



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:08 AM UTC

PDB ID : 6I49 / pdb_00006i49
Title : Structure of *P. aeruginosa* LpxC with compound 17a: (2R)-N-Hydroxy-2-methyl-2-(methylsulfonyl)-4(6((4(morpholinomethyl)phenyl)ethynyl)-3-oxo-1H-pyrrolo[1,2-c]imidazol-2(3H)yl)butanamide
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Deposited on : 2018-11-09
Resolution : 1.94 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)

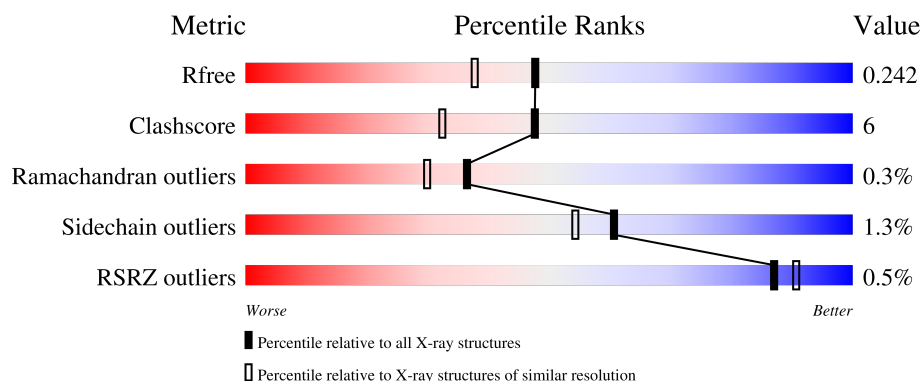
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.94 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	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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	AAA	299	 80% 19% .
1	BBB	299	 79% 19% .

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

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9470 atoms, of which 4644 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 UDP-3-O-acyl-N-acetylglucosamine deacetylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	299	Total	C	H	N	O	S	99	3	0
			4612	1465	2311	396	433	7			
1	BBB	298	Total	C	H	N	O	S	103	4	0
			4570	1453	2281	393	437	6			

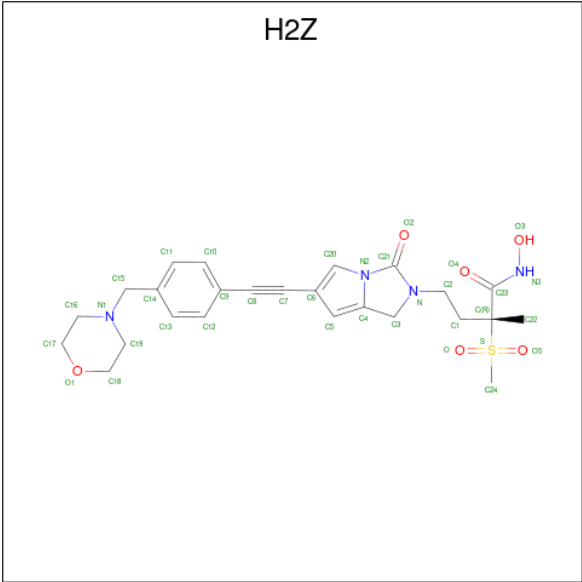
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	40	SER	CYS	engineered mutation	UNP B7UZI4
BBB	40	SER	CYS	engineered mutation	UNP B7UZI4

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	AAA	1	Total	Zn	0	0
			1	1		
2	BBB	1	Total	Zn	0	0
			1	1		

- Molecule 3 is (2 {R})-2-methyl-2-methylsulfonyl-4-[6-[2-[4-(morpholin-4-ylmethyl)phenyl]ethynyl]-3-oxidanylidene-1 {H}-pyrrolo[1,2-c]imidazol-2-yl]- {N}-oxidanyl-butanamide (CCD ID: H2Z) (formula: C₂₅H₃₀N₄O₆S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	AAA	1	Total	C	H	N	O	S	0	0
			66	25	30	4	6	1		
3	BBB	1	Total	C	H	N	O	S	1	0
			52	21	22	3	5	1		

