



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:51 AM UTC

PDB ID : 7CJL / pdb_00007cjl
Title : Metallo-Beta-Lactamase VIM-2 in complex with (S)-N-(3-(2H-tetrazol-5-yl)phenyl)-3-mercapto-2-methylpropanamide
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Deposited on : 2020-07-11
Resolution : 1.79 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

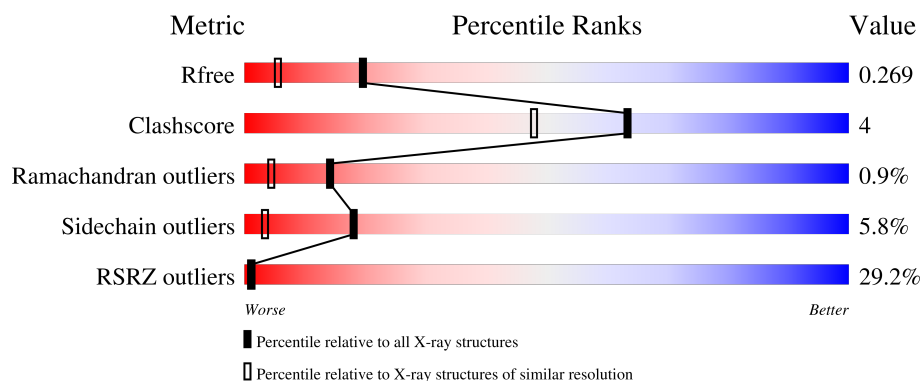
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.79 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	1365 (1.78-1.78)
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

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	231	33% 83% 16%
1	B	231	25% 85% 13%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3749 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.

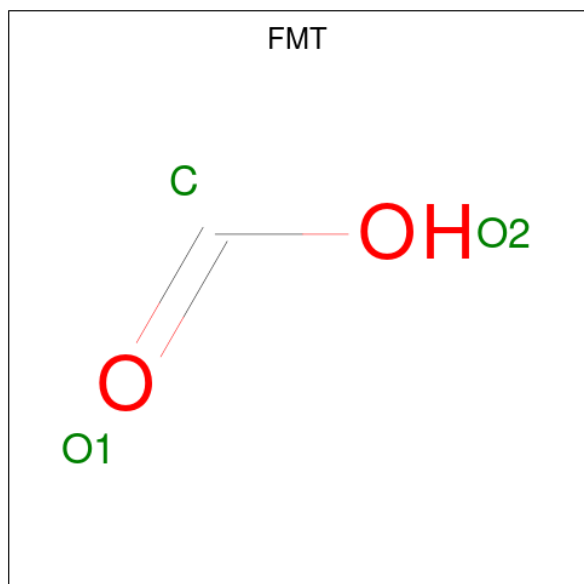
- Molecule 1 is a protein called Beta-lactamase class B VIM-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	231	Total	C	N	O	S	0	0	0
			1730	1093	299	337	1			
1	A	231	Total	C	N	O	S	0	0	0
			1726	1090	298	337	1			

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

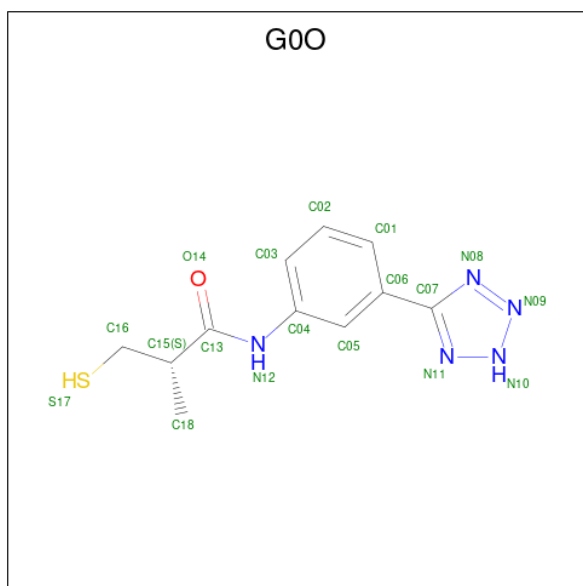
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is FORMIC ACID (CCD ID: FMT) (formula: CH₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			3	1	2		

- Molecule 4 is (S)-N-(3-(2H-tetrazol-5-yl)phenyl)-3-mercapto-2-methylpropanamide (CCD ID: G0O) (formula: C₁₁H₁₃N₅OS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			18	11	5	1	1		
4	A	1	Total	C	N	O	S	0	0
			18	11	5	1	1		

