-C	5.20	1.59	1.52
1	A	4	VAL	CA-CB	-5.20	1.48	1.54
1	A	26	LYS	CA-CB	5.19	1.61	1.53
1	A	40	ASP	CB-CG	5.19	1.65	1.52
1	A	177	ARG	CA-C	-5.16	1.46	1.52
1	A	11	LEU	CA-C	5.14	1.59	1.52
1	A	70	ILE	CG1-CD1	5.14	1.71	1.51
1	A	149	ASP	CB-CG	5.14	1.65	1.52
1	A	18	ILE	C-O	5.14	1.31	1.24
1	A	57	VAL	N-CA	5.07	1.51	1.46
1	A	13	ALA	CA-CB	5.06	1.62	1.53
1	A	148	THR	CB-CG2	5.05	1.69	1.52
1	A	163	GLU	N-CA	-5.05	1.40	1.46
1	A	17	ARG	C-O	-5.02	1.17	1.24
1	A	157	GLU	N-CA	5.01	1.52	1.46
1	A	58	PHE	N-CA	-5.01	1.40	1.46

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	16	LYS	CG-CD-CE	-9.74	88.89	111.30
1	A	6	TYR	CA-C-N	9.04	148.70	127.00
1	A	6	TYR	C-N-CA	9.04	148.70	127.00
1	A	46	ALA	CA-C-N	-9.02	110.98	119.82
1	A	46	ALA	C-N-CA	-9.02	110.98	119.82
1	A	6	TYR	C-N-CD	-8.68	101.51	120.60
1	A	34	ASP	CB-CG-OD2	-8.57	98.68	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	141	VAL	CB-CA-C	-8.57	98.06	110.83
1	A	88	ASP	N-CA-C	-8.53	97.17	109.96
1	A	8	ASP	CA-C-N	8.29	127.98	119.19
1	A	8	ASP	C-N-CA	8.29	127.98	119.19
1	A	30	ASP	CB-CG-OD2	-7.81	100.43	118.40
1	A	130	ILE	CB-CA-C	-7.79	98.51	111.29
1	A	31	ALA	CA-C-N	-7.58	110.58	120.44
1	A	31	ALA	C-N-CA	-7.58	110.58	120.44
1	A	154	SER	CA-C-N	-7.34	111.76	122.69
1	A	154	SER	C-N-CA	-7.34	111.76	122.69
1	A	165	LYS	N-CA-C	-7.15	103.49	111.28
1	A	35	VAL	CB-CA-C	-7.13	101.11	112.16
1	A	19	ASP	CA-CB-CG	-7.12	105.48	112.60
1	A	63	GLU	CA-C-N	-7.07	112.47	119.76
1	A	63	GLU	C-N-CA	-7.07	112.47	119.76
1	A	16	LYS	CD-CE-NZ	-7.00	89.49	111.90
1	A	17	ARG	CA-C-N	-6.97	111.41	122.64
1	A	17	ARG	C-N-CA	-6.97	111.41	122.64
1	A	34	ASP	OD1-CG-OD2	6.92	139.51	122.90
1	A	59	ASN	CA-C-N	6.82	128.37	119.84
1	A	59	ASN	C-N-CA	6.82	128.37	119.84
1	A	78	LYS	N-CA-C	-6.77	103.82	111.14
1	A	154	SER	N-CA-C	6.67	120.28	111.75
1	A	30	ASP	N-CA-CB	6.37	119.21	109.91
1	A	29	VAL	CA-C-N	-6.34	112.28	120.65
1	A	29	VAL	C-N-CA	-6.34	112.28	120.65
1	A	52	ASN	N-CA-C	6.26	119.34	109.39
1	A	97	ILE	N-CA-CB	-6.25	103.87	111.00
