



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:07 PM UTC

PDB ID : 8GPW / pdb_00008gpw
Title : Structure of Penicillin-binding protein 3 (PBP3) from *Klebsiella pneumoniae* with ligand 18G
Authors : Song, D.Q.; Li, Y.H.
Deposited on : 2022-08-27
Resolution : 2.06 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

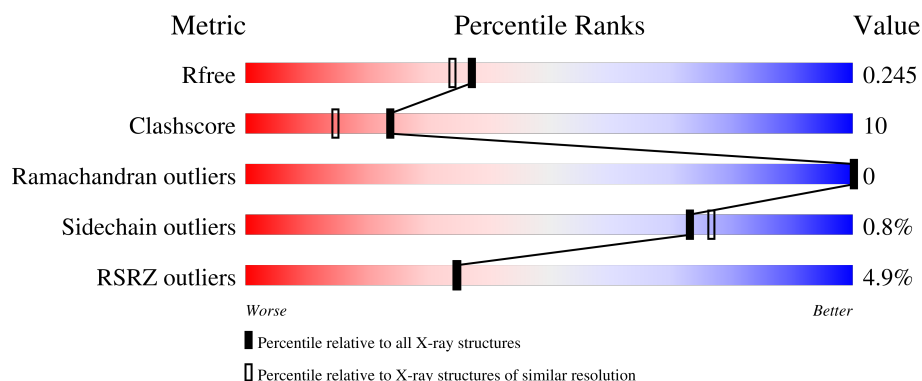
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.06 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	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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	410	4% 84% 12% .
1	B	410	6% 76% 20% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6240 atoms, of which 32 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 Peptidoglycan D,D-transpeptidase FtsI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	399	Total	C	N	O	S	0	0	0
			3005	1903	529	562	11			
1	B	395	Total	C	N	O	S	0	0	0
			2979	1888	523	557	11			

There are 94 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	68	SER	-	expression tag	UNP A0A483LPP8
A	69	THR	-	expression tag	UNP A0A483LPP8
A	70	SER	-	expression tag	UNP A0A483LPP8
A	71	ARG	-	expression tag	UNP A0A483LPP8
A	72	GLY	-	expression tag	UNP A0A483LPP8
A	73	MET	-	expression tag	UNP A0A483LPP8
A	74	ILE	-	expression tag	UNP A0A483LPP8
A	75	THR	-	expression tag	UNP A0A483LPP8
A	76	ASP	-	expression tag	UNP A0A483LPP8
A	77	ARG	-	expression tag	UNP A0A483LPP8
A	78	SER	-	expression tag	UNP A0A483LPP8
A	79	GLY	-	expression tag	UNP A0A483LPP8
A	80	ARG	-	expression tag	UNP A0A483LPP8
A	81	PRO	-	expression tag	UNP A0A483LPP8
A	82	LEU	-	expression tag	UNP A0A483LPP8
A	83	ALA	-	expression tag	UNP A0A483LPP8
A	84	VAL	-	expression tag	UNP A0A483LPP8
A	85	SER	-	expression tag	UNP A0A483LPP8
A	86	VAL	-	expression tag	UNP A0A483LPP8
A	87	PRO	-	expression tag	UNP A0A483LPP8
A	160	VAL	-	expression tag	UNP A0A483LPP8
A	161	GLY	-	expression tag	UNP A0A483LPP8
A	162	GLY	-	expression tag	UNP A0A483LPP8
A	163	GLY	-	expression tag	UNP A0A483LPP8
A	225	GLY	PRO	conflict	UNP A0A483LPP8