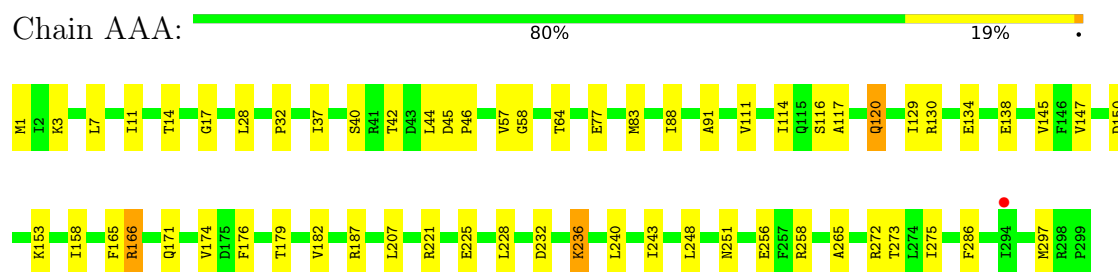
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	76	Total	O	0	0
			76	76		
4	BBB	92	Total	O	0	0
			92	92		

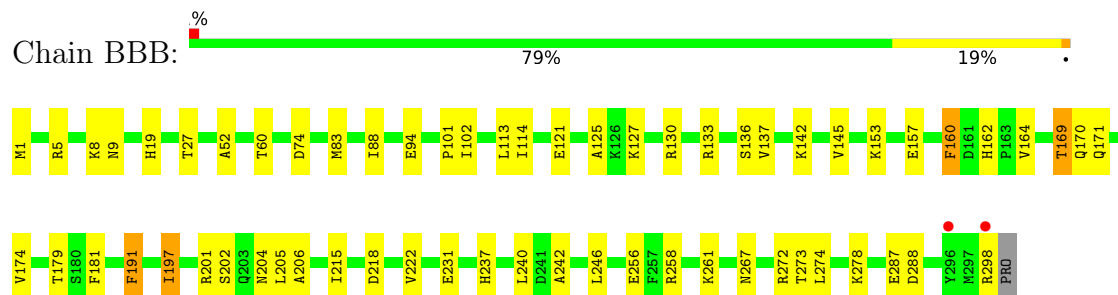
3 Residue-property plots [i](#)

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: UDP-3-O-acyl-N-acetylglucosamine deacetylase



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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	167.31Å 89.18Å 35.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.12 – 1.94 43.12 – 1.94	Depositor EDS
% Data completeness (in resolution range)	98.2 (43.12-1.94) 98.2 (43.12-1.94)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.8.0238 2018/15/10	Depositor
R, R_{free}	0.183 , 0.243 0.183 , 0.242	Depositor DCC
R_{free} test set	1982 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	23.1	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 27.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9470	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.04% 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: H2Z, 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	AAA	1.45	14/2341 (0.6%)	1.58	28/3171 (0.9%)
1	BBB	1.42	18/2334 (0.8%)	1.54	14/3162 (0.4%)
All	All	1.43	32/4675 (0.7%)	1.56	42/6333 (0.7%)

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	77	GLU	C-O	-9.76	1.12	1.24
1	AAA	207	LEU	C-O	-7.10	1.14	1.24
1	AAA	225	GLU	C-O	-6.93	1.15	1.24
1	BBB	267	ASN	C-O	6.64	1.31	1.24
1	AAA	17	GLY	C-O	-6.42	1.18	1.24
1	BBB	125	ALA	C-O	6.40	1.31	1.23
1	AAA	158	ILE	C-O	-6.30	1.15	1.24
1	BBB	222	VAL	C-O	-6.15	1.18	1.24
1	BBB	202	SER	C-O	6.01	1.31	1.24
1	BBB	60	THR	C-O	-5.95	1.17	1.23
1	BBB	272	ARG	NE-CZ	5.87	1.39	1.33
1	BBB	74	ASP	CG-OD1	5.84	1.36	1.25
1	BBB	191	PHE	C-O	5.83	1.30	1.23
1	AAA	228	LEU	C-O	5.80	1.30	1.23
1	BBB	113	LEU	C-O	-5.80	1.17	1.24
1	AAA	150	ASP	C-O	-5.79	1.17	1.23
1	BBB	121	GLU	C-O	-5.61	1.17	1.23
1	BBB	160	PHE	C-O	5.55	1.30	1.24
1	BBB	9	ASN	C-O	5.53	1.30	1.23
1	BBB	127	LYS	C-O	5.50	1.30	1.24
1	BBB	237	HIS	CE1-NE2	5.45	1.38	1.32
1	AAA	265	ALA	C-O	5.30	1.30	1.24
1	AAA	272	ARG	NE-CZ	5.27	1.38	1.33
1	BBB	52	ALA	C-O	5.23	1.29	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	111	VAL	C-O	5.18	1.30	1.24
1	BBB	278	LYS	C-O	-5.16	1.17	1.24
1	AAA	91	ALA	CA-CB	-5.13	1.45	1.53
1	AAA	138	GLU	C-O	5.09	1.30	1.23
1	BBB	157	GLU	C-O	-5.08	1.18	1.24
1	BBB	101	PRO	C-O	5.06	1.29	1.23
1	AAA	32	PRO	C-O	-5.05	1.17	1.23
1	AAA	221	ARG	C-O	5.02	1.30	1.23

