



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:19 PM UTC

PDB ID : 1KR3 / pdb_00001kr3
Title : Crystal Structure of the Metallo beta-Lactamase from *Bacteroides fragilis* (CfiA) in Complex with the Tricyclic Inhibitor SB-236050.
Authors : Payne, D.J.; Hueso-Rodriguez, J.A.; Boyd, H.; Concha, N.O.; Janson, C.A.; Gilpin, M.; Bateson, J.H.; Cheever, C.; Niconovich, N.L.; Pearson, S.; Rittenhouse, S.; Tew, D.; Dez, E.; Prez, P.; de la Fuente, J.; Rees, M.; Rivera-Sagredo, A.
Deposited on : 2002-01-08
Resolution : 2.50 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

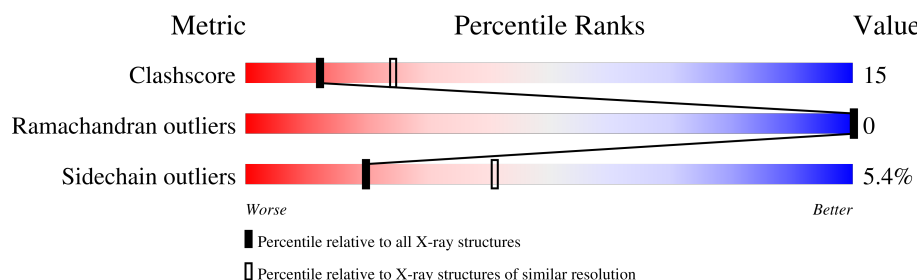
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	232	
1	B	232	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3576 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, type II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	S	40	0	0
			1742	1104	288	341	9			
1	B	227	Total	C	N	O	S	15	0	0
			1742	1104	288	341	9			

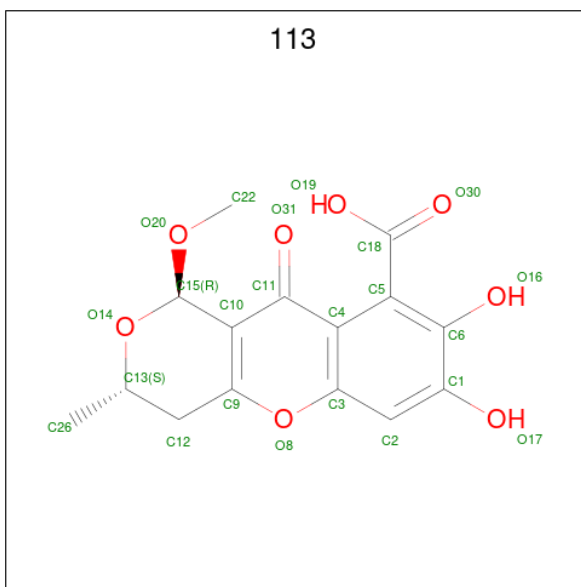
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 4 is 7,8-DIHYDROXY-1-METHOXY-3-METHYL-10-OXO-4,10-DIHYDRO-1H,3H-PYRANO[4,3-B]CHROMENE-9-CARBOXYLIC ACID (CCD ID: 113) (formula: C₁₅H₁₄O₈).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			23	15	8		
4	B	1	Total	C	O	0	0
			23	15	8		

- Molecule 5 is water.

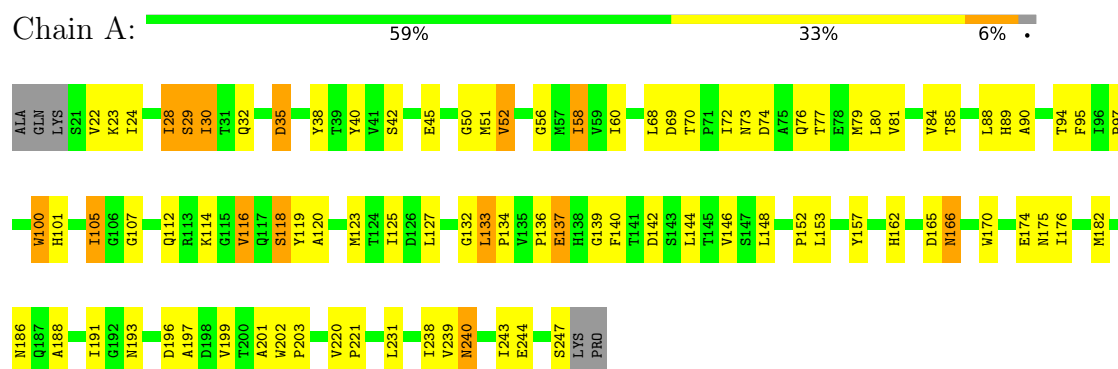
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	17	Total	O	0	0
			17	17		
5	B	23	Total	O	0	0
			23	23		