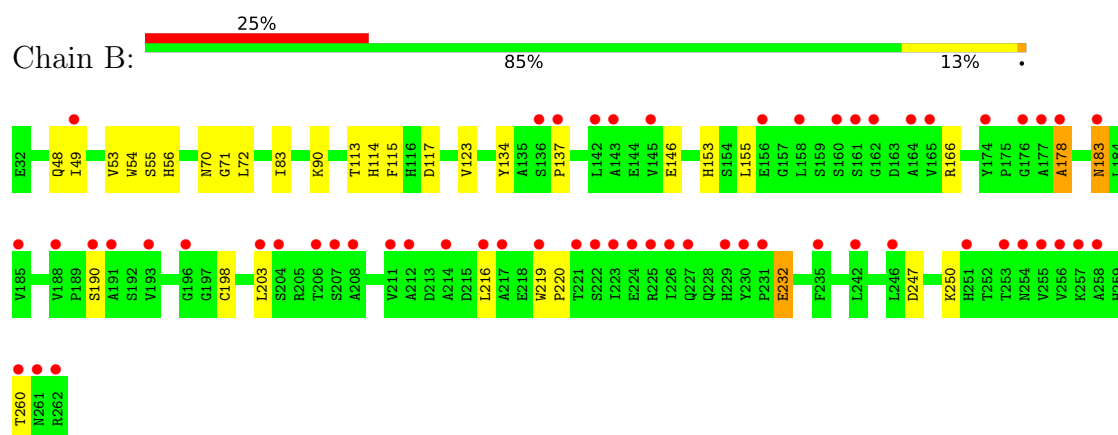
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	128	Total	O	0	0
			128	128		
5	A	122	Total	O	0	0
			122	122		

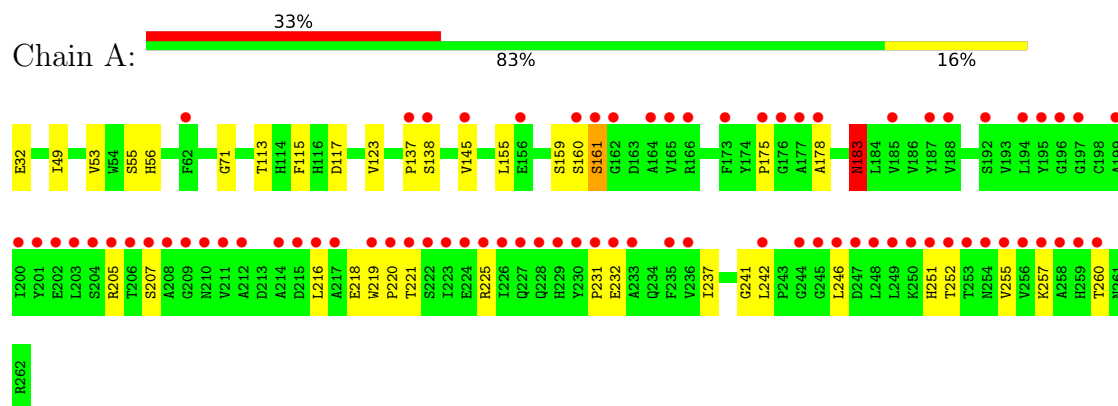
3 Residue-property plots

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: Beta-lactamase class B VIM-2



• Molecule 1: Beta-lactamase class B VIM-2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	45.36Å 90.13Å 125.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.07 – 1.79 45.07 – 1.79	Depositor EDS
% Data completeness (in resolution range)	85.5 (45.07-1.79) 66.6 (45.07-1.79)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 1.79Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.205 , 0.246 (Not available) , 0.269	Depositor DCC
R_{free} test set	2000 reflections (4.03%)	wwPDB-VP
Wilson B-factor (Å ²)	20.2	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 45.0	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	0.94	EDS
Total number of atoms	3749	wwPDB-VP
Average B, all atoms (Å ²)	29.0	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 40.56 % 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 2.6858e-04. 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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: FMT, G0O, 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	0.75	4/1767 (0.2%)	0.78	3/2421 (0.1%)
1	B	0.76	5/1771 (0.3%)	0.74	3/2425 (0.1%)
All	All	0.76	9/3538 (0.3%)	0.76	6/4846 (0.1%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	183	ASN	C-O	-5.74	1.16	1.23
1	B	54	TRP	C-O	-5.54	1.16	1.23
1	A	53	VAL	C-O	-5.51	1.18	1.24
1	B	53	VAL	C-O	-5.43	1.18	1.24
1	A	113	THR	C-O	-5.36	1.17	1.24
1	B	113	THR	C-O	-5.36	1.17	1.24
1	B	115	PHE	C-O	-5.21	1.17	1.24
1	A	241	GLY	C-O	-5.18	1.17	1.23
1	B	70	ASN	C-O	-5.08	1.17	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	183	ASN	N-CA-C	6.78	120.13	109.96
1	B	115	PHE	N-CA-C	6.25	120.76	113.20
1	A	242	LEU	N-CA-C	6.19	117.60	109.93
1	B	113	THR	N-CA-C	5.75	120.14	113.18
1	A	115	PHE	N-CA-C	5.71	120.11	113.20
1	A	183	ASN	N-CA-C	5.37	118.26	110.42