1	A	138	LEU	N-CA-C	-6.19	104.99	112.54
1	A	16	LYS	N-CA-C	6.17	119.21	110.50
1	A	27	ASN	CA-C-O	-6.06	114.65	120.90
1	A	140	GLY	N-CA-C	-6.02	107.09	114.92
1	A	75	PRO	CB-CA-C	-6.00	103.39	111.12
1	A	107	VAL	N-CA-C	5.97	117.36	108.46
1	A	20	ILE	CB-CA-C	5.91	119.78	111.63
1	A	94	PHE	CA-C-N	5.88	127.19	119.84
1	A	94	PHE	C-N-CA	5.88	127.19	119.84
1	A	57	VAL	CA-C-O	-5.86	115.51	121.67
1	A	65	GLY	N-CA-C	-5.86	107.01	115.27
1	A	122	SER	N-CA-C	-5.79	101.43	110.17
1	A	58	PHE	N-CA-C	5.71	116.83	108.14
1	A	51	LEU	CA-CB-CG	-5.64	96.55	116.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	69	GLU	CG-CD-OE1	5.62	131.31	118.40
1	A	91	CYS	N-CA-C	-5.59	99.56	109.06
1	A	25	LEU	CB-CA-C	5.55	119.69	110.81
1	A	9	PRO	CB-CA-C	-5.53	104.04	112.11
1	A	97	ILE	N-CA-C	5.53	116.69	108.23
1	A	4	VAL	CB-CA-C	-5.51	102.60	111.59
1	A	57	VAL	N-CA-C	-5.40	100.04	108.95
1	A	28	LEU	CA-C-N	-5.40	111.76	120.62
1	A	28	LEU	C-N-CA	-5.40	111.76	120.62
1	A	85	VAL	CA-C-N	-5.38	115.03	120.85
1	A	85	VAL	C-N-CA	-5.38	115.03	120.85
1	A	30	ASP	CA-CB-CG	-5.38	107.22	112.60
1	A	118	ARG	NE-CZ-NH2	5.38	124.04	119.20
1	A	5	GLU	N-CA-C	5.31	118.24	109.85
1	A	147	MET	CG-SD-CE	5.26	112.47	100.90
1	A	30	ASP	CA-C-N	-5.23	112.75	120.28
1	A	30	ASP	C-N-CA	-5.23	112.75	120.28
1	A	61	ALA	CA-C-N	5.19	127.95	120.11
1	A	61	ALA	C-N-CA	5.19	127.95	120.11
1	A	33	PHE	CA-C-N	-5.11	113.03	120.29
1	A	33	PHE	C-N-CA	-5.11	113.03	120.29
1	A	98	TYR	N-CA-C	5.08	117.18	108.90
1	A	55	LEU	CB-CG-CD2	-5.07	95.49	110.70
1	A	54	GLN	CA-CB-CG	-5.07	103.96	114.10
1	A	69	GLU	OE1-CD-OE2	-5.05	110.78	122.90
1	A	41	GLY	CA-C-N	-5.04	112.90	121.97
1	A	41	GLY	C-N-CA	-5.04	112.90	121.97
1	A	151	VAL	N-CA-CB	5.04	116.11	110.62

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	118	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	1377	0	1306	146	1
2	A	6	0	0	1	0
3	A	15	0	8	2	0
4	A	84	0	0	4	0
All	All	1482	0	1314	146	1

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 54.