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	58	GLY	CA-C-N	7.31	131.25	120.87
1	AAA	58	GLY	C-N-CA	7.31	131.25	120.87
1	AAA	187	ARG	NE-CZ-NH2	7.15	125.64	119.20
1	AAA	44	LEU	CA-C-O	-6.93	113.18	121.56
1	BBB	206	ALA	CA-C-O	-6.78	112.53	119.78
1	AAA	273	THR	CA-CB-OG1	-6.60	99.70	109.60
1	AAA	275	ILE	CA-C-N	6.52	129.01	120.28
1	AAA	275	ILE	C-N-CA	6.52	129.01	120.28
1	AAA	116	SER	CA-C-O	-6.49	114.01	120.82
1	AAA	166	ARG	CA-C-N	6.42	130.68	121.56
1	AAA	166	ARG	C-N-CA	6.42	130.68	121.56
1	BBB	274	LEU	N-CA-C	-6.31	104.31	111.07
1	BBB	205	LEU	N-CA-C	-6.28	100.40	110.14
1	AAA	57	VAL	CA-C-O	-6.09	113.91	120.85
1	AAA	221	ARG	CG-CD-NE	6.08	125.39	112.00
1	AAA	182	VAL	CA-C-O	-5.99	114.82	121.17
1	AAA	165	PHE	CB-CA-C	5.97	120.22	110.24
1	BBB	169	THR	CB-CA-C	5.95	119.28	109.70
1	BBB	231	GLU	N-CA-C	-5.80	105.04	111.71
1	BBB	287	GLU	N-CA-C	-5.69	105.83	112.89
1	BBB	1	MET	CG-SD-CE	-5.69	88.39	100.90
1	BBB	288	ASP	CA-C-O	-5.68	114.19	120.33
1	AAA	176	PHE	CA-C-N	5.61	128.11	120.54
1	AAA	176	PHE	C-N-CA	5.61	128.11	120.54
1	BBB	197	ILE	CA-C-O	-5.60	114.91	120.85
1	AAA	44	LEU	CA-C-N	5.59	130.05	122.56
1	AAA	44	LEU	C-N-CA	5.59	130.05	122.56
1	AAA	120	GLN	CB-CG-CD	-5.51	103.23	112.60
1	BBB	181	PHE	N-CA-C	-5.48	105.20	111.07
1	AAA	165	PHE	CA-CB-CG	-5.46	108.34	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	218	ASP	CA-CB-CG	5.42	118.02	112.60
1	BBB	5	ARG	CG-CD-NE	-5.41	100.11	112.00
1	AAA	42	THR	CA-CB-OG1	-5.35	101.57	109.60
1	AAA	243	ILE	CA-C-O	-5.20	115.66	121.17
1	AAA	44	LEU	O-C-N	5.18	129.78	123.10
1	AAA	187	ARG	NE-CZ-NH1	-5.15	116.35	121.50
1	BBB	298	ARG	CA-C-O	5.13	129.52	120.80
1	BBB	133	ARG	NE-CZ-NH2	5.12	123.81	119.20
1	AAA	286	PHE	CB-CA-C	5.07	118.28	110.62
1	AAA	14	THR	CA-CB-OG1	-5.04	102.04	109.60
1	AAA	236	LYS	CB-CA-C	5.03	119.14	110.79
1	AAA	176	PHE	CB-CA-C	5.01	120.39	110.17

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	AAA	2301	2311	2276	26	0
1	BBB	2289	2281	2247	25	0
2	AAA	1	0	0	0	0
2	BBB	1	0	0	0	0
3	AAA	36	30	0	1	0
3	BBB	30	22	0	1	0
4	AAA	76	0	0	2	0
4	BBB	92	0	0	3	0
All	All	4826	4644	4523	51	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 6.