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	1726	0	1663	15	0
1	B	1730	0	1674	12	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	B	3	0	1	0	0
4	A	18	0	0	0	0
4	B	18	0	0	0	0
5	A	122	0	0	2	1
5	B	128	0	0	2	0
All	All	3749	0	3338	27	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 4.

All (27) 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:32:GLU:N	5:A:401:HOH:O	2.03	0.91
1:A:251:HIS:O	1:A:255:VAL:HG23	1.99	0.62
1:A:216:LEU:H	1:A:216:LEU:HD12	1.68	0.58
1:B:216:LEU:O	5:B:401:HOH:O	2.18	0.56
1:B:247:ASP:OD1	1:B:247:ASP:N	2.39	0.53
1:A:56:HIS:CE1	1:A:71:GLY:HA3	2.44	0.53
1:A:49:ILE:HD13	1:A:237:ILE:HD11	1.93	0.51
1:A:221:THR:O	1:A:225:ARG:HG3	2.10	0.50
1:A:49:ILE:HD11	1:A:55:SER:HB3	1.96	0.48
1:B:178:ALA:HB1	1:B:219:TRP:CD1	2.48	0.48
1:B:56:HIS:CE1	1:B:71:GLY:HA3	2.49	0.48
1:A:257:LYS:O	1:A:260:THR:N	2.47	0.47
1:B:232:GLU:CD	1:B:232:GLU:H	2.23	0.47
1:A:145:VAL:O	5:A:402:HOH:O	2.20	0.46
1:A:183:ASN:HD22	1:A:183:ASN:C	2.22	0.46
1:B:219:TRP:HB3	1:B:220:PRO:HD3	1.99	0.44
1:A:219:TRP:HB3	1:A:220:PRO:HD3	1.99	0.43
1:A:231:PRO:O	1:A:246:LEU:HD11	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:TYR:CD2	1:B:153:HIS:HB2	2.55	0.42
1:A:137:PRO:HD3	1:A:155:LEU:O	2.20	0.42
1:B:90:LYS:HE2	5:B:514:HOH:O	2.18	0.42
1:B:114:HIS:HE1	1:B:198:CYS:SG	2.43	0.41
1:B:49:ILE:HD11	1:B:55:SER:HB3	2.02	0.41
1:B:72:LEU:HB3	1:B:83:ILE:HB	2.03	0.41
1:A:160:SER:O	1:A:161:SER:C	2.63	0.41
1:B:137:PRO:HD3	1:B:155:LEU:O	2.21	0.40
1:A:231:PRO:O	1:A:246:LEU:CD1	2.69	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)
5:A:486:HOH:O	5:A:500:HOH:O[4_476]	2.03	0.17

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	229/231 (99%)	215 (94%)	11 (5%)	3 (1%)	9	2
1	B	229/231 (99%)	223 (97%)	5 (2%)	1 (0%)	30	16
All	All	458/462 (99%)	438 (96%)	16 (4%)	4 (1%)	14	4

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	178	ALA
1	B	178	ALA
1	A	161	SER
1	A	175	PRO

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	180/184 (98%)	170 (94%)	10 (6%)	19	4
1	B	181/184 (98%)	170 (94%)	11 (6%)	17	3
All	All	361/368 (98%)	340 (94%)	21 (6%)	18	3