3 Residue-property plots

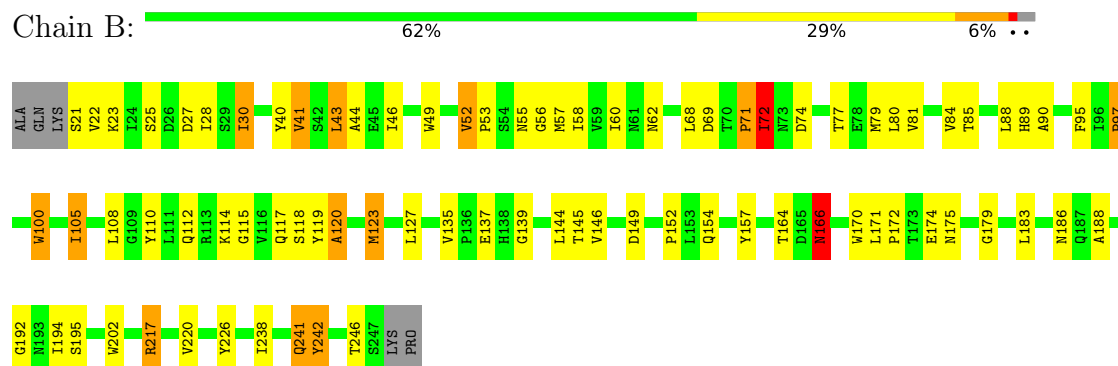
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

• Molecule 1: beta-Lactamase, type II



• Molecule 1: beta-Lactamase, type II



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	41.80 Å 44.20 Å 58.50 Å 92.80° 95.30° 98.00°	Depositor
Resolution (Å)	29.07 – 2.50	Depositor
% Data completeness (in resolution range)	73.7 (29.07-2.50)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
Refinement program	CNX 2000.1	Depositor
R, R_{free}	0.152 , 0.222	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3576	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 113, ZN, NA

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	2/1782 (0.1%)	1.31	22/2430 (0.9%)
1	B	0.96	3/1782 (0.2%)	1.37	22/2430 (0.9%)
All	All	0.93	5/3564 (0.1%)	1.34	44/4860 (0.9%)

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
1	B	0	2
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	123	MET	SD-CE	7.23	1.97	1.79
1	B	146	VAL	CA-CB	6.59	1.62	1.54
1	B	123	MET	SD-CE	5.65	1.93	1.79
1	A	116	VAL	CA-CB	5.24	1.60	1.54
1	B	220	VAL	CA-C	5.15	1.57	1.53