All (51) 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:AAA:147[A]:VAL:HG21	1:AAA:256:GLU:OE1	1.66	0.94
1:BBB:88:ILE:HD11	1:BBB:114:ILE:HG21	1.49	0.94
1:AAA:130:ARG:HD2	4:AAA:471:HOH:O	1.79	0.83
1:AAA:37:ILE:HD12	1:AAA:83[A]:MET:HE3	1.60	0.81
1:BBB:19:HIS:HE1	3:BBB:302:H2Z:O2	1.66	0.78
1:AAA:83[A]:MET:SD	1:AAA:88:ILE:HD12	2.23	0.77
1:BBB:261:LYS:CB	4:BBB:491:HOH:O	2.33	0.76
1:AAA:147[A]:VAL:CG2	1:AAA:256:GLU:OE1	2.35	0.74
1:BBB:83[B]:MET:HE2	1:BBB:88:ILE:HD12	1.75	0.67
1:AAA:147[A]:VAL:HG22	1:AAA:256:GLU:HB3	1.77	0.66
1:AAA:134:GLU:OE1	1:BBB:169:THR:HA	1.96	0.66
1:AAA:37:ILE:CD1	1:AAA:83[A]:MET:HE3	2.26	0.66
1:BBB:174:VAL:HG13	1:BBB:179:THR:OG1	1.97	0.65
1:BBB:142:LYS:HE3	1:BBB:261:LYS:O	1.96	0.65
1:BBB:145:VAL:CG1	1:BBB:258:ARG:HB2	2.28	0.64
1:BBB:242:ALA:O	1:BBB:246:LEU:HG	1.98	0.63
1:BBB:160:PHE:H	1:BBB:170:GLN:HE22	1.49	0.60
1:BBB:83[B]:MET:HE2	1:BBB:88:ILE:CD1	2.31	0.59
1:BBB:130:ARG:HD2	4:BBB:488:HOH:O	2.03	0.58
1:AAA:130:ARG:CD	4:AAA:471:HOH:O	2.45	0.57
1:BBB:83[A]:MET:SD	1:BBB:88:ILE:HD12	2.44	0.57
1:BBB:240:LEU:C	1:BBB:240:LEU:HD23	2.30	0.57
1:AAA:37:ILE:HD12	1:AAA:83[A]:MET:CE	2.31	0.57
1:AAA:240:LEU:C	1:AAA:240:LEU:HD23	2.30	0.56
1:AAA:174:VAL:HG13	1:AAA:179:THR:OG1	2.06	0.55
1:BBB:197:ILE:O	1:BBB:201:ARG:HG3	2.07	0.55
1:AAA:129:ILE:HG12	1:AAA:251:ASN:HB2	1.89	0.54
1:AAA:232:ASP:OD1	1:AAA:236:LYS:HD2	2.10	0.52
1:AAA:145:VAL:CG1	1:AAA:258:ARG:HB2	2.40	0.51
1:AAA:11:ILE:HB	1:AAA:28:LEU:HB2	1.92	0.51
1:AAA:147[A]:VAL:CG2	1:AAA:256:GLU:HB3	2.40	0.51
1:BBB:83[B]:MET:HE3	1:BBB:114:ILE:HD11	1.93	0.51
3:AAA:302:H2Z:C11	3:AAA:302:H2Z:C19	2.91	0.48
1:AAA:88:ILE:HD11	1:AAA:114:ILE:HG21	1.95	0.47
1:AAA:153:LYS:HE2	4:BBB:421:HOH:O	2.15	0.47
1:BBB:137:VAL:HG13	1:BBB:273[A]:THR:HG21	1.98	0.45
1:BBB:162:HIS:CE1	1:BBB:164:VAL:HG23	2.51	0.45
1:BBB:83[A]:MET:SD	1:BBB:88:ILE:CD1	3.06	0.43
1:BBB:153:LYS:O	1:BBB:256:GLU:HA	2.19	0.43
1:AAA:45:ASP:HA	1:AAA:46:PRO:HA	1.88	0.43
1:BBB:145:VAL:HG13	1:BBB:258:ARG:HB2	1.98	0.43
1:AAA:1:MET:HE3	1:AAA:3:LYS:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:120:GLN:NE2	1:AAA:120:GLN:HA	2.35	0.42
1:AAA:64:THR:HG21	1:AAA:248:LEU:HD11	2.02	0.42
1:BBB:102:ILE:HG13	1:BBB:102:ILE:O	2.21	0.41
1:BBB:27:THR:HB	1:BBB:94:GLU:HB2	2.01	0.41
1:AAA:11:ILE:HG13	1:AAA:117:ALA:HB2	2.01	0.40
1:BBB:191:PHE:HA	1:BBB:215:ILE:O	2.21	0.40
1:AAA:153:LYS:O	1:AAA:256:GLU:HA	2.22	0.40
1:AAA:7:LEU:HD13	1:AAA:11:ILE:CD1	2.50	0.40
1:BBB:83[B]:MET:HA	1:BBB:88:ILE:HD12	2.02	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	AAA	300/299 (100%)	290 (97%)	8 (3%)	2 (1%)	18	9
1	BBB	300/299 (100%)	288 (96%)	12 (4%)	0	100	100
All	All	600/598 (100%)	578 (96%)	20 (3%)	2 (0%)	36	30

