



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 7, 2021 – 10:11 AM JST

PDB ID : 6JKA  
Title : Crystal structure of metallo-beta-lactamase, IMP-1, in complex with a thiazole-bearing inhibitor  
Authors : Kamo, T.; Kuroda, K.; Kondo, S.; Hayashi, U.; Fudo, S.; Nukaga, M.; Hoshino, T.  
Deposited on : 2019-02-28  
Resolution : 2.01 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.24
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.24

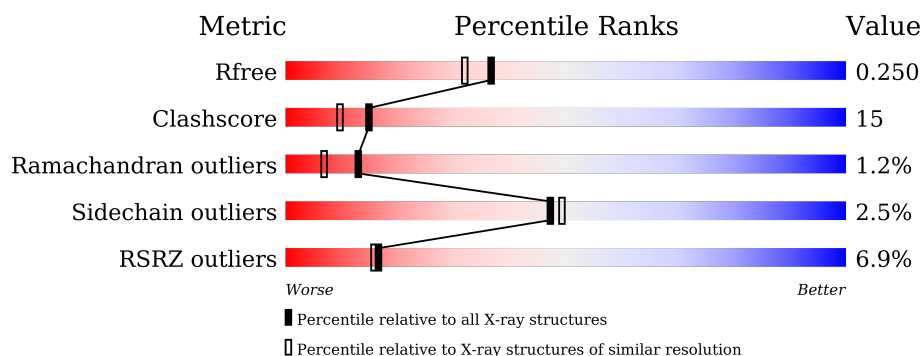
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.01 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))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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  $\geq 3$ , 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	228	<div> <div>4%</div> <div>79%</div> <div>18%</div> <div>.</div> </div>
1	B	228	<div> <div>2%</div> <div>77%</div> <div>16%</div> <div>.</div> <div>.</div> </div>
1	C	228	<div> <div>6%</div> <div>74%</div> <div>21%</div> <div>5%</div> </div>
1	D	228	<div> <div>14%</div> <div>53%</div> <div>34%</div> <div>10%</div> <div>.</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	BS0	A	303	-	-	X	X
3	BS0	C	303	-	-	X	-
4	BQU	B	303	-	-	X	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7419 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 Metallo-beta-lactamase type 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	S	0	0	0
			1763	1142	291	329	1			
1	B	220	Total	C	N	O	S	0	0	0
			1721	1116	284	320	1			
1	C	228	Total	C	N	O	S	0	0	0
			1769	1145	292	331	1			
1	D	220	Total	C	N	O	S	0	0	0
			1722	1118	284	319	1			

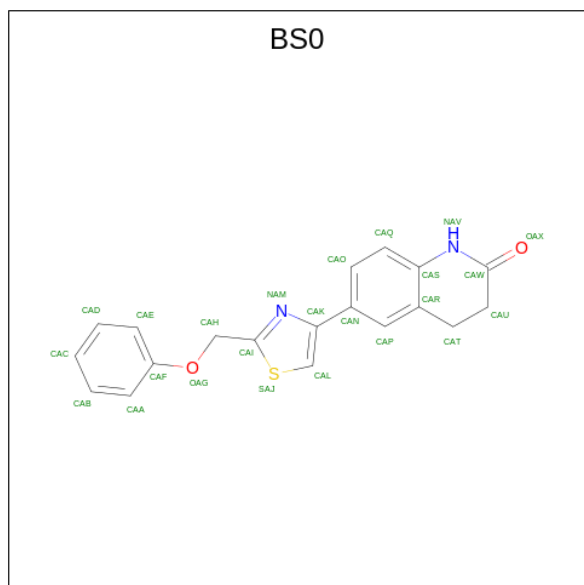
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P52699
A	2	PRO	-	expression tag	UNP P52699
A	3	GLY	-	expression tag	UNP P52699
A	4	VAL	-	expression tag	UNP P52699
A	5	GLY	-	expression tag	UNP P52699
B	1	GLY	-	expression tag	UNP P52699
B	2	PRO	-	expression tag	UNP P52699
B	3	GLY	-	expression tag	UNP P52699
B	4	VAL	-	expression tag	UNP P52699
B	5	GLY	-	expression tag	UNP P52699
C	1	GLY	-	expression tag	UNP P52699
C	2	PRO	-	expression tag	UNP P52699
C	3	GLY	-	expression tag	UNP P52699
C	4	VAL	-	expression tag	UNP P52699
C	5	GLY	-	expression tag	UNP P52699
D	1	GLY	-	expression tag	UNP P52699
D	2	PRO	-	expression tag	UNP P52699
D	3	GLY	-	expression tag	UNP P52699
D	4	VAL	-	expression tag	UNP P52699
D	5	GLY	-	expression tag	UNP P52699

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

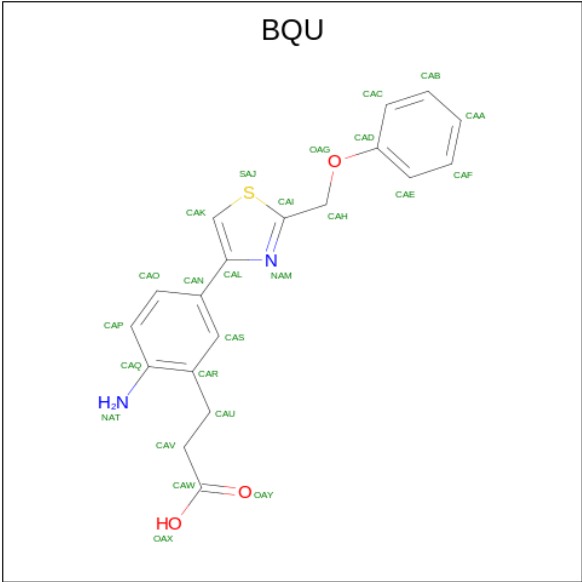
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		

- Molecule 3 is 6-[2-(phenoxyethyl)-1,3-thiazol-4-yl]-3,4-dihydro-1H-quinolin-2-one (three-letter code: BS0) (formula: C<sub>19</sub>H<sub>16</sub>N<sub>2</sub>O<sub>2</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			24	19	2	2	1		
3	C	1	Total	C	N	O	S	0	0
			24	19	2	2	1		

- Molecule 4 is 3-[2-azanyl-5-[2-(phenoxyethyl)-1,3-thiazol-4-yl]phenyl]propanoic acid (three-letter code: BQU) (formula: C<sub>19</sub>H<sub>18</sub>N<sub>2</sub>O<sub>3</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			25	19	2	3	1		

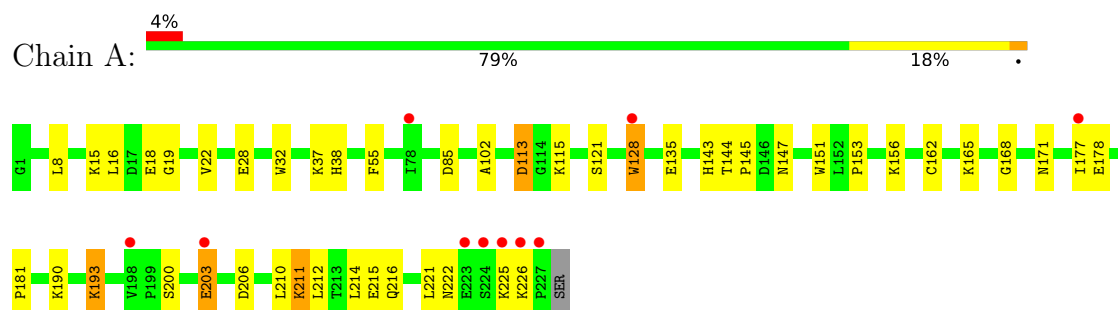
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	139	Total	O	0	0
			139	139		
5	B	85	Total	O	0	0
			85	85		
5	C	101	Total	O	0	0
			101	101		
5	D	38	Total	O	0	0
			38	38		