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	135	VAL	N-CA-C	9.52	118.58	107.73
1	B	171	LEU	CA-C-N	8.70	129.23	119.32
1	B	171	LEU	C-N-CA	8.70	129.23	119.32
1	B	100	TRP	N-CA-C	8.18	122.36	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	ASN	N-CA-C	7.68	121.55	110.10
1	A	182	MET	N-CA-C	-7.62	103.44	112.89
1	B	246	THR	N-CA-C	-7.60	104.24	113.97
1	B	72	ILE	N-CA-C	7.43	122.19	112.76
1	B	186	ASN	N-CA-C	7.34	119.28	111.28
1	A	133	LEU	CA-C-N	-7.12	112.44	119.78
1	A	133	LEU	C-N-CA	-7.12	112.44	119.78
1	A	52	VAL	CA-C-N	7.08	130.87	120.46
1	A	52	VAL	C-N-CA	7.08	130.87	120.46
1	A	186	ASN	N-CA-C	6.96	121.39	112.34
1	A	101	HIS	N-CA-C	6.59	118.51	110.41
1	B	74	ASP	N-CA-C	6.57	118.44	111.28
1	A	100	TRP	N-CA-C	6.36	120.76	113.19
1	B	217	ARG	N-CA-C	-6.35	103.62	112.45
1	B	152	PRO	N-CA-C	6.30	120.32	110.80
1	A	58	ILE	N-CA-C	-6.18	99.15	108.17
1	B	137	GLU	N-CA-C	6.15	120.79	113.16
1	A	137	GLU	N-CA-C	6.09	120.71	113.28
1	B	71	PRO	N-CA-C	-6.09	102.70	111.22
1	A	28	ILE	N-CA-C	5.95	116.57	107.77
1	B	120	ALA	N-CA-C	5.94	117.57	108.42
1	B	81	VAL	N-CA-C	5.89	116.07	110.42
1	A	193	ASN	N-CA-C	5.82	119.17	108.58
1	A	220	VAL	CA-C-N	5.82	127.13	120.85
1	A	220	VAL	C-N-CA	5.82	127.13	120.85
1	A	79	MET	N-CA-C	-5.77	104.89	111.07
1	A	140	PHE	N-CA-C	-5.70	101.08	109.81
1	B	166	ASN	N-CA-C	5.70	118.50	110.23
1	B	220	VAL	N-CA-C	5.54	114.04	107.73
1	B	115	GLY	N-CA-C	5.51	122.97	115.30
1	B	27	ASP	N-CA-C	5.34	119.95	113.38
1	B	28	ILE	N-CA-C	5.34	115.58	108.11
1	B	192	GLY	N-CA-C	5.28	121.82	112.53
1	A	231	LEU	N-CA-C	-5.25	106.13	112.54
1	B	127	LEU	N-CA-C	5.25	116.69	111.07
1	A	148	LEU	N-CA-C	-5.21	98.82	107.99
1	A	105	ILE	CB-CA-C	-5.13	105.33	112.36
1	A	94	THR	N-CA-C	5.01	117.58	109.06
1	A	191	ILE	N-CA-C	-5.01	105.54	112.50
1	B	105	ILE	CB-CA-C	-5.00	105.03	111.88

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	157	TYR	Sidechain
1	B	157	TYR	Sidechain
1	B	242	TYR	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	1742	0	1699	56	0
1	B	1742	0	1699	51	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	23	0	13	0	0
4	B	23	0	13	0	0
5	A	17	0	0	0	0
5	B	23	0	0	0	0
All	All	3576	0	3424	106	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 15.