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	48	GLN
1	B	117	ASP
1	B	123	VAL
1	B	146	GLU
1	B	166	ARG
1	B	183	ASN
1	B	190	SER
1	B	203	LEU
1	B	232	GLU
1	B	250	LYS
1	B	260	THR
1	A	117	ASP
1	A	123	VAL
1	A	138	SER
1	A	159	SER
1	A	183	ASN
1	A	205	ARG
1	A	207	SER
1	A	218	GLU
1	A	232	GLU
1	A	252	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	48	GLN

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Mol	Chain	Res	Type
1	A	48	GLN

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 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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	FMT	B	303	-	2,2,2	0.61	0	1,1,1	0.49	0
4	G0O	B	304	2	19,19,19	2.19	6 (31%)	24,25,25	2.04	8 (33%)
4	G0O	A	303	2	19,19,19	2.16	7 (36%)	24,25,25	2.24	10 (41%)

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	G0O	A	303	2	-	0/14/14/14	0/2/2/2
4	G0O	B	304	2	-	0/14/14/14	0/2/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	304	G0O	C13-N12	4.83	1.46	1.35
4	A	303	G0O	C13-N12	4.48	1.45	1.35
4	B	304	G0O	C06-C07	-4.30	1.40	1.47
4	B	304	G0O	N10-N09	4.13	1.37	1.31
4	A	303	G0O	N10-N09	3.73	1.37	1.31
4	A	303	G0O	C06-C07	-3.54	1.41	1.47
4	A	303	G0O	N08-N09	3.36	1.38	1.32
4	A	303	G0O	N10-N11	3.25	1.37	1.33
4	B	304	G0O	N08-N09	3.07	1.38	1.32
4	A	303	G0O	C04-N12	2.99	1.47	1.41
4	B	304	G0O	N10-N11	2.79	1.37	1.33
4	B	304	G0O	C04-N12	2.46	1.46	1.41
4	A	303	G0O	C16-S17	2.02	1.85	1.81

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	303	G0O	N11-C07-N08	-4.77	107.38	112.10
4	B	304	G0O	C01-C06-C07	-4.48	115.14	120.78
4	A	303	G0O	C07-N08-N09	4.13	109.34	105.65
4	A	303	G0O	C07-N11-N10	3.87	110.03	102.32
4	A	303	G0O	C01-C06-C07	-3.58	116.28	120.78
4	A	303	G0O	N11-N10-N09	-3.48	106.24	113.52
4	B	304	G0O	N11-N10-N09	-3.43	106.35	113.52
4	B	304	G0O	C07-N11-N10	3.38	109.07	102.32
4	B	304	G0O	N11-C07-N08	-3.30	108.83	112.10
4	A	303	G0O	C05-C06-C07	3.25	124.63	120.27
4	B	304	G0O	C07-N08-N09	2.96	108.29	105.65
4	A	303	G0O	C06-C07-N08	2.92	128.11	123.94
4	B	304	G0O	C06-C07-N08	2.55	127.58	123.94
4	B	304	G0O	C05-C06-C07	2.53	123.66	120.27
4	B	304	G0O	C02-C03-C04	2.35	122.44	119.73
4	A	303	G0O	C15-C16-S17	2.24	116.94	114.04
4	A	303	G0O	C05-C04-N12	2.24	127.41	120.13
4	A	303	G0O	C03-C04-N12	-2.23	112.91	120.41