All (146) 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:152:LEU:CG	1:A:152:LEU:CD1	1.78	1.58
1:A:121:ILE:CD1	1:A:121:ILE:CG1	1.74	1.56
1:A:16:LYS:CD	1:A:16:LYS:CE	1.85	1.52
1:A:1:MET:CE	1:A:35:VAL:CG2	2.31	1.09
1:A:42:ILE:HG13	1:A:130:ILE:HD13	1.36	1.06
1:A:1:MET:CE	1:A:35:VAL:HG23	1.86	1.05
1:A:16:LYS:CE	1:A:16:LYS:CG	2.42	0.97
1:A:19:ASP:N	1:A:19:ASP:OD1	1.92	0.97
1:A:1:MET:HE1	1:A:35:VAL:HG23	1.47	0.93
1:A:121:ILE:HG23	1:A:123:LEU:HD12	1.51	0.90
1:A:158:GLU:HG2	4:A:256:HOH:O	1.71	0.89
1:A:103:ARG:HG3	1:A:129:ARG:NH1	1.91	0.86
1:A:1:MET:HE3	1:A:35:VAL:CG2	2.06	0.83
1:A:152:LEU:CD1	1:A:152:LEU:HG	2.07	0.83
1:A:126:LEU:O	1:A:127:PRO:O	1.98	0.82
1:A:16:LYS:CD	1:A:16:LYS:NZ	2.43	0.81
1:A:127:PRO:O	1:A:128:ALA:C	2.26	0.79
1:A:54:GLN:HA	1:A:138:LEU:HD22	1.65	0.78
1:A:1:MET:HE1	1:A:35:VAL:CG2	2.07	0.77
1:A:178:VAL:O	1:A:178:VAL:HG22	1.84	0.77
1:A:12:ARG:HD2	1:A:176:GLU:OE2	1.83	0.77
1:A:1:MET:CE	1:A:35:VAL:HG21	2.16	0.75
1:A:113:ASP:OD1	1:A:113:ASP:C	2.30	0.74
1:A:1:MET:HE3	1:A:35:VAL:HG21	1.67	0.74
1:A:113:ASP:HB3	1:A:119:PHE:HE1	1.52	0.74
1:A:155:ILE:HG13	1:A:159:LEU:CD1	2.19	0.73
1:A:114:ILE:O	1:A:114:ILE:HG13	1.89	0.72
1:A:121:ILE:CG2	1:A:123:LEU:HD12	2.20	0.72
1:A:1:MET:SD	1:A:31:ALA:HB1	2.30	0.71
1:A:32:MET:HB3	1:A:44:LEU:HD23	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:PHE:HA	1:A:147:MET:CG	2.23	0.69
1:A:5:GLU:HA	1:A:93:SER:HB3	1.75	0.69
1:A:104:PRO:HD2	1:A:132:GLN:HE22	1.58	0.68
1:A:144:PHE:HA	1:A:147:MET:HG3	1.75	0.68
1:A:113:ASP:HB3	1:A:119:PHE:CE1	2.29	0.67
1:A:33:PHE:CZ	1:A:69:GLU:HB3	2.30	0.67
1:A:136:ASP:HB3	1:A:141:VAL:HB	1.76	0.66
1:A:160:GLU:OE2	2:A:203:ZN:ZN	1.43	0.66
1:A:155:ILE:HG13	1:A:159:LEU:HD12	1.76	0.66
1:A:92:LEU:N	3:A:300:BB4:O2	2.22	0.65
1:A:57:VAL:HG12	1:A:71:VAL:HG22	1.79	0.65
1:A:134:GLU:OE1	3:A:300:BB4:N1	2.26	0.65
1:A:6:TYR:HB2	1:A:94:PHE:CE2	2.34	0.63
1:A:155:ILE:CG1	1:A:159:LEU:HD11	2.29	0.63
1:A:178:VAL:O	1:A:178:VAL:CG2	2.47	0.62
1:A:113:ASP:OD1	1:A:114:ILE:N	2.31	0.62
1:A:150:GLN:O	1:A:153:ASP:HB2	1.98	0.62
1:A:6:TYR:CB	1:A:94:PHE:CE2	2.83	0.62
1:A:126:LEU:O	1:A:127:PRO:C	2.41	0.62