All (106) 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:B:100:TRP:O	1:B:105:ILE:HD11	1.85	0.77
1:A:152:PRO:O	1:A:153:LEU:HD23	1.89	0.73
1:B:84:VAL:HG13	1:B:88:LEU:HD12	1.70	0.73
1:B:60:ILE:HD11	1:B:88:LEU:HD13	1.72	0.72
1:B:179:GLY:HA3	1:B:183:LEU:HD12	1.72	0.71
1:A:70:THR:HG23	1:A:95:PHE:CE2	2.25	0.71
1:B:46:ILE:HD12	1:B:52:VAL:HG21	1.71	0.70
1:B:44:ALA:HB1	1:B:72:ILE:HD11	1.73	0.69
1:A:45:GLU:OE1	1:A:51:MET:HG2	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:LEU:O	1:A:69:ASP:HB2	1.94	0.66
1:B:40:TYR:CE2	1:B:56:GLY:HA3	2.31	0.65
1:B:22:VAL:HG12	1:B:30:ILE:HG22	1.79	0.65
1:B:154:GLN:NE2	1:B:170:TRP:HD1	1.93	0.64
1:A:85:THR:O	1:A:89:HIS:HA	1.98	0.63
1:B:40:TYR:CZ	1:B:56:GLY:HA3	2.33	0.63
1:A:170:TRP:CH2	1:A:175:ASN:HA	2.35	0.62
1:B:46:ILE:HD12	1:B:52:VAL:CG2	2.29	0.62
1:A:152:PRO:C	1:A:153:LEU:HD23	2.24	0.61
1:A:35:ASP:OD2	1:A:35:ASP:N	2.33	0.61
1:A:24:ILE:HD11	1:A:28:ILE:CG2	2.32	0.60
1:B:44:ALA:CB	1:B:72:ILE:HD11	2.32	0.60
1:B:71:PRO:HD2	1:B:77:THR:OG1	2.01	0.60
1:B:241:GLN:O	1:B:241:GLN:HG2	2.01	0.59
1:B:21:SER:HA	1:B:30:ILE:O	2.02	0.59
1:A:162:HIS:O	1:A:197:ALA:HA	2.02	0.59
1:A:85:THR:HG22	1:A:90:ALA:O	2.03	0.59
1:A:24:ILE:HD11	1:A:28:ILE:HG22	1.85	0.58
1:A:120:ALA:O	1:A:139:GLY:HA2	2.03	0.58
1:B:170:TRP:CH2	1:B:175:ASN:HA	2.41	0.56
1:A:58:ILE:HD11	1:A:80:LEU:HD11	1.89	0.55
1:A:85:THR:HA	1:A:90:ALA:H	1.71	0.55
1:A:95:PHE:CZ	1:A:97:PRO:HB3	2.42	0.55
1:A:42:SER:HB2	1:A:76:GLN:OE1	2.07	0.54
1:A:100:TRP:CD1	1:A:127:LEU:HD13	2.43	0.54
1:B:202:TRP:O	1:B:202:TRP:HD1	1.92	0.53
1:B:85:THR:O	1:B:89:HIS:HA	2.09	0.53
1:B:226:TYR:CD1	1:B:226:TYR:C	2.87	0.52
1:B:62:ASN:HB2	1:B:149:ASP:OD2	2.11	0.51
1:B:188:ALA:O	1:B:238:ILE:HD11	2.10	0.51
1:A:29:SER:O	1:A:30:ILE:HD12	2.10	0.51
1:A:77:THR:O	1:A:81:VAL:HG23	2.10	0.51
1:A:72:ILE:HD12	1:A:73:ASN:N	2.24	0.51
1:A:132:GLY:O	1:B:217:ARG:HD2	2.11	0.50
1:A:174:GLU:O	1:A:176:ILE:HG13	2.12	0.49
1:A:50:GLY:O	1:A:52:VAL:HG13	2.12	0.49
1:B:57:MET:HE2	1:B:68:LEU:HD12	1.94	0.49
1:B:68:LEU:O	1:B:69:ASP:HB2	2.13	0.49
1:B:154:GLN:NE2	1:B:172:PRO:HG3	2.27	0.48
1:A:243:ILE:O	1:A:247:SER:HB2	2.14	0.48
1:B:110:TYR:CZ	1:B:114:LYS:HD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ALA:O	1:A:238:ILE:HD11	2.13	0.47
1:A:40:TYR:CE2	1:A:56:GLY:HA3	2.49	0.47
1:B:95:PHE:O	1:B:118:SER:HA	2.14	0.46
1:B:166:ASN:C	1:B:166:ASN:HD22	2.23	0.46