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	166	ARG
1	AAA	297	MET

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	AAA	241/253 (95%)	239 (99%)	2 (1%)	73	71
1	BBB	240/253 (95%)	236 (98%)	4 (2%)	53	44
All	All	481/506 (95%)	475 (99%)	6 (1%)	61	57

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	40	SER
1	AAA	171	GLN
1	BBB	8	LYS
1	BBB	136	SER
1	BBB	171	GLN
1	BBB	204	ASN

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

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 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	$\# Z > 2$
3	H2Z	AAA	302	2	36,39,39	4.32	20 (55%)	34,57,57	2.11	3 (8%)
3	H2Z	BBB	302	2	29,32,39	5.05	17 (58%)	25,48,57	2.54	3 (12%)

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	H2Z	AAA	302	2	-	3/25/52/52	0/4/4/4
3	H2Z	BBB	302	2	-	2/21/40/52	0/3/3/4

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	BBB	302	H2Z	C4-N2	-20.12	1.18	1.39
3	AAA	302	H2Z	C4-N2	-12.97	1.26	1.39
3	BBB	302	H2Z	C24-S	-11.74	1.62	1.76
3	AAA	302	H2Z	C3-N	9.37	1.57	1.45
3	AAA	302	H2Z	C15-C14	7.33	1.64	1.51
3	AAA	302	H2Z	C24-S	-6.84	1.68	1.76
3	AAA	302	H2Z	C5-C6	6.75	1.49	1.40
3	AAA	302	H2Z	C15-N1	6.66	1.60	1.47
3	AAA	302	H2Z	C7-C6	-5.89	1.36	1.43
3	AAA	302	H2Z	C3-C4	5.63	1.61	1.50
3	BBB	302	H2Z	C1-C2	-5.61	1.40	1.52
3	AAA	302	H2Z	O5-S	-4.83	1.40	1.44
3	AAA	302	H2Z	C23-N3	-4.73	1.25	1.34
3	AAA	302	H2Z	C20-C6	4.32	1.45	1.38
3	BBB	302	H2Z	C9-C8	-4.18	1.34	1.44
3	AAA	302	H2Z	C1-C	4.06	1.59	1.54
3	BBB	302	H2Z	C21-N	-4.01	1.30	1.36
3	AAA	302	H2Z	O-S	3.77	1.47	1.44
3	BBB	302	H2Z	C12-C13	3.67	1.44	1.38
3	BBB	302	H2Z	C5-C6	3.51	1.45	1.40
3	AAA	302	H2Z	C12-C13	3.42	1.44	1.38
3	BBB	302	H2Z	C23-N3	-3.41	1.27	1.34
3	BBB	302	H2Z	O5-S	-3.41	1.41	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	BBB	302	H2Z	C11-C10	3.36	1.44	1.38
3	BBB	302	H2Z	O2-C21	3.31	1.28	1.22
3	BBB	302	H2Z	C3-N	3.22	1.50	1.45
3	BBB	302	H2Z	C7-C6	-3.01	1.39	1.43
3	BBB	302	H2Z	C3-C4	2.73	1.55	1.50
3	AAA	302	H2Z	C11-C10	2.64	1.43	1.38
3	BBB	302	H2Z	C21-N2	-2.64	1.36	1.39
3	AAA	302	H2Z	C1-C2	-2.62	1.47	1.52
3	AAA	302	H2Z	O3-N3	-2.62	1.33	1.40
3	BBB	302	H2Z	C11-C14	2.31	1.44	1.38
3	AAA	302	H2Z	C19-N1	-2.21	1.40	1.46
3	BBB	302	H2Z	C12-C9	2.15	1.43	1.39
3	AAA	302	H2Z	C9-C8	-2.10	1.39	1.44
3	AAA	302	H2Z	O1-C18	2.07	1.50	1.42