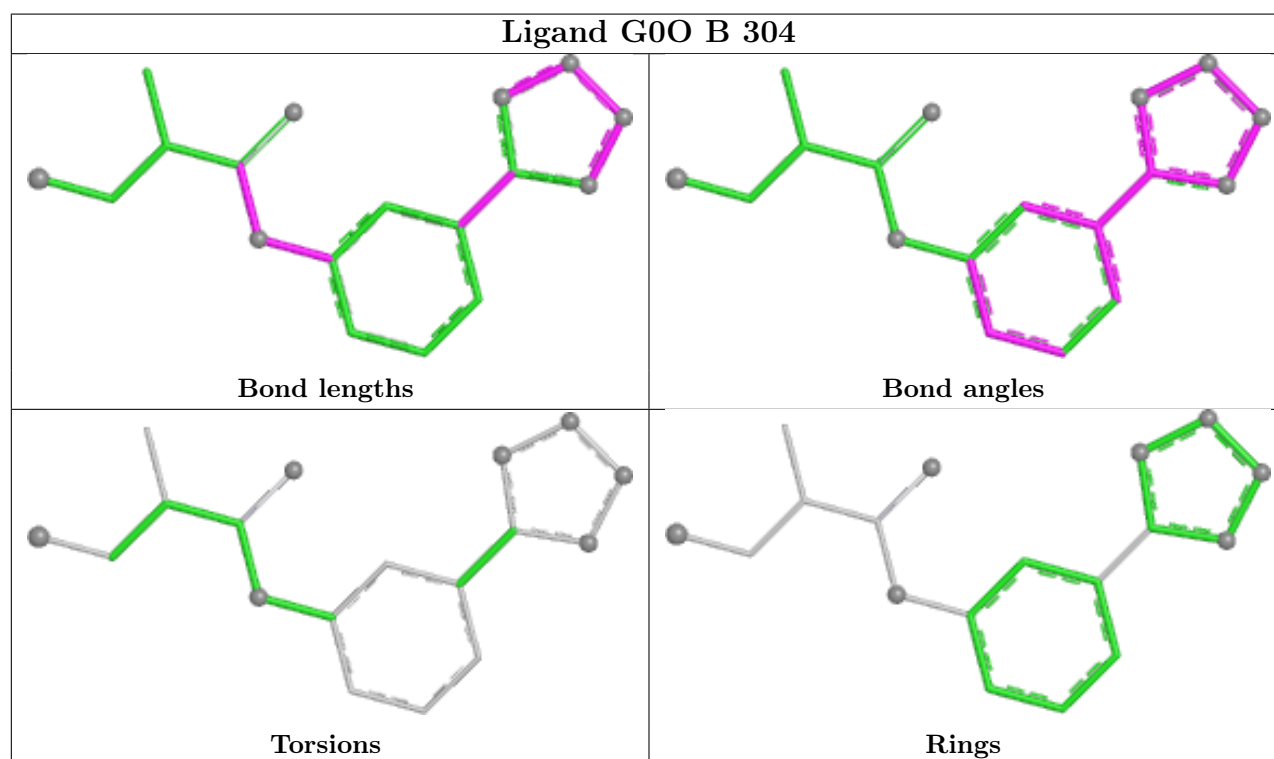
There are no chirality outliers.

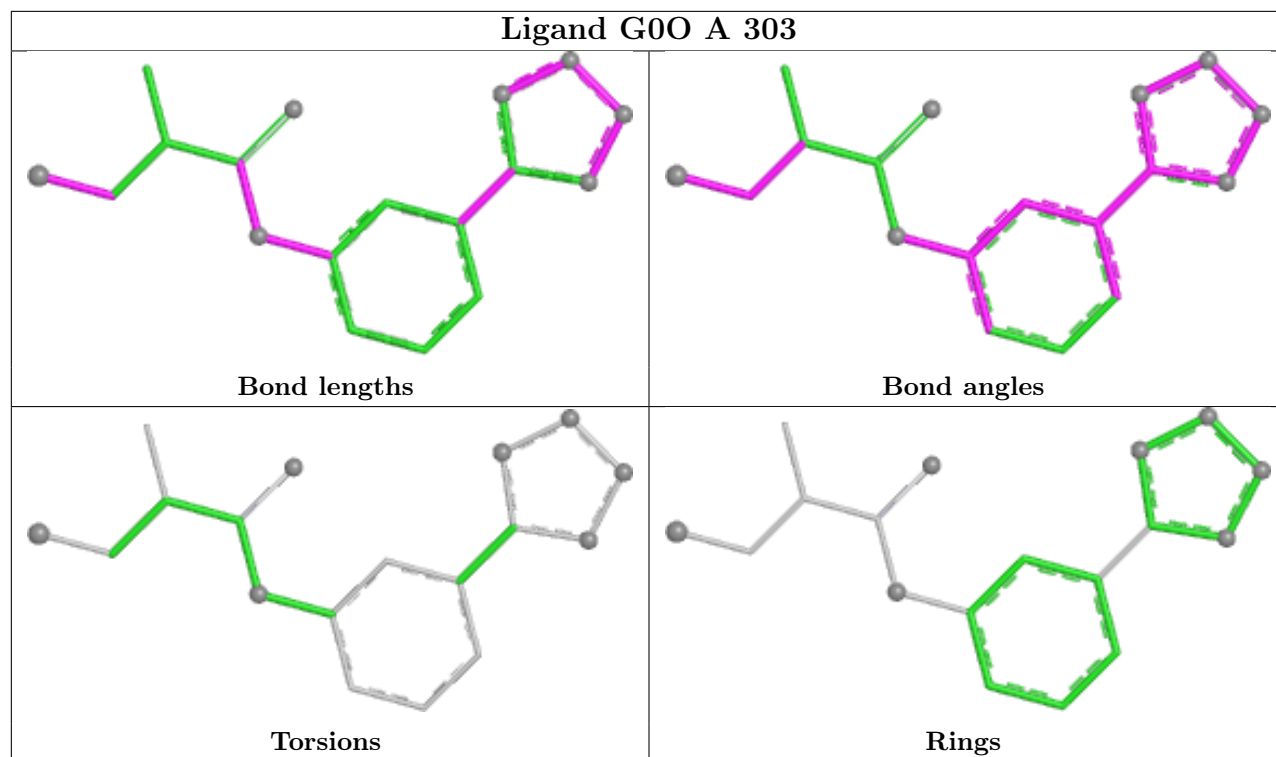
There are no torsion outliers.