1:B:154:GLN:HE21	1:B:170:TRP:HD1	1.63	0.46
1:B:117:GLN:OE1	1:B:117:GLN:HA	2.15	0.46
1:B:60:ILE:HD11	1:B:88:LEU:HB3	1.98	0.45
1:A:85:THR:CG2	1:A:90:ALA:O	2.64	0.45
1:A:22:VAL:HG12	1:A:23:LYS:N	2.32	0.44
1:A:133:LEU:O	1:A:134:PRO:C	2.59	0.44
1:A:202:TRP:HB3	1:A:203:PRO:HD3	1.99	0.44
1:B:120:ALA:O	1:B:139:GLY:HA2	2.16	0.44
1:A:100:TRP:HZ2	1:A:196:ASP:OD1	2.01	0.44
1:B:144:LEU:HG	1:B:145:THR:N	2.31	0.44
1:A:201:ALA:O	1:A:202:TRP:C	2.61	0.44
1:B:22:VAL:HG22	1:B:23:LYS:N	2.31	0.44
1:B:43:LEU:HD22	1:B:53:PRO:HB3	2.00	0.44
1:A:114:LYS:HB3	1:A:114:LYS:HE2	1.72	0.44
1:B:110:TYR:OH	1:B:114:LYS:HD2	2.18	0.44
1:A:72:ILE:HD12	1:A:72:ILE:C	2.42	0.43
1:B:174:GLU:O	1:B:175:ASN:HB2	2.18	0.43
1:B:49:TRP:HB3	1:B:52:VAL:HG11	2.00	0.43
1:A:125:ILE:HD12	1:A:139:GLY:HA3	1.99	0.43
1:B:85:THR:HG22	1:B:90:ALA:O	2.19	0.43
1:A:119:TYR:HD2	1:A:144:LEU:HD21	1.82	0.43
1:B:123:MET:HE1	1:B:164:THR:HB	2.00	0.43
1:A:112:GLN:C	1:A:114:LYS:N	2.75	0.43
1:B:80:LEU:O	1:B:84:VAL:HG23	2.19	0.43
1:B:57:MET:CE	1:B:68:LEU:HD12	2.48	0.43
1:A:24:ILE:CD1	1:A:30:ILE:HD13	2.48	0.43
1:A:24:ILE:HD11	1:A:28:ILE:HG21	2.01	0.43
1:A:80:LEU:O	1:A:84:VAL:HG23	2.18	0.42
1:A:74:ASP:OD1	1:A:107:GLY:HA2	2.19	0.42
1:B:41:VAL:HG13	1:B:55:ASN:OD1	2.19	0.42
1:A:24:ILE:HD13	1:A:30:ILE:HD13	2.02	0.42
1:B:88:LEU:O	1:B:89:HIS:C	2.61	0.42
1:B:194:ILE:O	1:B:195:SER:C	2.59	0.42
1:A:32:GLN:NE2	1:A:38:TYR:CZ	2.88	0.41
1:A:97:PRO:HD2	1:A:119:TYR:O	2.20	0.41
1:A:118:SER:HB2	1:A:136:PRO:HB3	2.03	0.41
1:B:79:MET:O	1:B:80:LEU:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:ILE:CD1	1:A:73:ASN:HD22	2.34	0.41
1:A:97:PRO:HB3	1:A:105:ILE:HG22	2.02	0.41
1:A:144:LEU:HG	1:A:146:VAL:CG2	2.51	0.41
1:B:97:PRO:HD2	1:B:119:TYR:O	2.20	0.41
1:A:239:VAL:O	1:A:240:ASN:C	2.62	0.41
1:A:22:VAL:CG1	1:A:23:LYS:N	2.83	0.41
1:A:40:TYR:CZ	1:A:56:GLY:HA3	2.56	0.41
1:A:60:ILE:HD12	1:A:88:LEU:HB3	2.03	0.41
1:B:202:TRP:CD1	1:B:202:TRP:C	2.99	0.41
1:A:119:TYR:CD2	1:A:144:LEU:HD21	2.55	0.41
1:B:23:LYS:HG2	1:B:25:SER:O	2.21	0.41
1:A:72:ILE:CD1	1:A:73:ASN:ND2	2.85	0.40
1:A:100:TRP:HD1	1:A:165:ASP:OD2	2.03	0.40
1:B:108:LEU:O	1:B:112:GLN:HG3	2.22	0.40
1:B:242:TYR:CD2	1:B:242:TYR:C	3.00	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	225/232 (97%)	203 (90%)	22 (10%)	0	100	100
1	B	225/232 (97%)	212 (94%)	13 (6%)	0	100	100
All	All	450/464 (97%)	415 (92%)	35 (8%)	0	100	100