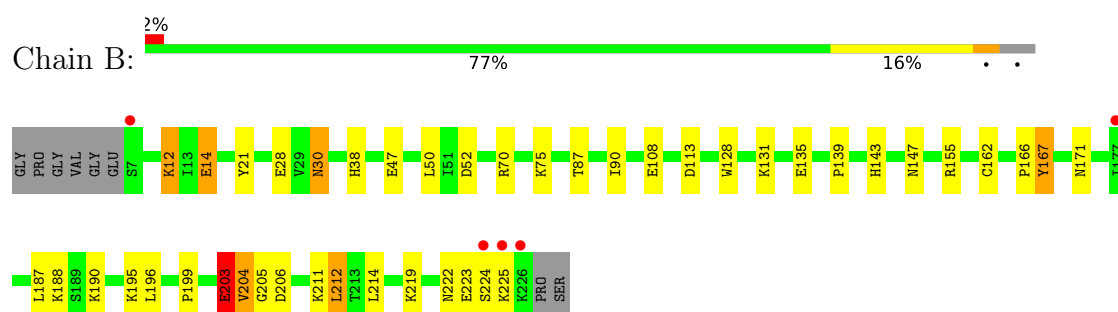
### 3 Residue-property plots [i](#)

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.

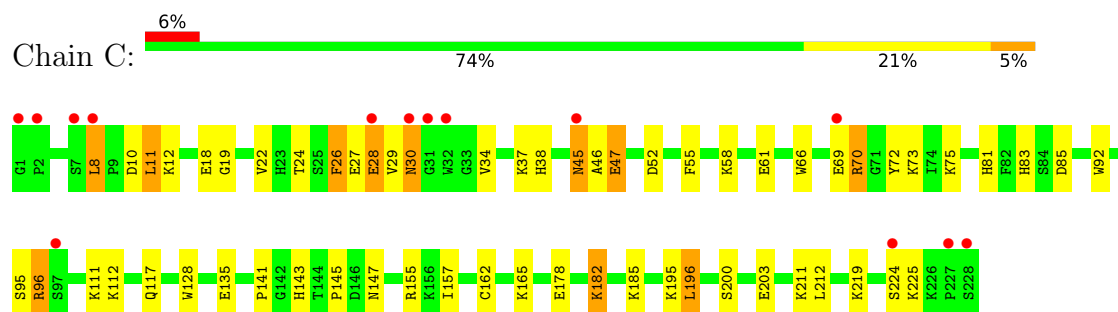
#### • Molecule 1: Metallo-beta-lactamase type 2



#### • Molecule 1: Metallo-beta-lactamase type 2

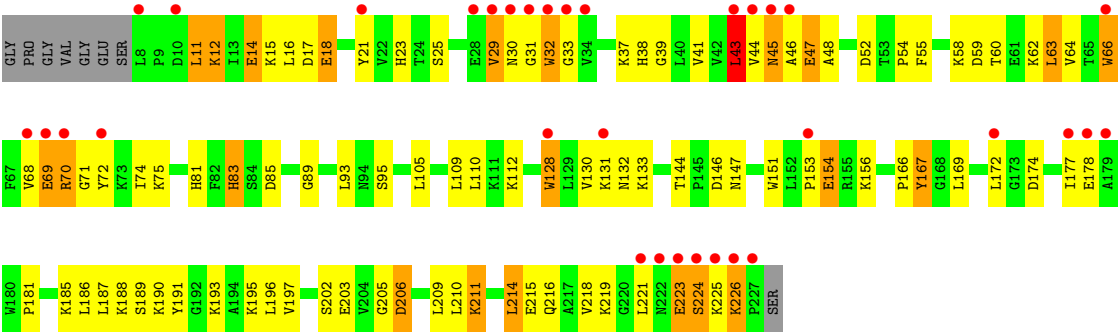


#### • Molecule 1: Metallo-beta-lactamase type 2



#### • Molecule 1: Metallo-beta-lactamase type 2







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	48.48Å 77.76Å 261.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.68 – 2.01 33.68 – 2.01	Depositor EDS
% Data completeness (in resolution range)	88.6 (33.68-2.01) 88.6 (33.68-2.01)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.75 (at 2.01Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, $R_{free}$	0.193 , 0.250 0.193 , 0.250	Depositor DCC
$R_{free}$ test set	2919 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.7	Xtriage
Anisotropy	0.545	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 73.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7419	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: ZN, BS0, BQU

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	0.81	6/1809 (0.3%)	1.11	12/2455 (0.5%)
1	B	0.89	7/1765 (0.4%)	1.20	15/2394 (0.6%)
1	C	1.00	10/1815 (0.6%)	1.20	18/2463 (0.7%)
1	D	1.21	17/1767 (1.0%)	1.35	18/2398 (0.8%)
All	All	0.99	40/7156 (0.6%)	1.22	63/9710 (0.6%)

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	1
1	C	0	2
1	D	0	7
All	All	0	11

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	128	TRP	CB-CG	12.91	1.73	1.50
1	C	27	GLU	CB-CG	10.87	1.72	1.52
1	A	203	GLU	CB-CG	10.04	1.71	1.52
1	D	32	TRP	CB-CG	9.00	1.66	1.50
1	B	108	GLU	CB-CG	8.92	1.69	1.52
1	D	66	TRP	CB-CG	8.34	1.65	1.50
1	D	47	GLU	CB-CG	8.15	1.67	1.52
1	C	27	GLU	CG-CD	8.14	1.64	1.51
1	A	203	GLU	CG-CD	7.85	1.63	1.51
1	C	26	PHE	CD2-CE2	-7.83	1.23	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	167	TYR	CD2-CE2	7.69	1.50	1.39
1	D	178	GLU	CB-CG	7.50	1.66	1.52
1	D	151	TRP	CB-CG	-7.25	1.37	1.50
1	C	30	ASN	CB-CG	6.94	1.67	1.51
1	B	203	GLU	CB-CG	6.79	1.65	1.52
1	A	193	LYS	CB-CG	6.67	1.70	1.52
1	C	69	GLU	CB-CG	-6.49	1.39	1.52
1	D	14	GLU	CB-CG	6.39	1.64	1.52
1	B	108	GLU	CG-CD	6.09	1.61	1.51
1	D	12	LYS	CD-CE	6.07	1.66	1.51
1	D	47	GLU	CG-CD	6.07	1.61	1.51
1	C	28	GLU	CB-CG	5.93	1.63	1.52
1	D	12	LYS	CG-CD	5.92	1.72	1.52
1	D	178	GLU	CG-CD	5.63	1.60	1.51
1	B	219	LYS	CB-CG	5.55	1.67	1.52
1	D	21	TYR	CD2-CE2	5.43	1.47	1.39
1	A	113	ASP	CB-CG	5.40	1.63	1.51
1	B	167	TYR	CG-CD2	5.39	1.46	1.39
1	D	128	TRP	C-O	5.38	1.33	1.23
1	C	26	PHE	CE1-CZ	-5.38	1.27	1.37
1	C	219	LYS	CD-CE	5.27	1.64	1.51
1	D	193	LYS	CB-CG	5.25	1.66	1.52
1	B	70	ARG	CB-CG	-5.24	1.38	1.52
1	D	211	LYS	CB-CG	5.23	1.66	1.52
1	A	128	TRP	CE3-CZ3	5.14	1.47	1.38
1	D	12	LYS	CB-CG	5.12	1.66	1.52
1	C	178	GLU	CG-CD	-5.12	1.44	1.51
1	C	47	GLU	CB-CG	-5.07	1.42	1.52
1	A	203	GLU	CD-OE1	5.05	1.31	1.25
1	D	12	LYS	CA-CB	5.01	1.65	1.53