1:A:57:VAL:O	1:A:58:PHE:HB3	1.99	0.61
1:A:123:LEU:HD23	1:A:127:PRO:HB2	1.83	0.61
1:A:32:MET:HE2	1:A:57:VAL:HG13	1.83	0.60
1:A:15:ASN:HD21	1:A:47:PRO:HG3	1.67	0.60
1:A:123:LEU:HD23	1:A:128:ALA:H	1.67	0.60
1:A:123:LEU:HD23	1:A:128:ALA:N	2.18	0.59
1:A:148:THR:OG1	1:A:151:VAL:HG23	2.02	0.59
1:A:155:ILE:CG1	1:A:159:LEU:CD1	2.81	0.58
1:A:42:ILE:CG1	1:A:130:ILE:HD13	2.22	0.58
1:A:33:PHE:CE1	1:A:69:GLU:HB3	2.39	0.58
1:A:177:ARG:O	1:A:180:ALA:HB3	2.04	0.58
1:A:59:ASN:OD1	1:A:59:ASN:C	2.43	0.58
1:A:136:ASP:O	1:A:137:HIS:C	2.48	0.56
1:A:1:MET:HE2	1:A:35:VAL:HG23	1.86	0.56
1:A:77:ILE:HD12	1:A:135:TYR:CD2	2.41	0.55
1:A:7:PRO:O	1:A:8:ASP:C	2.49	0.55
1:A:77:ILE:HD13	1:A:80:TYR:CZ	2.41	0.55
1:A:6:TYR:CG	1:A:94:PHE:CE2	2.94	0.55
1:A:16:LYS:CE	1:A:16:LYS:HG2	2.34	0.54
1:A:116:GLY:O	1:A:117:GLU:C	2.51	0.53
1:A:11:LEU:HD23	1:A:11:LEU:N	2.22	0.53
1:A:113:ASP:CB	1:A:119:PHE:HE1	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:LEU:CD2	1:A:128:ALA:N	2.72	0.52
1:A:6:TYR:CD2	1:A:6:TYR:C	2.87	0.52
1:A:77:ILE:HD12	1:A:135:TYR:CE2	2.45	0.52
1:A:56:MET:HE3	1:A:75:PRO:HG2	1.93	0.51
1:A:127:PRO:O	1:A:129:ARG:N	2.43	0.50
1:A:147:MET:HE1	1:A:155:ILE:CD1	2.42	0.50
1:A:128:ALA:O	1:A:131:PHE:HB3	2.12	0.50
1:A:147:MET:HE1	1:A:155:ILE:HD13	1.93	0.50
1:A:104:PRO:HD2	1:A:132:GLN:NE2	2.24	0.49
1:A:123:LEU:C	1:A:128:ALA:HB2	2.37	0.49
1:A:144:PHE:HB3	1:A:147:MET:HE2	1.95	0.49
1:A:8:ASP:C	1:A:8:ASP:OD2	2.55	0.49
1:A:61:ALA:HB2	1:A:67:GLY:HA3	1.95	0.49
1:A:130:ILE:O	1:A:131:PHE:C	2.53	0.49
1:A:61:ALA:HB2	1:A:67:GLY:CA	2.43	0.48
1:A:32:MET:O	1:A:33:PHE:C	2.53	0.48
1:A:166:TYR:CE1	1:A:170:THR:HG21	2.50	0.47
1:A:46:ALA:HB2	1:A:55:LEU:HD23	1.97	0.47
1:A:152:LEU:O	1:A:153:ASP:C	2.57	0.47
1:A:148:THR:O	1:A:149:ASP:C	2.58	0.47
1:A:142:LEU:N	1:A:145:ASP:OD1	2.41	0.46
1:A:15:ASN:ND2	1:A:47:PRO:HG3	2.31	0.46
1:A:20:ILE:HG12	1:A:22:ASP:OD2	2.15	0.46
1:A:42:ILE:O	1:A:58:PHE:HB2	2.15	0.46
1:A:73:VAL:HG23	1:A:74:ASN:N	2.30	0.46
1:A:155:ILE:O	1:A:156:ARG:C	2.58	0.46
1:A:147:MET:CE	1:A:155:ILE:CD1	2.93	0.46
1:A:43:GLY:HA2	1:A:58:PHE:CB	2.46	0.46