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 [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

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	231/231 (100%)	1.48	77 (33%)  	10, 25, 56, 84	0
1	B	231/231 (100%)	1.25	58 (25%)  	11, 26, 47, 83	0
All	All	462/462 (100%)	1.36	135 (29%)  	10, 26, 51, 84	0

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	256	VAL	7.0
1	B	217	ALA	6.0
1	A	255	VAL	6.0
1	A	219	TRP	5.9
1	A	211	VAL	5.5
1	A	223	ILE	5.3
1	B	208	ALA	5.2
1	A	216	LEU	5.1
1	A	249	LEU	4.8
1	A	208	ALA	4.8
1	B	177	ALA	4.7
1	A	246	LEU	4.7
1	B	258	ALA	4.5
1	A	206	THR	4.5
1	A	253	THR	4.4
1	A	196	GLY	4.4
1	A	251	HIS	4.3
1	A	203	LEU	4.3
1	A	200	ILE	4.3
1	A	242	LEU	4.3
1	A	231	PRO	4.3
1	B	161	SER	4.2
1	B	211	VAL	4.2
1	A	259	HIS	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	160	SER	4.0
1	B	219	TRP	4.0
1	A	230	TYR	4.0
1	A	258	ALA	4.0
1	A	217	ALA	3.9
1	A	252	THR	3.8
1	A	222	SER	3.8
1	A	210	ASN	3.7
1	A	178	ALA	3.6
1	B	223	ILE	3.6
1	A	177	ALA	3.6
1	B	226	ILE	3.6
1	B	255	VAL	3.6
1	A	247	ASP	3.5
1	A	161	SER	3.5
1	B	260	THR	3.5
1	A	221	THR	3.5
1	B	235	PHE	3.4
1	B	206	THR	3.4
1	A	194	LEU	3.4
1	A	228	GLN	3.4
1	A	214	ALA	3.3
1	A	257	LYS	3.3
1	A	229	HIS	3.2
1	A	224	GLU	3.2
1	A	226	ILE	3.2
1	A	235	PHE	3.2
1	B	137	PRO	3.1
1	A	227	GLN	3.1
1	B	253	THR	3.1
1	B	165	VAL	3.1
1	B	256	VAL	3.1
1	A	137	PRO	3.1
1	A	220	PRO	3.1
1	A	192	SER	3.1
1	B	246	LEU	3.1
1	A	162	GLY	3.0
1	A	248	LEU	3.0
1	B	160	SER	3.0
1	A	173	PHE	3.0
1	A	254	ASN	3.0
1	A	204	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	231	PRO	3.0
1	B	221	THR	2.9
1	B	164	ALA	2.9
1	B	242	LEU	2.9
1	B	230	TYR	2.9
1	A	233	ALA	2.9
1	A	201	TYR	2.9
1	A	209	GLY	2.9
1	A	225	ARG	2.8
1	B	188	VAL	2.8
1	B	212	ALA	2.8
1	A	164	ALA	2.8
1	A	205	ARG	2.8
1	A	212	ALA	2.8
1	A	166	ARG	2.8
1	B	204	SER	2.8
1	B	174	TYR	2.8
1	B	227	GLN	2.8
1	A	250	LYS	2.8
1	B	251	HIS	2.8
1	A	176	GLY	2.7
1	A	244	GLY	2.7
1	A	245	GLY	2.7
1	A	145	VAL	2.7
1	A	236	VAL	2.7
1	B	216	LEU	2.7
1	B	156	GLU	2.7
1	B	229	HIS	2.7
1	B	261	ASN	2.7
1	A	156	GLU	2.6
1	A	175	PRO	2.6
1	A	62	PHE	2.6
1	A	260	THR	2.5
1	A	138	SER	2.5
1	A	195	TYR	2.5
1	A	188	VAL	2.5
1	B	49	ILE	2.5
1	B	158	LEU	2.5
1	B	214	ALA	2.5
1	B	162	GLY	2.5
1	B	193	VAL	2.5
1	B	207	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	254	ASN	2.4
1	A	207	SER	2.4
1	A	165	VAL	2.3
1	B	176	GLY	2.3
1	A	202	GLU	2.3
1	A	232	GLU	2.3
1	A	199	ALA	2.3
1	B	203	LEU	2.3
1	B	196	GLY	2.2
1	B	224	GLU	2.2
1	A	187	TYR	2.2
1	B	190	SER	2.2
1	B	143	ALA	2.1
1	A	197	GLY	2.1
1	B	257	LYS	2.1
1	B	262	ARG	2.1
1	B	178	ALA	2.1
1	B	191	ALA	2.1
1	B	136	SER	2.1
1	B	222	SER	2.1
1	A	215	ASP	2.1
1	B	183	ASN	2.0
1	B	185	VAL	2.0
1	B	225	ARG	2.0
1	A	185	VAL	2.0
1	B	142	LEU	2.0
1	B	145	VAL	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.