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	167	TYR	CB-CG-CD2	13.55	129.13	121.00
1	A	113	ASP	CB-CG-OD1	12.45	129.51	118.30
1	B	167	TYR	CB-CG-CD1	-11.46	114.13	121.00
1	A	214	LEU	CB-CG-CD2	-9.93	94.12	111.00
1	C	165	LYS	CD-CE-NZ	-9.28	90.35	111.70
1	B	70	ARG	NE-CZ-NH2	-9.25	115.68	120.30
1	C	11	LEU	CB-CG-CD2	-9.04	95.64	111.00
1	B	70	ARG	NE-CZ-NH1	8.92	124.76	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	ASP	CB-CG-OD2	-8.80	110.38	118.30
1	A	32	TRP	C-N-CA	-8.72	103.98	122.30
1	C	18	GLU	C-N-CA	-8.41	104.64	122.30
1	A	18	GLU	C-N-CA	-8.21	105.06	122.30
1	D	225	LYS	CD-CE-NZ	-8.10	93.08	111.70
1	B	113	ASP	CB-CG-OD1	7.82	125.34	118.30
1	C	8	LEU	CA-CB-CG	7.72	133.06	115.30
1	C	182	LYS	CD-CE-NZ	7.56	129.09	111.70
1	C	8	LEU	CB-CG-CD1	7.53	123.81	111.00
1	D	186	LEU	CB-CG-CD1	7.45	123.66	111.00
1	C	219	LYS	CD-CE-NZ	7.42	128.78	111.70
1	C	58	LYS	CD-CE-NZ	7.22	128.31	111.70
1	D	214	LEU	CB-CG-CD2	-7.21	98.74	111.00
1	D	11	LEU	CB-CG-CD1	-7.08	98.97	111.00
1	D	12	LYS	CA-CB-CG	7.03	128.87	113.40
1	A	211	LYS	CD-CE-NZ	7.01	127.83	111.70
1	D	187	LEU	CB-CG-CD2	-6.89	99.29	111.00
1	B	206	ASP	CB-CG-OD2	-6.81	112.17	118.30
1	C	211	LYS	CD-CE-NZ	-6.53	96.68	111.70
1	C	70	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	C	70	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	D	43	LEU	CA-CB-CG	-6.34	100.71	115.30
1	A	15	LYS	CD-CE-NZ	6.28	126.15	111.70
1	D	63	LEU	CA-CB-CG	6.27	129.72	115.30
1	B	155	ARG	CG-CD-NE	-6.26	98.65	111.80
1	D	206	ASP	CB-CG-OD2	-6.24	112.68	118.30
1	A	115	LYS	CD-CE-NZ	-6.12	97.63	111.70
1	B	113	ASP	CB-CG-OD2	-6.09	112.82	118.30
1	D	156	LYS	CD-CE-NZ	-5.98	97.94	111.70
1	A	203	GLU	OE1-CD-OE2	-5.98	116.13	123.30
1	C	112	LYS	CD-CE-NZ	-5.96	98.00	111.70
1	C	185	LYS	CD-CE-NZ	5.94	125.37	111.70
1	D	17	ASP	N-CA-C	-5.94	94.96	111.00
1	D	219	LYS	CD-CE-NZ	5.80	125.05	111.70
1	B	14	GLU	CA-CB-CG	5.77	126.08	113.40
1	B	214	LEU	CB-CG-CD2	-5.74	101.24	111.00
1	A	190	LYS	CD-CE-NZ	5.74	124.90	111.70
1	B	50	LEU	CB-CG-CD1	-5.70	101.30	111.00
1	C	196	LEU	CB-CG-CD1	-5.65	101.39	111.00
1	C	45	ASN	CB-CA-C	-5.62	99.15	110.40
1	C	8	LEU	CB-CG-CD2	-5.62	101.44	111.00
1	B	206	ASP	CB-CG-OD1	5.60	123.34	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	69	GLU	CA-CB-CG	-5.59	101.10	113.40
1	D	185	LYS	CA-CB-CG	5.46	125.41	113.40
1	D	52	ASP	CB-CG-OD2	5.43	123.19	118.30
1	B	204	VAL	CA-CB-CG1	-5.42	102.77	110.90
1	B	12	LYS	CA-CB-CG	5.36	125.19	113.40
1	D	70	ARG	CA-CB-CG	5.34	125.15	113.40
1	A	203	GLU	CG-CD-OE2	5.31	128.92	118.30
1	D	52	ASP	CB-CG-OD1	-5.25	113.58	118.30
1	D	154	GLU	CA-CB-CG	5.24	124.92	113.40
1	A	210	LEU	CB-CG-CD1	5.15	119.76	111.00
1	D	11	LEU	CA-CB-CG	5.10	127.03	115.30
1	B	212	LEU	CA-CB-CG	-5.05	103.69	115.30
1	C	73	LYS	CD-CE-NZ	5.03	123.26	111.70

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	19	GLY	Peptide
1	B	225	LYS	Peptide
1	C	19	GLY	Peptide
1	C	29	VAL	Peptide
1	D	202	SER	Peptide
1	D	223	GLU	Peptide
1	D	224	SER	Peptide
1	D	29	VAL	Peptide
1	D	33	GLY	Peptide
1	D	44	VAL	Peptide
1	D	71	GLY	Peptide