1:A:148:THR:HG1	1:A:151:VAL:HG23	1.80	0.46
1:A:28:LEU:O	1:A:29:VAL:C	2.56	0.45
1:A:21:PHE:HB3	4:A:246:HOH:O	2.15	0.45
1:A:121:ILE:CD1	1:A:121:ILE:CB	2.82	0.45
1:A:92:LEU:C	1:A:94:PHE:H	2.24	0.45
1:A:144:PHE:HD2	1:A:144:PHE:H	1.63	0.45
1:A:9:PRO:O	1:A:10:ILE:C	2.55	0.45
1:A:87:PHE:HD2	1:A:87:PHE:HA	1.69	0.45
1:A:24:ASN:O	1:A:25:LEU:C	2.60	0.45
1:A:134:GLU:O	1:A:135:TYR:C	2.59	0.45
1:A:151:VAL:O	1:A:154:SER:N	2.51	0.44
1:A:91:CYS:HB2	1:A:133:HIS:HE1	1.81	0.44
1:A:21:PHE:CE2	1:A:116:GLY:HA2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:LEU:HA	1:A:142:LEU:HD23	1.57	0.43
1:A:177:ARG:O	1:A:180:ALA:CB	2.66	0.43
1:A:152:LEU:O	1:A:155:ILE:N	2.49	0.43
1:A:98:TYR:N	1:A:98:TYR:CD1	2.86	0.43
1:A:32:MET:HE3	1:A:44:LEU:HD23	2.01	0.43
1:A:30:ASP:O	1:A:31:ALA:C	2.59	0.43
1:A:53:VAL:O	1:A:53:VAL:CG2	2.67	0.43
1:A:61:ALA:CB	1:A:67:GLY:HA3	2.49	0.43
1:A:148:THR:HG23	4:A:210:HOH:O	2.18	0.43
1:A:32:MET:HE2	1:A:57:VAL:CG1	2.47	0.43
1:A:77:ILE:HD13	1:A:80:TYR:OH	2.19	0.42
1:A:133:HIS:CD2	1:A:133:HIS:C	2.98	0.42
1:A:151:VAL:O	1:A:152:LEU:C	2.63	0.42
1:A:163:GLU:OE1	1:A:177:ARG:HG2	2.19	0.42
1:A:147:MET:CE	1:A:155:ILE:HD13	2.49	0.42
1:A:32:MET:HB3	1:A:32:MET:HE3	1.71	0.42
1:A:6:TYR:CG	1:A:94:PHE:HE2	2.36	0.42
1:A:56:MET:HE2	1:A:138:LEU:CD1	2.50	0.42
1:A:108:LYS:HA	1:A:122:SER:HA	2.02	0.41
1:A:166:TYR:O	1:A:170:THR:HG23	2.20	0.41
1:A:138:LEU:HD23	1:A:138:LEU:HA	1.91	0.41
1:A:51:LEU:HD23	1:A:51:LEU:HA	1.94	0.41
1:A:56:MET:CE	1:A:138:LEU:HD12	2.51	0.41
1:A:92:LEU:C	1:A:94:PHE:N	2.75	0.41
1:A:1:MET:HG2	4:A:290:HOH:O	2.20	0.41
1:A:59:ASN:O	1:A:62:GLY:N	2.42	0.41
1:A:123:LEU:O	1:A:128:ALA:HB2	2.21	0.41
1:A:29:VAL:O	1:A:30:ASP:C	2.61	0.41
1:A:129:ARG:HG3	1:A:130:ILE:N	2.36	0.41
1:A:23:GLU:O	1:A:24:ASN:C	2.63	0.40
1:A:144:PHE:CD2	1:A:144:PHE:N	2.87	0.40
1:A:4:VAL:H	1:A:4:VAL:HG23	1.44	0.40
1:A:53:VAL:O	1:A:53:VAL:HG23	2.21	0.40
1:A:45:SER:HB3	1:A:134:GLU:OE2	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:ASP:OD1	1:A:69:GLU:OE1[8_554]	1.62	0.58

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	178/193 (92%)	142 (80%)	30 (17%)	6 (3%)	3	17