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	BBB	302	H2Z	O-S-O5	-10.20	109.63	118.01
3	AAA	302	H2Z	O-S-O5	-9.75	110.00	118.01
3	BBB	302	H2Z	C3-N-C2	-5.76	114.88	123.00
3	AAA	302	H2Z	C3-N-C2	-5.54	115.19	123.00
3	BBB	302	H2Z	C2-N-C21	4.00	131.78	123.07
3	AAA	302	H2Z	C2-N-C21	3.90	131.56	123.07

There are no chirality outliers.

All (5) torsion outliers are listed below:

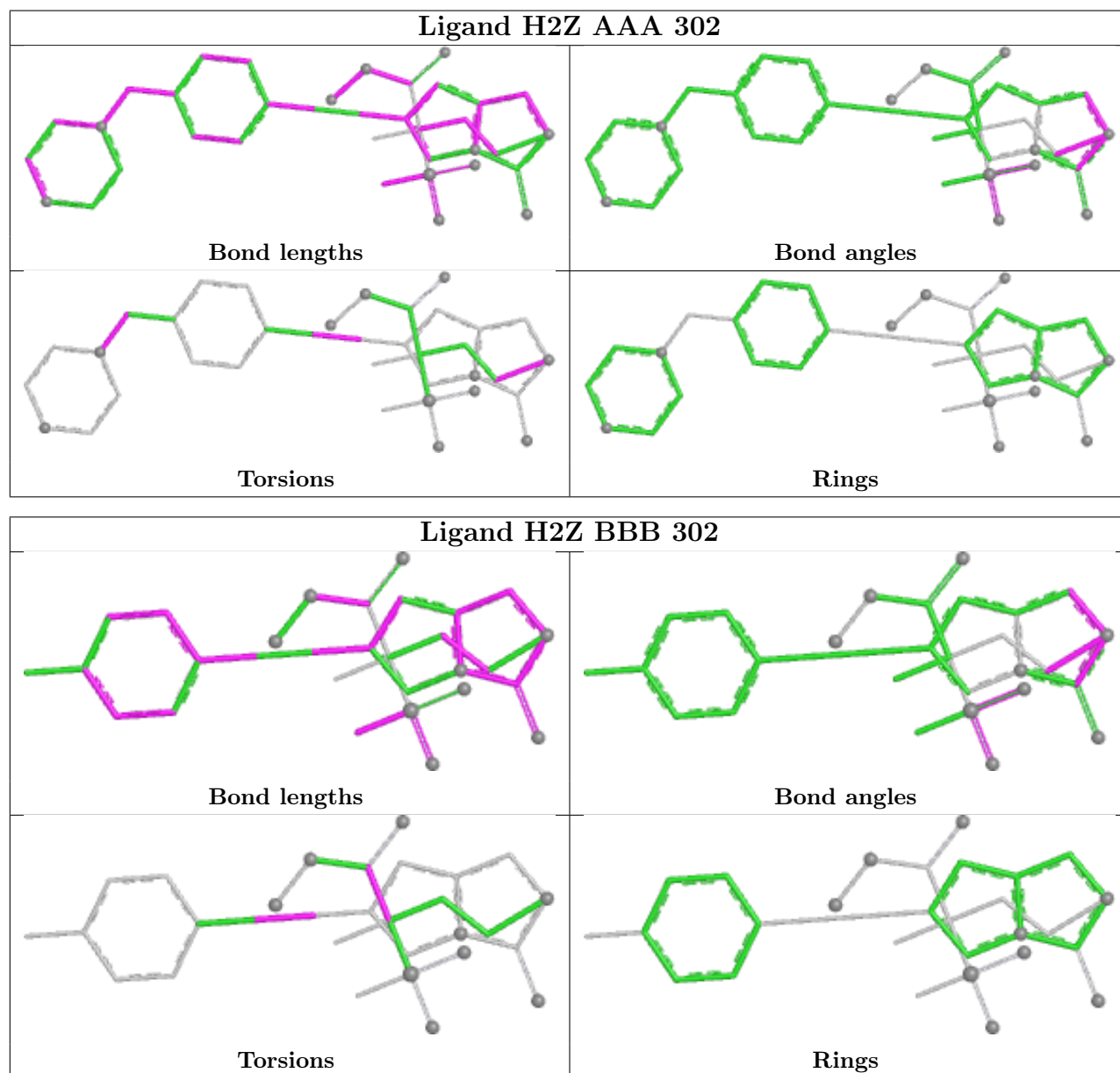
Mol	Chain	Res	Type	Atoms
3	AAA	302	H2Z	C6-C7-C8-C9
3	AAA	302	H2Z	C14-C15-N1-C19
3	BBB	302	H2Z	C6-C7-C8-C9
3	AAA	302	H2Z	C1-C2-N-C3
3	BBB	302	H2Z	C22-C-C23-O4