## 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	1763	0	1777	42	0
1	B	1721	0	1736	34	0
1	C	1769	0	1782	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1722	0	1738	87	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	24	0	0	12	0
3	C	24	0	0	13	0
4	B	25	0	0	18	0
5	A	139	0	0	6	0
5	B	85	0	0	4	0
5	C	101	0	0	5	0
5	D	38	0	0	3	0
All	All	7419	0	7033	214	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 (214) 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:177:ILE:CD1	1:A:221:LEU:HD13	1.65	1.26
1:C:38:HIS:NE2	3:C:303:BS0:SAJ	2.11	1.23
1:C:38:HIS:CD2	3:C:303:BS0:SAJ	2.31	1.23
1:A:177:ILE:HD13	1:A:221:LEU:HD13	1.27	1.14
4:B:303:BQU:OAY	4:B:303:BQU:CAQ	1.97	1.13
1:A:177:ILE:HD13	1:A:221:LEU:CD1	1.88	1.02
1:D:58:LYS:H	1:D:58:LYS:HD2	1.22	1.02
1:A:177:ILE:CD1	1:A:221:LEU:CD1	2.41	0.99
1:A:143:HIS:HE1	3:A:303:BS0:CAL	1.75	0.98
1:D:64:VAL:HG13	1:D:74:ILE:HG13	1.46	0.95
1:B:171:ASN:HB3	4:B:303:BQU:CAP	1.97	0.93
1:B:171:ASN:H	4:B:303:BQU:CAO	1.84	0.90
1:A:177:ILE:HD12	1:A:178:GLU:N	1.88	0.89
1:B:171:ASN:HB3	4:B:303:BQU:CAQ	2.01	0.89
4:B:303:BQU:OAY	4:B:303:BQU:NAT	2.06	0.89
1:A:143:HIS:CE1	3:A:303:BS0:CAL	2.57	0.88
1:D:128:TRP:CD2	1:D:131:LYS:NZ	2.42	0.87
1:D:38:HIS:HE1	5:D:415:HOH:O	1.61	0.83
1:D:128:TRP:HE3	1:D:131:LYS:HA	1.44	0.82
1:A:171:ASN:HB3	3:A:303:BS0:CAL	2.09	0.82
1:A:177:ILE:HD12	1:A:177:ILE:C	2.01	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:LEU:HD21	1:D:48:ALA:HB2	1.64	0.80
1:D:169:LEU:HB3	1:D:172:LEU:HD21	1.63	0.79
1:B:203:GLU:OE1	5:B:401:HOH:O	2.01	0.77
1:D:133:LYS:CD	1:D:154:GLU:OE2	2.33	0.77
1:D:47:GLU:OE2	1:D:75:LYS:HD3	1.83	0.77
1:D:43:LEU:HD23	1:D:47:GLU:O	1.84	0.77
1:A:165:LYS:NZ	3:A:303:BS0:SAJ	2.57	0.76
1:D:223:GLU:HA	1:D:226:LYS:HD3	1.65	0.76
1:D:223:GLU:HG3	1:D:226:LYS:NZ	2.01	0.76
4:B:303:BQU:NAT	4:B:303:BQU:CAW	2.48	0.76
1:C:8:LEU:HD11	1:C:28:GLU:HB2	1.68	0.75
1:A:38:HIS:NE2	1:A:203:GLU:OE1	2.19	0.75
1:D:128:TRP:CE3	1:D:131:LYS:NZ	2.55	0.75
1:A:177:ILE:HD12	1:A:221:LEU:HD13	1.67	0.73
4:B:303:BQU:SAJ	1:D:203:GLU:HG3	2.28	0.73
1:B:167:TYR:HB2	4:B:303:BQU:CAB	2.20	0.72
1:D:133:LYS:HZ2	1:D:154:GLU:CD	1.94	0.71
1:A:153:PRO:O	1:A:156:LYS:HD3	1.90	0.71
4:B:303:BQU:OAY	4:B:303:BQU:CAR	2.39	0.70
1:D:12:LYS:NZ	5:D:401:HOH:O	2.17	0.70
1:D:133:LYS:O	1:D:153:PRO:HD2	1.92	0.70
1:D:60:THR:O	1:D:64:VAL:HG23	1.93	0.69
1:B:167:TYR:H	4:B:303:BQU:CAA	2.05	0.69
4:B:303:BQU:CAQ	4:B:303:BQU:CAW	2.70	0.68
3:A:303:BS0:SAJ	5:A:461:HOH:O	2.50	0.68
1:D:69:GLU:CG	1:D:69:GLU:O	2.41	0.68
1:C:45:ASN:O	1:C:46:ALA:HB3	1.92	0.68
3:A:303:BS0:CAC	1:C:203:GLU:CG	2.72	0.67
1:D:130:VAL:HG13	1:D:133:LYS:HB2	1.77	0.67
1:D:128:TRP:CE3	1:D:131:LYS:HG3	2.31	0.66
1:D:128:TRP:CZ3	1:D:131:LYS:HG3	2.31	0.66
1:C:128:TRP:CZ3	1:C:135:GLU:HB2	2.30	0.66
1:D:23:HIS:NE2	1:D:39:GLY:HA3	2.11	0.65
3:A:303:BS0:CAC	1:C:203:GLU:HG2	2.27	0.65
1:C:26:PHE:CE2	3:C:303:BS0:CAD	2.80	0.65
1:D:66:TRP:CD2	1:D:70:ARG:NH1	2.64	0.65
1:A:8:LEU:HD21	1:A:28:GLU:HG3	1.79	0.65
1:B:143:HIS:HE1	4:B:303:BQU:NAT	1.96	0.64
1:C:26:PHE:CZ	3:C:303:BS0:CAD	2.80	0.64
1:D:69:GLU:O	1:D:69:GLU:HG3	1.98	0.63
1:D:15:LYS:HE2	1:D:18:GLU:HA	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:LYS:HD2	1:D:154:GLU:OE2	1.97	0.63
1:D:133:LYS:HZ3	1:D:154:GLU:CG	2.12	0.63
1:D:66:TRP:CE2	1:D:70:ARG:NH2	2.67	0.63
1:D:133:LYS:HD3	1:D:154:GLU:OE2	1.98	0.62
1:D:188:LYS:HE3	1:D:211:LYS:HA	1.80	0.62
1:D:133:LYS:NZ	1:D:154:GLU:CD	2.52	0.61
1:D:64:VAL:HG13	1:D:74:ILE:CG1	2.28	0.61
1:A:211:LYS:NZ	1:A:215:GLU:OE2	2.32	0.60
1:D:11:LEU:HD12	1:D:59:ASP:HB3	1.83	0.60
1:A:177:ILE:HD13	1:A:221:LEU:HD12	1.82	0.60
1:D:66:TRP:CE2	1:D:70:ARG:CZ	2.85	0.60
1:D:66:TRP:NE1	1:D:70:ARG:NH2	2.49	0.60
1:D:214:LEU:O	1:D:218:VAL:HG22	2.02	0.60
1:C:155:ARG:NH2	5:C:404:HOH:O	2.34	0.59
1:B:222:ASN:O	1:B:224:SER:N	2.34	0.59
1:C:12:LYS:NZ	3:C:303:BS0:CAF	2.65	0.59
1:D:128:TRP:CE3	1:D:131:LYS:HA	2.31	0.59
1:C:182:LYS:NZ	5:C:401:HOH:O	2.17	0.59
1:D:133:LYS:NZ	1:D:154:GLU:CG	2.66	0.58
1:D:66:TRP:CG	1:D:70:ARG:NH1	2.71	0.58
1:B:171:ASN:N	4:B:303:BQU:CAO	2.63	0.57
3:A:303:BS0:CAC	1:C:203:GLU:HG3	2.34	0.57
1:C:26:PHE:CZ	3:C:303:BS0:CAE	2.88	0.56
1:D:47:GLU:HB3	1:D:75:LYS:CG	2.34	0.56
1:D:131:LYS:HG2	1:D:132:ASN:ND2	2.20	0.56
1:D:47:GLU:HB3	1:D:75:LYS:HG3	1.86	0.56
1:A:38:HIS:NE2	1:A:203:GLU:CD	2.59	0.56
1:D:223:GLU:HG3	1:D:226:LYS:HZ1	1.69	0.56
1:B:188:LYS:NZ	1:B:211:LYS:HE3	2.21	0.55
1:C:111:LYS:HE2	1:C:117:GLN:OE1	2.06	0.55
1:A:128:TRP:CE3	1:A:135:GLU:HB3	2.42	0.55
1:D:16:LEU:HD21	1:D:196:LEU:HD12	1.87	0.55
1:B:143:HIS:CE1	4:B:303:BQU:NAT	2.76	0.54
1:D:166:PRO:HB2	1:D:167:TYR:CE1	2.43	0.54
1:A:171:ASN:HB3	3:A:303:BS0:CAK	2.37	0.54
1:A:144:THR:HB	1:A:145:PRO:CD	2.38	0.54
1:A:37:LYS:HE2	1:A:200:SER:OG	2.08	0.54
1:D:205:GLY:N	1:D:209:LEU:HD11	2.23	0.53
1:D:11:LEU:HD12	1:D:59:ASP:CB	2.38	0.53
1:C:96:ARG:NH2	5:C:402:HOH:O	2.22	0.53
1:B:139:PRO:HG3	1:B:187:LEU:HD13	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:LYS:NZ	1:B:14:GLU:OE2	2.41	0.53