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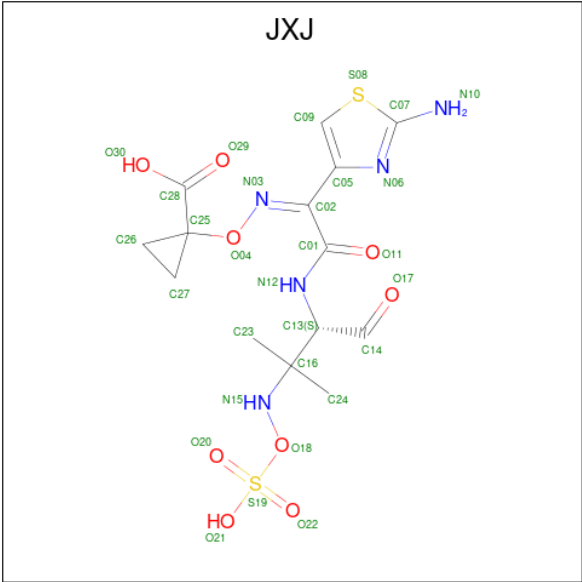
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLU	deletion	UNP A0A483LPP8
A	?	-	ARG	deletion	UNP A0A483LPP8
A	?	-	ILE	deletion	UNP A0A483LPP8
A	?	-	VAL	deletion	UNP A0A483LPP8
A	?	-	ARG	deletion	UNP A0A483LPP8
A	?	-	LYS	deletion	UNP A0A483LPP8
A	?	-	ASP	deletion	UNP A0A483LPP8
A	?	-	ARG	deletion	UNP A0A483LPP8
A	?	-	TYR	deletion	UNP A0A483LPP8
A	?	-	GLY	deletion	UNP A0A483LPP8
A	?	-	ARG	deletion	UNP A0A483LPP8
A	?	-	VAL	deletion	UNP A0A483LPP8
A	?	-	ILE	deletion	UNP A0A483LPP8
A	?	-	GLU	deletion	UNP A0A483LPP8
A	?	-	ASP	deletion	UNP A0A483LPP8
A	?	-	ILE	deletion	UNP A0A483LPP8
A	?	-	SER	deletion	UNP A0A483LPP8
A	?	-	SER	deletion	UNP A0A483LPP8
A	?	-	THR	deletion	UNP A0A483LPP8
A	?	-	ASP	deletion	UNP A0A483LPP8
A	?	-	SER	deletion	UNP A0A483LPP8
A	227	GLY	GLN	conflict	UNP A0A483LPP8
B	68	SER	-	expression tag	UNP A0A483LPP8
B	69	THR	-	expression tag	UNP A0A483LPP8
B	70	SER	-	expression tag	UNP A0A483LPP8
B	71	ARG	-	expression tag	UNP A0A483LPP8
B	72	GLY	-	expression tag	UNP A0A483LPP8
B	73	MET	-	expression tag	UNP A0A483LPP8
B	74	ILE	-	expression tag	UNP A0A483LPP8
B	75	THR	-	expression tag	UNP A0A483LPP8
B	76	ASP	-	expression tag	UNP A0A483LPP8
B	77	ARG	-	expression tag	UNP A0A483LPP8
B	78	SER	-	expression tag	UNP A0A483LPP8
B	79	GLY	-	expression tag	UNP A0A483LPP8
B	80	ARG	-	expression tag	UNP A0A483LPP8
B	81	PRO	-	expression tag	UNP A0A483LPP8
B	82	LEU	-	expression tag	UNP A0A483LPP8
B	83	ALA	-	expression tag	UNP A0A483LPP8
B	84	VAL	-	expression tag	UNP A0A483LPP8
B	85	SER	-	expression tag	UNP A0A483LPP8
B	86	VAL	-	expression tag	UNP A0A483LPP8
B	87	PRO	-	expression tag	UNP A0A483LPP8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	160	VAL	-	expression tag	UNP A0A483LPP8
B	161	GLY	-	expression tag	UNP A0A483LPP8
B	162	GLY	-	expression tag	UNP A0A483LPP8
B	163	GLY	-	expression tag	UNP A0A483LPP8
B	204	GLY	PRO	conflict	UNP A0A483LPP8
B	?	-	GLU	deletion	UNP A0A483LPP8
B	?	-	ARG	deletion	UNP A0A483LPP8
B	?	-	ILE	deletion	UNP A0A483LPP8
B	?	-	VAL	deletion	UNP A0A483LPP8
B	?	-	ARG	deletion	UNP A0A483LPP8
B	?	-	LYS	deletion	UNP A0A483LPP8
B	?	-	ASP	deletion	UNP A0A483LPP8
B	?	-	ARG	deletion	UNP A0A483LPP8
B	?	-	TYR	deletion	UNP A0A483LPP8
B	?	-	GLY	deletion	UNP A0A483LPP8
B	?	-	ARG	deletion	UNP A0A483LPP8
B	?	-	VAL	deletion	UNP A0A483LPP8
B	?	-	ILE	deletion	UNP A0A483LPP8
B	?	-	GLU	deletion	UNP A0A483LPP8
B	?	-	ASP	deletion	UNP A0A483LPP8
B	?	-	ILE	deletion	UNP A0A483LPP8
B	?	-	SER	deletion	UNP A0A483LPP8
B	?	-	SER	deletion	UNP A0A483LPP8
B	?	-	THR	deletion	UNP A0A483LPP8
B	?	-	ASP	deletion	UNP A0A483LPP8
B	?	-	SER	deletion	UNP A0A483LPP8
B	227	GLY	GLN	conflict	UNP A0A483LPP8

- Molecule 2 is 1-[({Z})-[1-(2-azanyl-1,3-thiazol-4-yl)-2-[(2 {S})-3-methyl-1-oxidanylidene-3-(sulfooxyamino)butan-2-yl]amino]-2-oxidanylidene-ethylidene]amino]oxycyclopropane-1-carboxylic acid (CCD ID: JXJ) (formula: C₁₄H₁₉N₅O₉S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	S	0	0
			46	14	16	5	9	2		
2	B	1	Total	C	H	N	O	S	0	0
			46	14	16	5	9	2		