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AAA	302	H2Z	1	0
3	BBB	302	H2Z	1	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	AAA	299/299 (100%)	-0.34	1 (0%) 90 93	8, 24, 43, 67	3 (1%)
1	BBB	298/299 (99%)	-0.37	2 (0%) 84 88	8, 23, 41, 58	4 (1%)
All	All	597/598 (99%)	-0.35	3 (0%) 87 91	8, 24, 42, 67	7 (1%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	294	ILE	3.2
1	BBB	298	ARG	2.7
1	BBB	296	TYR	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(Å ²)	Q<0.9
3	H2Z	AAA	302	36/36	0.96	0.08	17,23,70,76	0
3	H2Z	BBB	302	30/36	0.97	0.07	15,23,40,46	1

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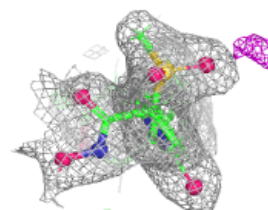
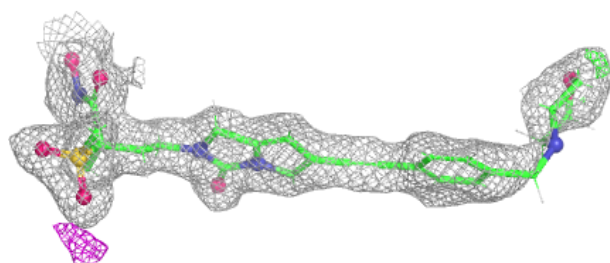
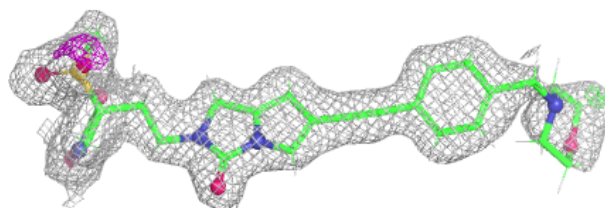
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	AAA	301	1/1	1.00	0.01	16,16,16,16	0
2	ZN	BBB	301	1/1	1.00	0.01	16,16,16,16	0

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.

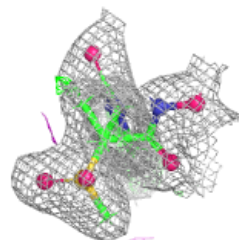
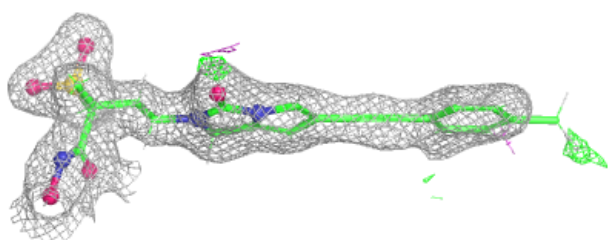
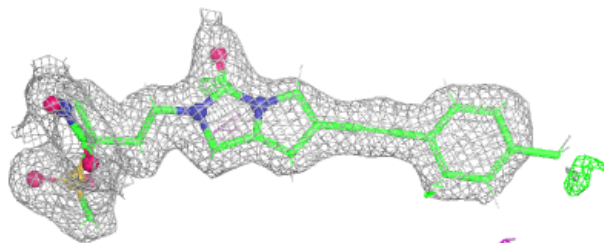
Electron density around H2Z AAA 302:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around H2Z BBB 302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.