1:D:29:VAL:O	1:D:31:GLY:HA2	2.09	0.53
1:D:167:TYR:HA	1:D:216:GLN:HE21	1.74	0.53
1:D:188:LYS:HA	1:D:210:LEU:HD13	1.90	0.53
1:A:162:CYS:HB3	5:A:461:HOH:O	2.09	0.52
1:C:111:LYS:HE2	1:C:117:GLN:CD	2.30	0.52
1:D:58:LYS:H	1:D:58:LYS:CD	2.05	0.52
1:D:38:HIS:CE1	5:D:415:HOH:O	2.46	0.51
1:D:45:ASN:OD1	1:D:46:ALA:N	2.39	0.51
1:B:128:TRP:CZ3	1:B:135:GLU:HB2	2.45	0.51
1:D:169:LEU:CB	1:D:172:LEU:HD21	2.35	0.51
1:B:47:GLU:HB3	1:B:75:LYS:CG	2.41	0.51
1:C:26:PHE:HZ	3:C:303:BS0:CAE	2.24	0.51
1:C:225:LYS:NZ	5:C:405:HOH:O	2.44	0.51
1:C:66:TRP:CE2	1:C:70:ARG:CZ	2.93	0.51
1:B:167:TYR:H	4:B:303:BQU:CAB	2.23	0.50
1:A:55:PHE:CE1	1:A:85:ASP:HB3	2.46	0.50
1:A:143:HIS:CE1	3:A:303:BS0:SAJ	3.05	0.50
1:A:102:ALA:O	1:A:121:SER:HA	2.11	0.49
1:B:47:GLU:HB3	1:B:75:LYS:HG3	1.94	0.49
1:C:111:LYS:HE2	1:C:117:GLN:NE2	2.28	0.49
1:C:8:LEU:HD12	1:C:34:VAL:HG22	1.96	0.48
1:A:216:GLN:NE2	3:C:303:BS0:OAX	2.37	0.48
1:C:12:LYS:HZ1	3:C:303:BS0:CAF	2.27	0.48
1:D:68:VAL:HG23	1:D:69:GLU:N	2.28	0.48
1:C:70:ARG:HG3	1:C:70:ARG:HH11	1.79	0.47
1:D:190:LYS:HE3	1:D:191:TYR:CZ	2.49	0.47
1:D:223:GLU:HG3	1:D:226:LYS:HZ2	1.76	0.47
1:A:151:TRP:CH2	1:A:156:LYS:HA	2.49	0.47
1:C:26:PHE:CE2	3:C:303:BS0:CAE	2.97	0.47
1:C:143:HIS:CD2	1:C:162:CYS:HB2	2.49	0.47
1:A:144:THR:HB	1:A:145:PRO:HD2	1.96	0.47
1:B:195:LYS:HG2	1:B:196:LEU:HG	1.96	0.47
1:C:141:PRO:HB3	1:C:145:PRO:HA	1.97	0.47
1:A:212:LEU:HD23	1:A:212:LEU:HA	1.68	0.47
1:B:167:TYR:CZ	1:D:206:ASP:HB3	2.49	0.47
1:D:109:LEU:HD23	1:D:109:LEU:HA	1.74	0.47
1:B:167:TYR:CB	4:B:303:BQU:CAB	2.92	0.46
1:D:89:GLY:O	1:D:93:LEU:HG	2.15	0.46
1:D:68:VAL:HG12	1:D:72:TYR:O	2.15	0.46
1:A:38:HIS:CE1	1:A:203:GLU:HA	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:LYS:NZ	1:B:14:GLU:CD	2.69	0.46
1:D:215:GLU:HA	1:D:218:VAL:CG2	2.46	0.46
1:A:165:LYS:HB3	1:A:168:GLY:O	2.16	0.45
1:B:21:TYR:CD1	1:B:21:TYR:N	2.84	0.45
1:B:38:HIS:NE2	5:B:401:HOH:O	2.16	0.45
1:B:143:HIS:CD2	1:B:162:CYS:HB2	2.51	0.45
1:D:167:TYR:HA	1:D:216:GLN:NE2	2.30	0.45
1:A:128:TRP:HE3	1:A:135:GLU:HB3	1.81	0.45
1:A:193:LYS:CG	1:A:193:LYS:O	2.64	0.45
1:A:177:ILE:HD11	1:A:221:LEU:CD1	2.39	0.45
1:C:46:ALA:HA	1:C:72:TYR:CD2	2.52	0.45
1:D:181:PRO:HG2	1:D:221:LEU:HD22	1.99	0.45
1:D:25:SER:HG	1:D:55:PHE:HD1	1.64	0.44
1:D:131:LYS:HB2	1:D:131:LYS:HE2	1.48	0.44
1:A:177:ILE:O	1:A:181:PRO:HD3	2.17	0.44
1:B:12:LYS:HG2	5:B:406:HOH:O	2.18	0.44
1:D:37:LYS:HE3	1:D:85:ASP:O	2.17	0.44
1:C:22:VAL:HG11	3:C:303:BSO:CAL	2.48	0.44
1:D:81:HIS:NE2	1:D:83:HIS:HB2	2.32	0.44
1:B:171:ASN:H	4:B:303:BQU:CAP	2.28	0.44
1:D:16:LEU:O	1:D:16:LEU:HG	2.07	0.44
1:D:177:ILE:HG13	1:D:221:LEU:HA	1.98	0.44
1:C:61:GLU:HG3	1:C:92:TRP:CZ2	2.53	0.44
1:C:195:LYS:HG2	1:C:196:LEU:HG	1.99	0.44
1:D:43:LEU:HD23	1:D:47:GLU:C	2.36	0.44
1:A:203:GLU:HG3	1:C:212:LEU:HD11	1.99	0.43
1:C:47:GLU:HB3	1:C:75:LYS:HG3	2.00	0.43
1:D:68:VAL:C	1:D:70:ARG:H	2.22	0.43
1:C:37:LYS:HE2	1:C:200:SER:OG	2.18	0.43
1:D:110:LEU:HD23	1:D:110:LEU:HA	1.83	0.43
1:A:222:ASN:ND2	5:A:411:HOH:O	2.47	0.43
1:C:28:GLU:OE1	1:C:30:ASN:HA	2.19	0.43
1:D:12:LYS:HG2	1:D:14:GLU:OE1	2.19	0.43
1:D:197:VAL:HB	1:D:209:LEU:HD12	2.01	0.43
1:D:205:GLY:CA	1:D:209:LEU:HD11	2.48	0.43
1:D:59:ASP:OD1	1:D:62:LYS:HE3	2.19	0.43
1:A:225:LYS:O	1:A:226:LYS:HG2	2.18	0.42
1:B:30:ASN:HD22	1:B:30:ASN:HA	1.55	0.42
1:C:45:ASN:O	1:C:46:ALA:CB	2.55	0.42
1:C:96:ARG:NE	5:C:402:HOH:O	2.47	0.42
1:D:41:VAL:CG2	1:D:63:LEU:HD11	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:303:BS0:CAL	5:A:461:HOH:O	2.68	0.42
1:C:12:LYS:HZ2	3:C:303:BS0:CAF	2.31	0.42
1:D:144:THR:HG22	1:D:174:ASP:HB2	2.02	0.42
1:B:166:PRO:HD2	4:B:303:BQU:CAF	2.49	0.42
1:C:24:THR:OG1	3:C:303:BS0:SAJ	2.67	0.41
1:C:55:PHE:CE2	1:C:85:ASP:HB3	2.55	0.41
1:D:41:VAL:HG21	1:D:63:LEU:HD11	2.02	0.41
1:C:155:ARG:HB2	1:C:157:ILE:HG13	2.01	0.41
1:C:81:HIS:NE2	1:C:83:HIS:HB2	2.35	0.41
1:D:105:LEU:HG	1:D:146:ASP:HB3	2.02	0.41
1:D:190:LYS:HE3	1:D:191:TYR:OH	2.20	0.41
1:B:87:THR:HB	1:B:90:ILE:HD12	2.03	0.41
1:D:47:GLU:OE2	1:D:75:LYS:CD	2.63	0.41
1:C:66:TRP:CE2	1:C:70:ARG:NH2	2.88	0.41
1:C:95:SER:OG	1:C:96:ARG:NH1	2.53	0.41
1:D:112:LYS:O	1:D:112:LYS:HG2	2.20	0.41
1:D:133:LYS:NZ	1:D:154:GLU:HG2	2.34	0.41
1:A:16:LEU:HB2	1:A:22:VAL:HG23	2.03	0.41
1:C:10:ASP:O	1:C:11:LEU:C	2.60	0.41
1:D:68:VAL:C	1:D:70:ARG:N	2.73	0.41
1:A:38:HIS:HE1	1:A:203:GLU:HA	1.85	0.41
3:A:303:BS0:CAI	5:A:461:HOH:O	2.69	0.41
1:B:212:LEU:HD23	1:B:212:LEU:HA	1.90	0.40
1:A:206:ASP:HB2	5:A:463:HOH:O	2.21	0.40
1:B:47:GLU:HB3	1:B:75:LYS:HG2	2.04	0.40
1:B:188:LYS:HZ1	1:B:211:LYS:HE3	1.84	0.40
1:B:204:VAL:HG12	1:B:205:GLY:N	2.36	0.40
1:A:143:HIS:CD2	1:A:162:CYS:HB2	2.57	0.40
1:B:47:GLU:OE2	5:B:402:HOH:O	2.22	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	225/228 (99%)	217 (96%)	8 (4%)	0	100	100
1	B	218/228 (96%)	209 (96%)	7 (3%)	2 (1%)	17	11
1	C	226/228 (99%)	212 (94%)	13 (6%)	1 (0%)	34	30
1	D	218/228 (96%)	192 (88%)	18 (8%)	8 (4%)	3	1
All	All	887/912 (97%)	830 (94%)	46 (5%)	11 (1%)	13	7