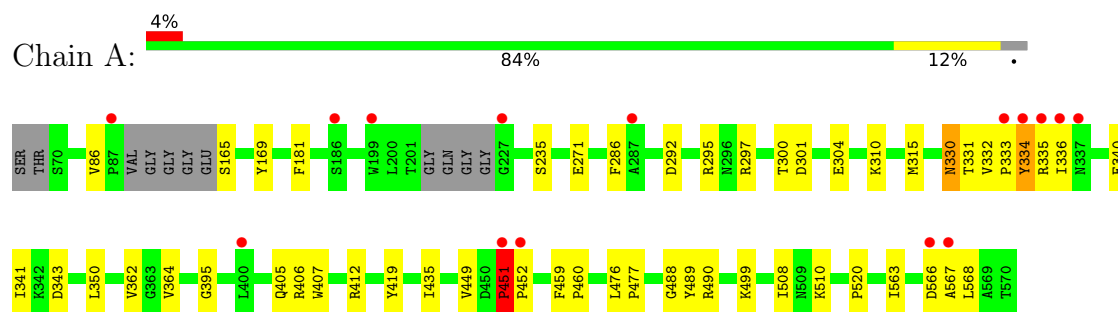
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	101	Total	O	0	0
			101	101		
3	B	63	Total	O	0	0
			63	63		

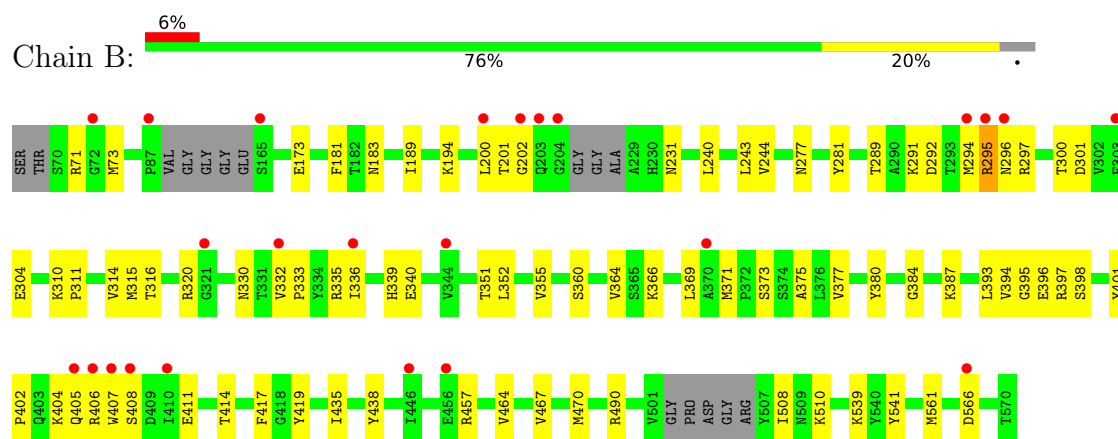
3 Residue-property plots [i](#)

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: Peptidoglycan D,D-transpeptidase FtsI



- Molecule 1: Peptidoglycan D,D-transpeptidase FtsI



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	95.40Å 103.66Å 80.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.54 – 2.06 43.54 – 2.06	Depositor EDS
% Data completeness (in resolution range)	99.3 (43.54-2.06) 99.3 (43.54-2.06)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.06Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.200 , 0.236 0.211 , 0.245	Depositor DCC
R_{free} test set	2000 reflections (4.01%)	wwPDB-VP
Wilson B-factor (Å ²)	38.7	Xtriage
Anisotropy	0.480	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6240	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: JXJ

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	0.42	1/3063 (0.0%)	0.64	1/4159 (0.0%)
1	B	0.35	0/3035	0.62	0/4119
All	All	0.38	1/6098 (0.0%)	0.63	1/8278 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	451	PRO	CA-C	-7.23	1.45	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	451	PRO	N-CA-C	12.87	126.40	110.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3005	0	3046	48	0
1	B	2979	0	3021	74	3
2	A	30	16	0	1	0
2	B	30	16	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	101	0	0	2	0
3	B	63	0	0	4	0
All	All	6208	32	6067	122	3

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 10.

All (122) 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:404:LYS:NZ	1:B:411:GLU:OE1	1.89	1.04
1:A:304:GLU:OE1	2:A:601:JXJ:N10	1.99	0.96
1:A:490:ARG:N	1:A:566:ASP:OD1	2.01	0.92
1:B:183:ASN:HD21	1:B:189:ILE:HG21	1.34	0.90
1:B:73:MET:H	1:B:231:ASN:HD22	1.20	0.88
1:A:520:PRO:HB3	1:A:566:ASP:OD2	1.79	0.83
1:A:335:ARG:HG2	1:A:340:GLU:HA	1.58	0.82
1:B:277:ASN:ND2	1:B:296:ASN:OD1	2.14	0.80
1:A:520:PRO:CB	1:A:566:