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	127	PRO
1	A	13	ALA
1	A	128	ALA
1	A	117	GLU
1	A	125	ARG

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	145/169 (86%)	105 (72%)	40 (28%)	0	2

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	3	ILE
1	A	5	GLU
1	A	12	ARG
1	A	18	ILE

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Mol	Chain	Res	Type
1	A	19	ASP
1	A	20	ILE
1	A	25	LEU
1	A	28	LEU
1	A	32	MET
1	A	38	LYS
1	A	42	ILE
1	A	44	LEU
1	A	55	LEU
1	A	56	MET
1	A	71	VAL
1	A	73	VAL
1	A	87	PHE
1	A	100	GLU
1	A	102	VAL
1	A	112	ARG
1	A	113	ASP
1	A	114	ILE
1	A	121	ILE
1	A	122	SER
1	A	123	LEU
1	A	124	SER
1	A	126	LEU
1	A	130	ILE
1	A	139	GLU
1	A	143	PHE
1	A	147	MET
1	A	152	LEU
1	A	155	ILE
1	A	156	ARG
1	A	167	GLU
1	A	168	GLU
1	A	169	LYS
1	A	172	LEU
1	A	177	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 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	$\# Z > 2$
3	BB4	A	300	2	16,16,16	5.44	10 (62%)	22,22,22	3.67	13 (59%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BB4	A	300	2	-	0/6/6/6	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	300	BB4	C12-C13	12.27	1.68	1.51
3	A	300	BB4	C13-N1	10.96	1.44	1.32
3	A	300	BB4	BR-C8	7.55	2.05	1.90
3	A	300	BB4	C7-C8	5.20	1.48	1.38
3	A	300	BB4	C12-C5	5.12	1.56	1.50
3	A	300	BB4	C6-C11	5.04	1.47	1.41
3	A	300	BB4	C11-N3	-4.69	1.30	1.37
3	A	300	BB4	C9-C8	4.52	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	300	BB4	C10-C9	2.86	1.43	1.38
3	A	300	BB4	C7-C6	2.55	1.43	1.39

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	300	BB4	C6-C5-C4	-6.89	99.11	106.16
3	A	300	BB4	C12-C5-C6	6.50	134.89	126.43
3	A	300	BB4	O14-N1-C13	6.28	129.08	119.79
3	A	300	BB4	C5-C4-N3	6.21	117.12	110.31
3	A	300	BB4	BR-C8-C9	5.33	126.55	119.30
3	A	300	BB4	C13-C12-C5	4.47	123.95	114.52
3	A	300	BB4	C11-C6-C5	4.33	111.54	107.17
3	A	300	BB4	C9-C8-C7	-3.75	116.13	121.53
3	A	300	BB4	C7-C6-C11	-3.44	116.03	119.39
3	A	300	BB4	C6-C11-N3	-2.75	105.23	107.52
3	A	300	BB4	C10-C9-C8	2.55	122.23	119.18
3	A	300	BB4	C11-N3-C4	-2.35	106.98	109.08
3	A	300	BB4	C6-C7-C8	2.24	122.86	118.99

There are no chirality outliers.