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	224	SER
1	B	223	GLU
1	D	30	ASN
1	C	52	ASP
1	D	45	ASN
1	D	95	SER
1	B	52	ASP
1	D	69	GLU
1	D	83	HIS
1	D	226	LYS
1	D	54	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	193/194 (100%)	191 (99%)	2 (1%)	76	81
1	B	189/194 (97%)	182 (96%)	7 (4%)	34	32
1	C	194/194 (100%)	191 (98%)	3 (2%)	65	69
1	D	189/194 (97%)	182 (96%)	7 (4%)	34	32
All	All	765/776 (99%)	746 (98%)	19 (2%)	47	49

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	113	ASP
1	A	147	ASN
1	B	28	GLU
1	B	30	ASN
1	B	131	LYS
1	B	147	ASN
1	B	190	LYS
1	B	199	PRO
1	B	203	GLU
1	C	96	ARG
1	C	147	ASN
1	C	224	SER
1	D	18	GLU
1	D	32	TRP
1	D	43	LEU
1	D	147	ASN
1	D	167	TYR
1	D	189	SER
1	D	195	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	171	ASN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 8 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	BS0	C	303	-	25,27,27	2.83	7 (28%)	30,37,37	3.61	17 (56%)
4	BQU	B	303	2	22,27,27	2.31	6 (27%)	26,36,36	2.29	10 (38%)
3	BS0	A	303	-	25,27,27	2.63	6 (24%)	30,37,37	3.04	13 (43%)

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	BS0	C	303	-	-	1/7/18/18	0/4/4/4
4	BQU	B	303	2	-	2/10/14/14	0/3/3/3
3	BS0	A	303	-	-	0/7/18/18	0/4/4/4

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	303	BS0	CAN-CAK	-9.13	1.34	1.48
3	A	303	BS0	CAN-CAK	-7.71	1.36	1.48
4	B	303	BQU	CAH-CAI	6.10	1.58	1.50
3	A	303	BS0	CAT-CAR	-6.01	1.40	1.51
3	C	303	BS0	CAS-CAR	5.58	1.47	1.40
3	C	303	BS0	CAT-CAR	-5.29	1.42	1.51
3	A	303	BS0	CAS-CAR	5.27	1.46	1.40
4	B	303	BQU	CAB-CAC	4.67	1.48	1.38
3	C	303	BS0	CAQ-CAS	-4.43	1.32	1.39
3	A	303	BS0	CAQ-CAS	-3.76	1.33	1.39
4	B	303	BQU	CAF-CAE	3.49	1.46	1.38
4	B	303	BQU	CAU-CAR	-3.34	1.45	1.51
3	A	303	BS0	CAH-CAI	3.29	1.54	1.50
4	B	303	BQU	CAA-CAB	2.70	1.45	1.38
3	C	303	BS0	CAU-CAW	-2.67	1.43	1.50
3	A	303	BS0	CAS-NAV	-2.37	1.35	1.39
4	B	303	BQU	CAN-CAL	-2.25	1.45	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	303	BS0	CAI-SAJ	-2.18	1.66	1.73
3	C	303	BS0	CAE-CAF	-2.07	1.34	1.38

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	303	BS0	CAU-CAW-NAV	-6.92	111.08	116.24
3	C	303	BS0	CAC-CAD-CAE	6.74	130.46	120.19
3	C	303	BS0	CAL-CAK-CAN	-6.59	120.28	129.44
3	C	303	BS0	CAU-CAW-NAV	-6.18	111.64	116.24
3	C	303	BS0	CAT-CAR-CAP	5.78	131.50	119.91
3	A	303	BS0	CAC-CAB-CAA	-5.52	111.78	120.19
3	A	303	BS0	CAT-CAR-CAP	5.43	130.78	119.91
3	A	303	BS0	CAT-CAR-CAS	-5.25	113.72	118.55
3	A	303	BS0	CAD-CAC-CAB	5.20	129.59	119.93
3	C	303	BS0	CAB-CAA-CAF	5.16	127.23	118.96
3	C	303	BS0	CAK-CAL-SAJ	-5.04	105.61	111.79
3	C	303	BS0	CAR-CAS-NAV	-5.03	115.10	119.11
3	C	303	BS0	CAP-CAR-CAS	-4.95	114.34	118.54
3	C	303	BS0	CAT-CAR-CAS	-4.78	114.14	118.55
4	B	303	BQU	CAK-CAL-CAN	-4.78	122.79	129.44
3	C	303	BS0	CAD-CAC-CAB	-4.78	111.05	119.93
4	B	303	BQU	CAP-CAO-CAN	-4.54	114.59	121.13
3	A	303	BS0	CAL-CAK-CAN	-4.45	123.25	129.44
4	B	303	BQU	CAR-CAQ-NAT	4.31	125.39	120.80
3	C	303	BS0	CAE-CAF-CAA	-4.11	113.85	120.18
4	B	303	BQU	CAP-CAQ-NAT	-3.70	112.96	120.13
3	A	303	BS0	CAP-CAR-CAS	-3.61	115.48	118.54
3	A	303	BS0	CAN-CAK-NAM	3.54	126.74	120.78
3	A	303	BS0	CAO-CAQ-CAS	3.20	125.83	119.64
3	C	303	BS0	CAO-CAQ-CAS	3.19	125.81	119.64
3	A	303	BS0	CAQ-CAS-CAR	-3.10	116.10	119.76
4	B	303	BQU	CAO-CAN-CAS	3.05	122.48	118.16
3	C	303	BS0	CAS-NAV-CAW	3.01	128.22	124.49
4	B	303	BQU	CAS-CAR-CAQ	-2.84	116.34	118.96
4	B	303	BQU	CAS-CAN-CAL	-2.79	116.55	120.59
4	B	303	BQU	CAA-CAF-CAE	-2.79	115.94	120.19
3	A	303	BS0	CAR-CAS-NAV	-2.75	116.92	119.11
3	C	303	BS0	CAQ-CAO-CAN	-2.72	117.22	121.13
3	A	303	BS0	CAC-CAD-CAE	-2.54	116.32	120.19
4	B	303	BQU	CAP-CAQ-CAR	2.39	121.63	119.12
3	C	303	BS0	OAX-CAW-CAU	2.33	127.15	122.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	303	BS0	OAG-CAF-CAE	2.30	131.25	119.94
3	C	303	BS0	CAN-CAK-NAM	2.25	124.56	120.78
4	B	303	BQU	CAV-CAU-CAR	-2.20	109.25	112.81
3	A	303	BS0	CAB-CAA-CAF	2.14	122.39	118.96