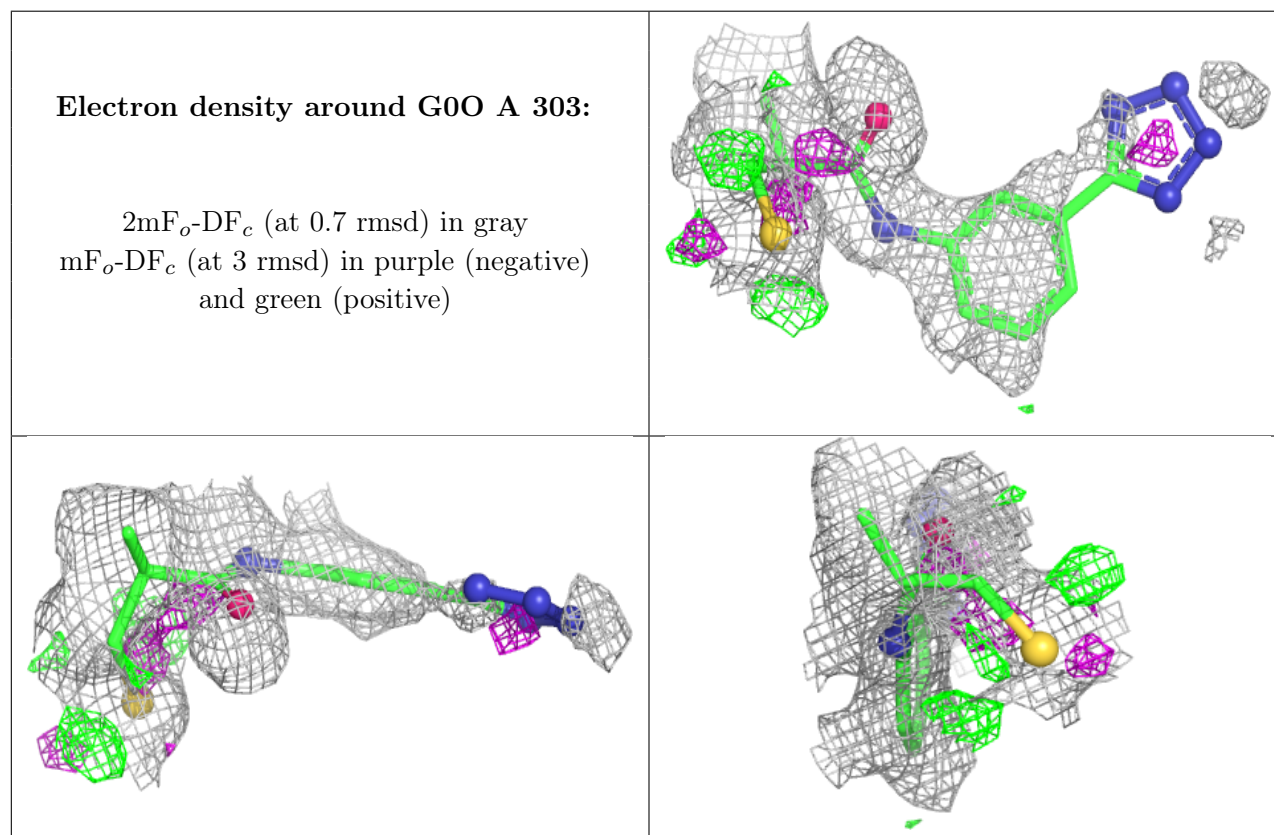
6.4 Ligands [i](#)