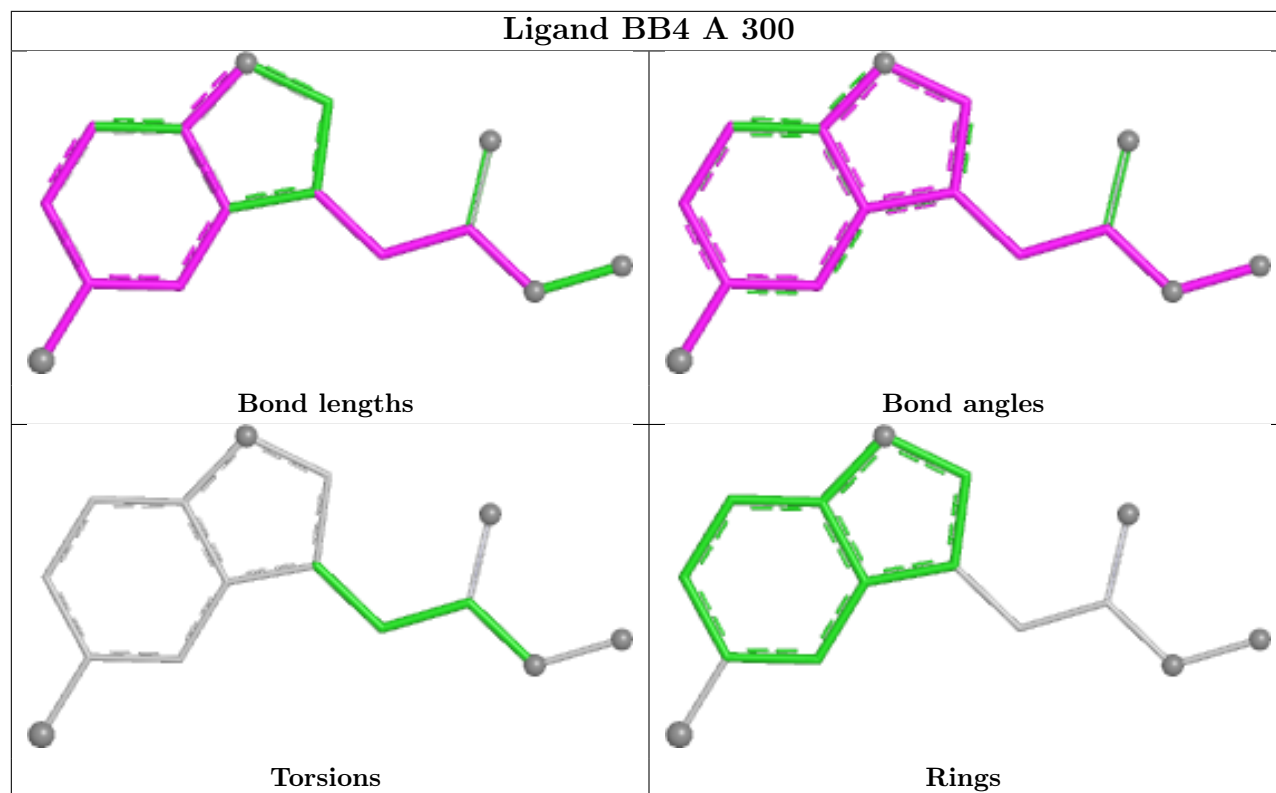
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	300	BB4	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	180/193 (93%)	0.01	8 (4%) 39 21	15, 67, 145, 189	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	82	ASP	3.3
1	A	81	SER	2.7
1	A	105	GLN	2.7
1	A	80	TYR	2.6
1	A	84	LEU	2.5
1	A	18	ILE	2.2
1	A	104	PRO	2.2
1	A	83	LYS	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](#)