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	303	BQU	CAC-CAD-OAG-CAH
4	B	303	BQU	CAE-CAD-OAG-CAH
3	C	303	BS0	CAA-CAF-OAG-CAH

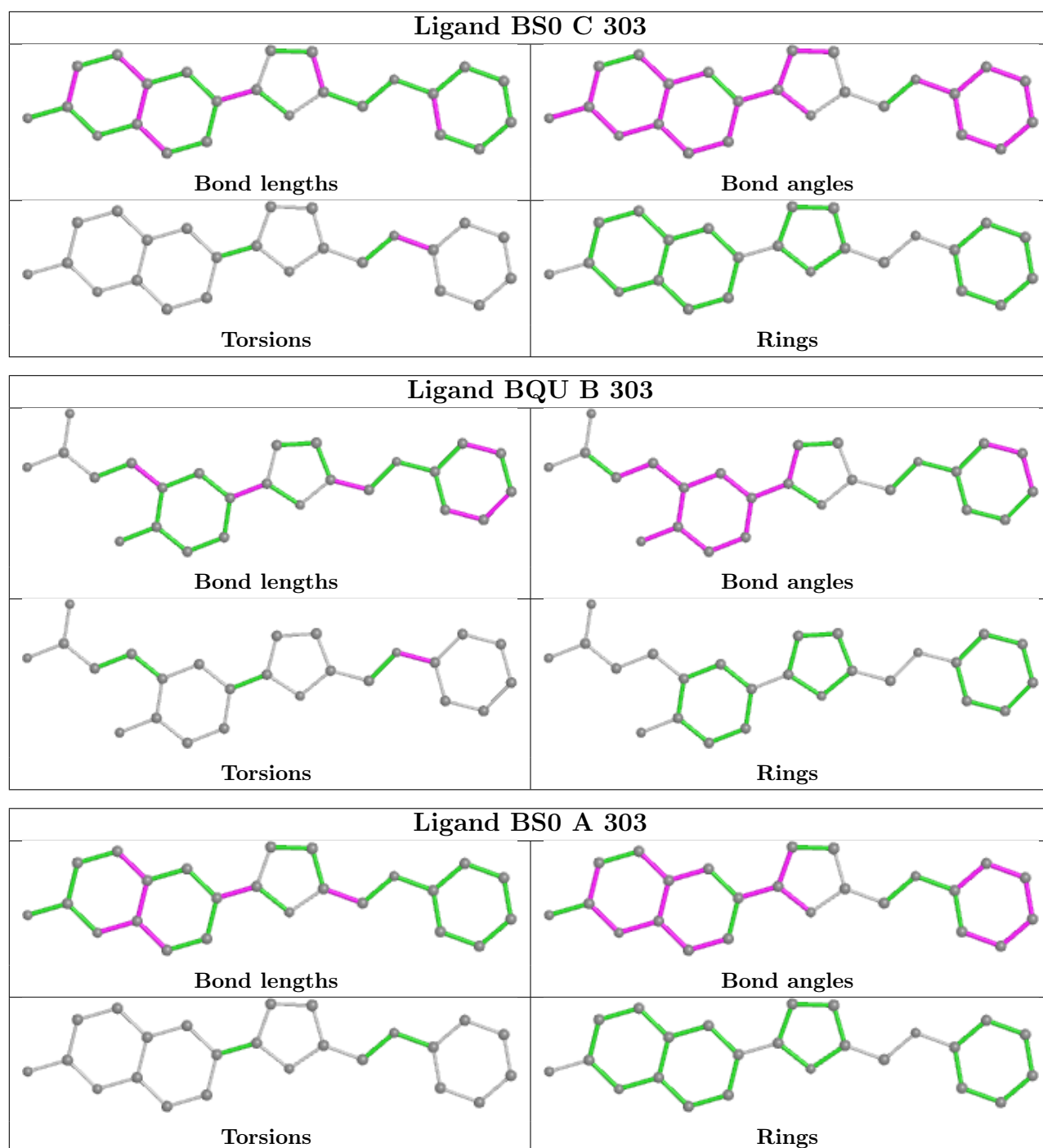
There are no ring outliers.

3 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	303	BS0	13	0
4	B	303	BQU	18	0
3	A	303	BS0	12	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

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	227/228 (99%)	0.29	10 (4%) 34 33	16, 25, 43, 80	0
1	B	220/228 (96%)	0.20	5 (2%) 60 59	18, 31, 49, 69	0
1	C	228/228 (100%)	0.37	14 (6%) 21 20	19, 30, 53, 74	0
1	D	220/228 (96%)	1.00	33 (15%) 2 2	26, 44, 70, 89	0
All	All	895/912 (98%)	0.46	62 (6%) 16 16	16, 32, 61, 89	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	29	VAL	8.5
1	D	33	GLY	7.5
1	D	32	TRP	7.0
1	D	227	PRO	6.3
1	D	72	TYR	6.3
1	C	227	PRO	6.1
1	C	32	TRP	5.9
1	D	225	LYS	5.7
1	D	177	ILE	5.7
1	D	66	TRP	5.6
1	D	221	LEU	5.2
1	D	226	LYS	4.9
1	D	222	ASN	4.8
1	D	30	ASN	4.7
1	C	7	SER	4.5
1	D	224	SER	4.5
1	C	8	LEU	4.4
1	A	227	PRO	4.4
1	B	225	LYS	4.3
1	D	31	GLY	4.3
1	D	68	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	31	GLY	4.2
1	D	223	GLU	4.1
1	B	226	LYS	3.9
1	D	46	ALA	3.9
1	D	8	LEU	3.8
1	D	128	TRP	3.8
1	D	172	LEU	3.7
1	A	177	ILE	3.5
1	A	226	LYS	3.5
1	C	2	PRO	3.4
1	C	228	SER	3.3
1	C	1	GLY	3.2
1	D	131	LYS	3.1
1	D	153	PRO	3.0
1	D	178	GLU	3.0
1	D	45	ASN	2.9
1	C	28	GLU	2.9
1	A	224	SER	2.9
1	D	43	LEU	2.8
1	B	177	ILE	2.7
1	D	28	GLU	2.7
1	D	10	ASP	2.5
1	C	69	GLU	2.5
1	D	44	VAL	2.5
1	B	7	SER	2.5
1	A	198	VAL	2.4
1	A	128	TRP	2.4
1	A	203	GLU	2.3
1	D	69	GLU	2.3
1	A	225	LYS	2.3
1	B	224	SER	2.3
1	D	34	VAL	2.2
1	C	97	SER	2.2
1	D	70	ARG	2.2
1	A	223	GLU	2.1
1	C	30	ASN	2.1
1	D	21	TYR	2.1
1	A	78	ILE	2.1
1	C	45	ASN	2.1
1	C	224	SER	2.0
1	D	179	ALA	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