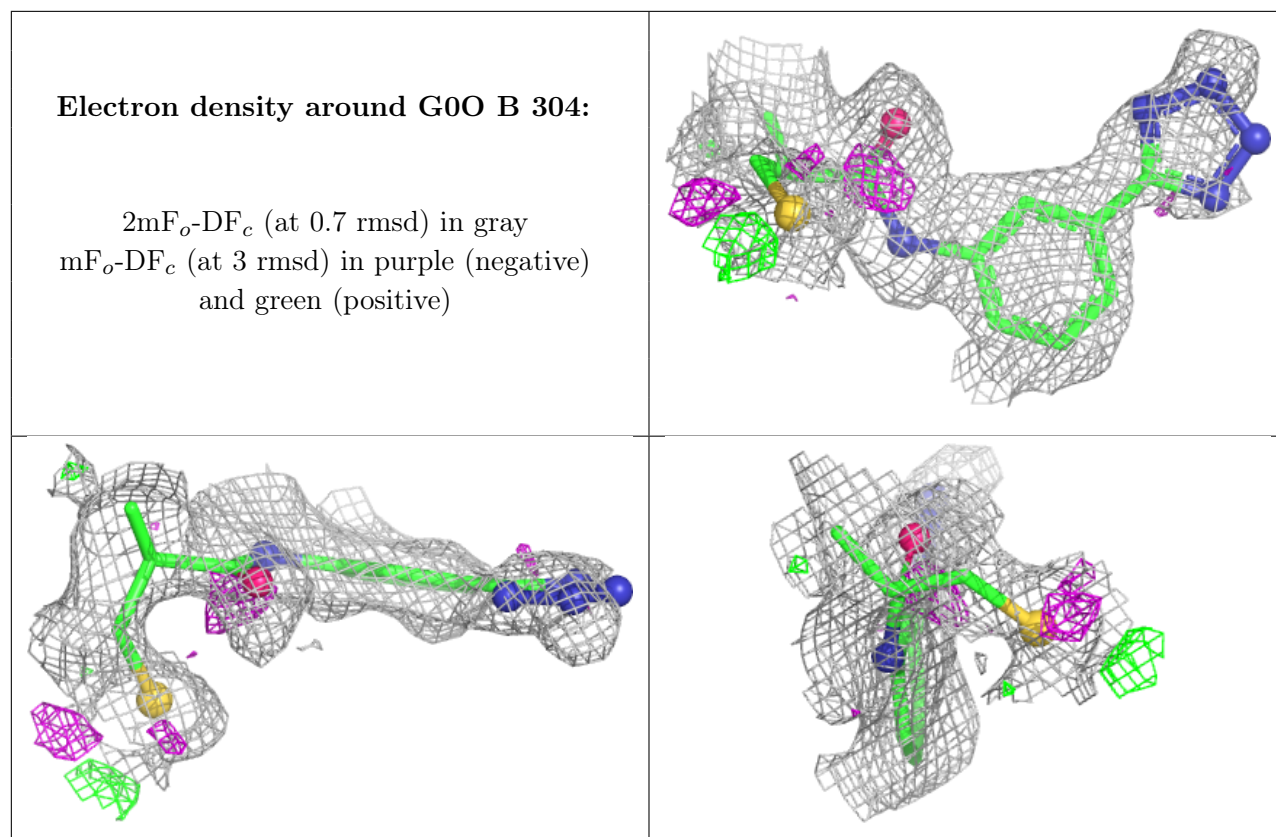
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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
3	FMT	B	303	3/3	0.77	0.17	26,26,39,49	0
4	G0O	A	303	18/18	0.92	0.14	28,44,61,62	0
4	G0O	B	304	18/18	0.93	0.11	27,32,55,55	0
2	ZN	A	301	1/1	0.95	0.06	27,27,27,27	0
2	ZN	A	302	1/1	0.97	0.04	28,28,28,28	0
2	ZN	B	301	1/1	0.98	0.04	21,21,21,21	0
2	ZN	B	302	1/1	0.99	0.02	23,23,23,23	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.