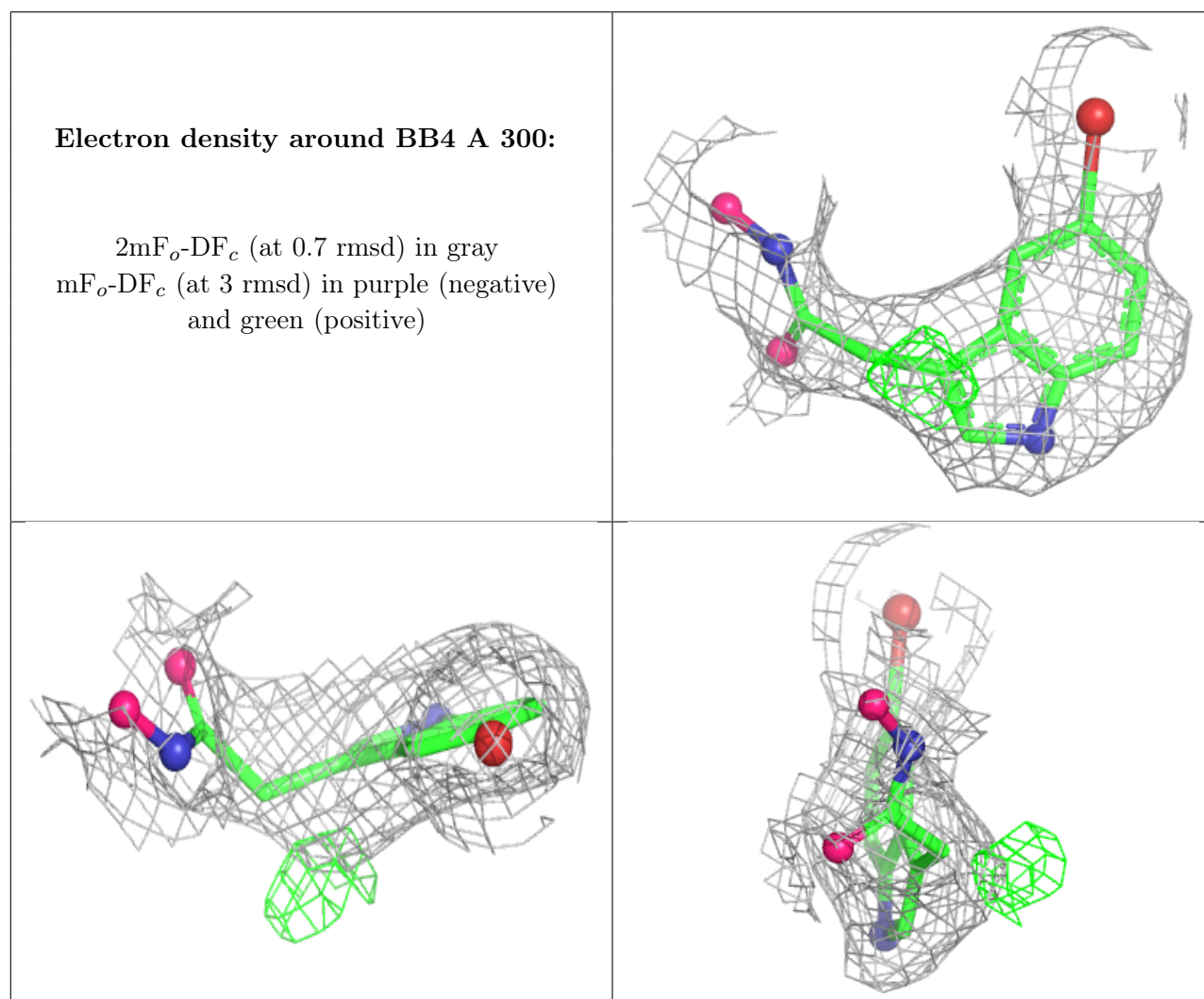
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
2	ZN	A	205	1/1	0.83	0.07	106,106,106,106	0
2	ZN	A	204	1/1	0.94	0.06	76,76,76,76	0
2	ZN	A	202	1/1	0.95	0.07	67,67,67,67	0
2	ZN	A	206	1/1	0.95	0.12	54,54,54,54	0
3	BB4	A	300	15/15	0.96	0.10	53,64,68,71	0
2	ZN	A	201	1/1	0.99	0.05	53,53,53,53	0
2	ZN	A	203	1/1	0.99	0.04	53,53,53,53	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 ⓘ

There are no such residues in this entry.