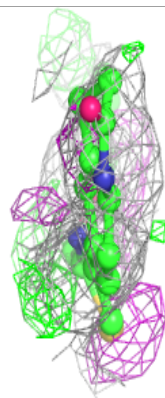
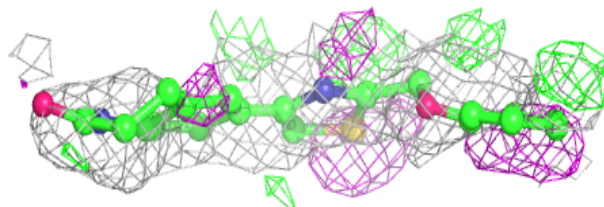
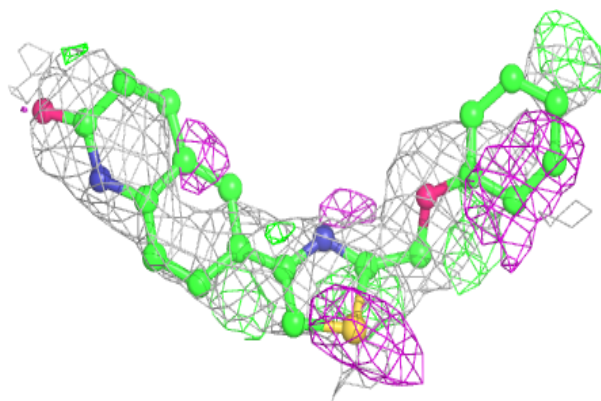
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	BS0	C	303	24/24	0.65	0.36	40,55,61,78	0
3	BS0	A	303	24/24	0.66	0.53	39,49,55,60	0
4	BQU	B	303	25/25	0.78	0.61	29,57,65,76	0
2	ZN	B	302	1/1	0.92	0.10	28,28,28,28	0
2	ZN	D	301	1/1	0.96	0.06	42,42,42,42	0
2	ZN	D	302	1/1	0.98	0.06	37,37,37,37	0
2	ZN	B	301	1/1	0.98	0.12	32,32,32,32	0
2	ZN	C	301	1/1	0.99	0.08	26,26,26,26	0
2	ZN	C	302	1/1	1.00	0.07	22,22,22,22	0
2	ZN	A	302	1/1	1.00	0.11	25,25,25,25	0
2	ZN	A	301	1/1	1.00	0.11	22,22,22,22	0

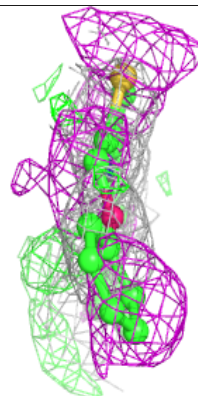
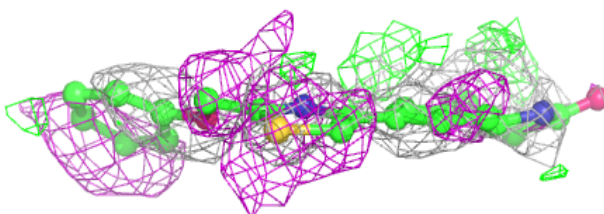
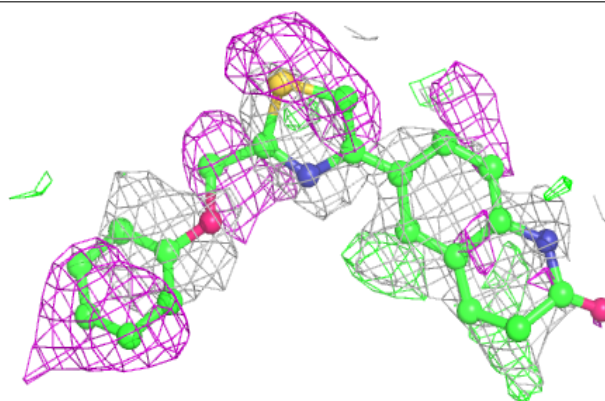
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

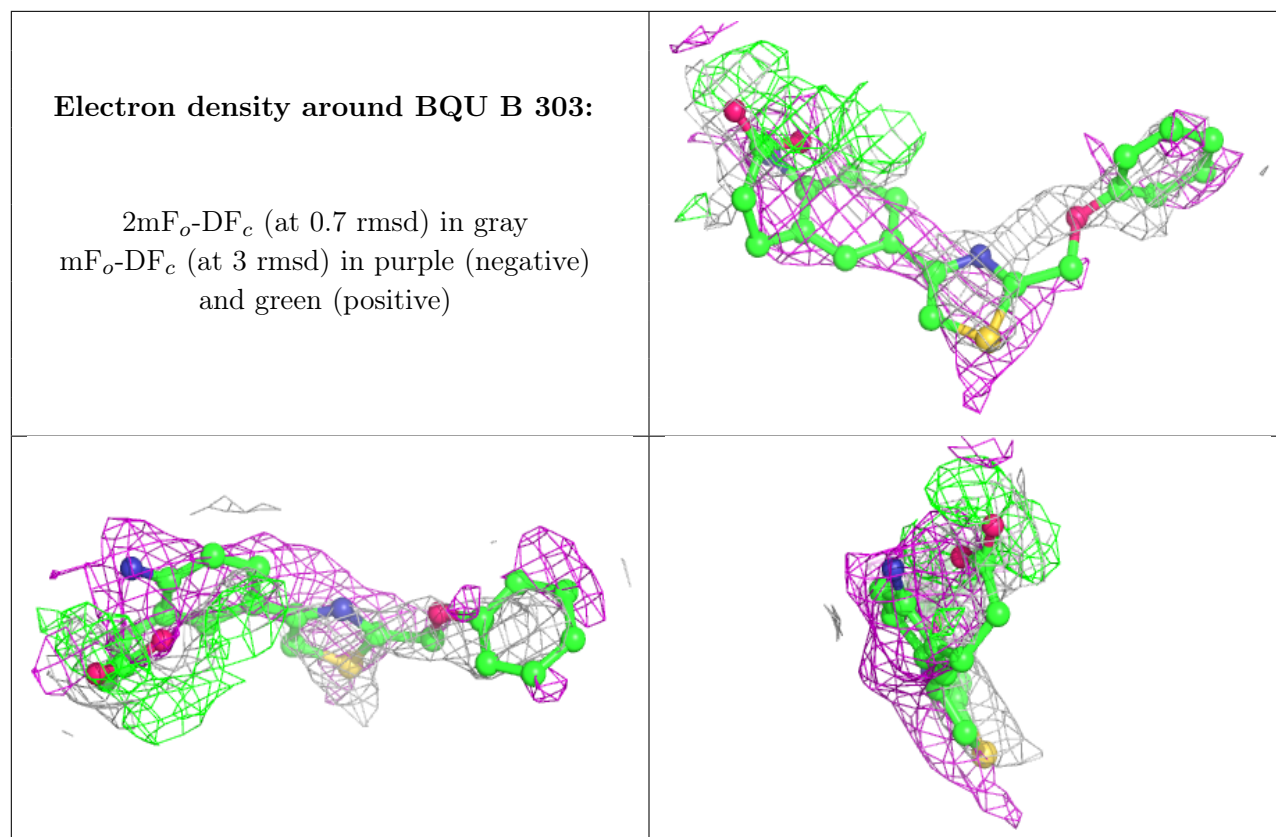
**Electron density around BS0 C 303:**

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

**Electron density around BS0 A 303:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.