There are no Ramachandran outliers to report.

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	193/197 (98%)	181 (94%)	12 (6%)	16	34
1	B	193/197 (98%)	184 (95%)	9 (5%)	23	47
All	All	386/394 (98%)	365 (95%)	21 (5%)	20	41

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

Mol	Chain	Res	Type
1	A	29	SER
1	A	30	ILE
1	A	35	ASP
1	A	116	VAL
1	A	118	SER
1	A	137	GLU
1	A	142	ASP
1	A	166	ASN
1	A	199	VAL
1	A	221	PRO
1	A	240	ASN
1	A	244	GLU
1	B	30	ILE
1	B	41	VAL
1	B	43	LEU
1	B	52	VAL
1	B	58	ILE
1	B	72	ILE
1	B	97	PRO
1	B	166	ASN
1	B	241	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	82	ASN
1	A	138	HIS
1	A	154	GLN
1	A	186	ASN

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Mol	Chain	Res	Type
1	A	240	ASN
1	A	241	GLN
1	B	154	GLN
1	B	166	ASN
1	B	187	GLN
1	B	240	ASN
1	B	241	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 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	113	A	602	2	25,25,25	1.13	1 (4%)	32,38,38	1.45	4 (12%)
4	113	B	601	2	25,25,25	1.12	1 (4%)	32,38,38	1.34	4 (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
4	113	A	602	2	-	1/6/18/18	0/3/3/3
4	113	B	601	2	-	0/6/18/18	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	601	113	O14-C15	2.20	1.44	1.41
4	A	602	113	C10-C11	2.17	1.51	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	601	113	C22-O20-C15	4.30	121.15	113.28
4	A	602	113	C22-O20-C15	4.26	121.07	113.28
4	A	602	113	O20-C15-C10	2.86	113.35	108.13
4	A	602	113	C3-O8-C9	2.75	122.04	118.70
4	A	602	113	O8-C3-C2	2.61	119.53	115.83
4	B	601	113	O20-C15-C10	2.48	112.66	108.13
4	B	601	113	C3-O8-C9	2.09	121.24	118.70
4	B	601	113	C3-C4-C11	-2.06	117.55	120.03

There are no chirality outliers.

All (1) torsion outliers are listed below:

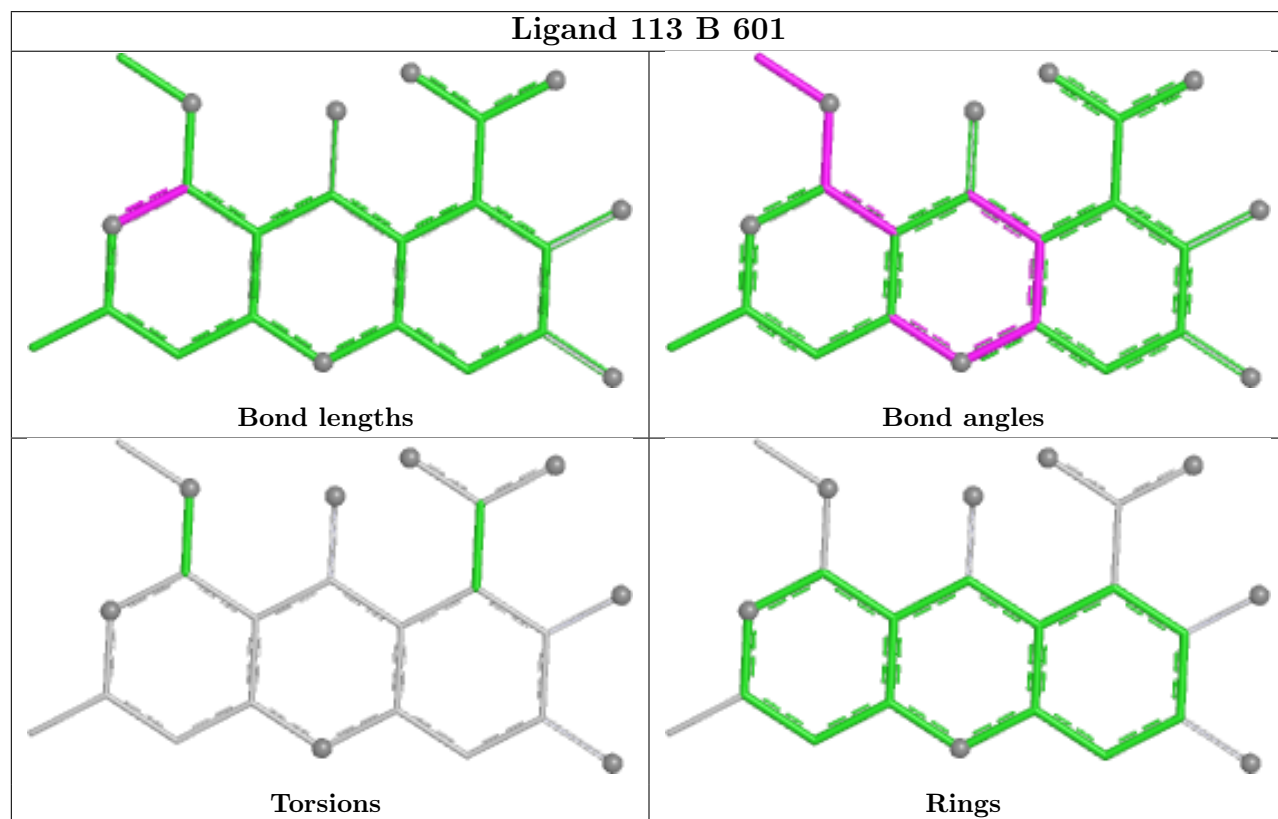
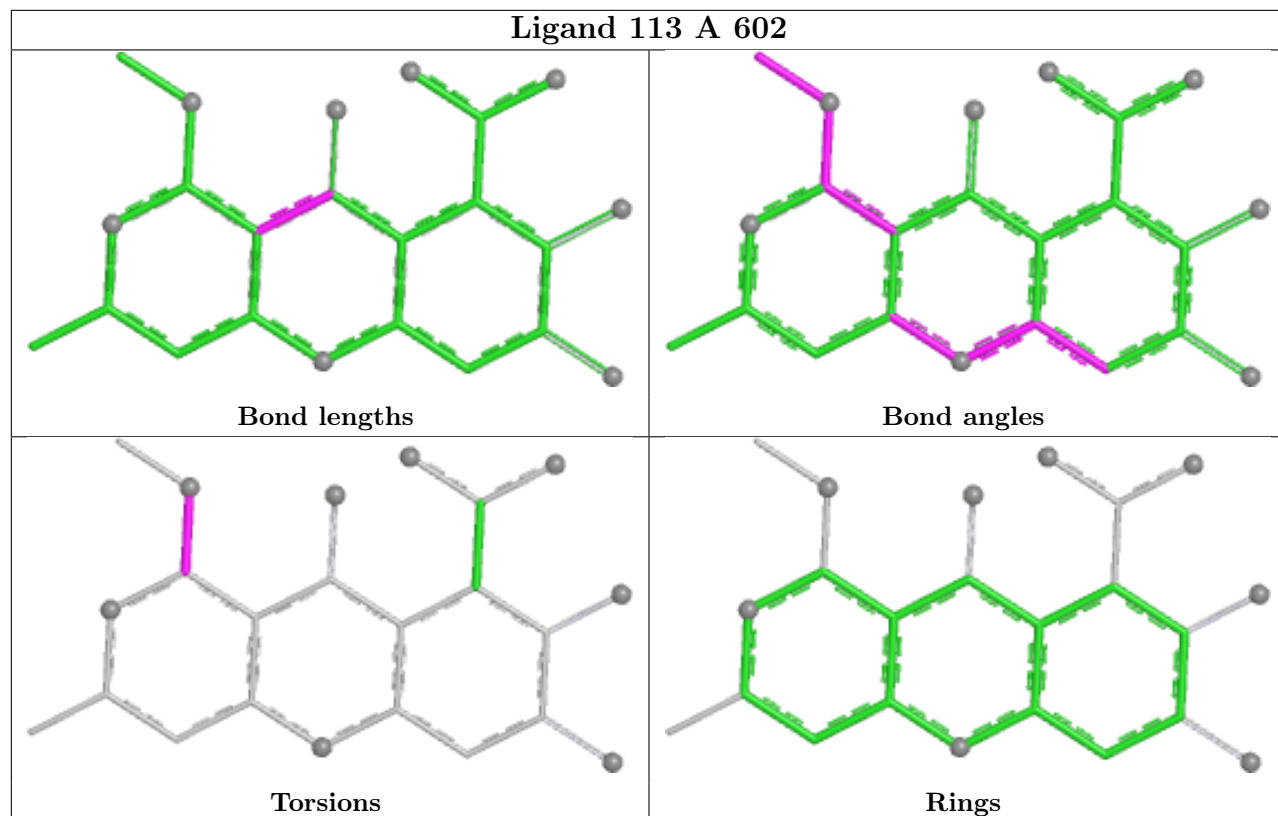
Mol	Chain	Res	Type	Atoms
4	A	602	113	C10-C15-O20-C22

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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.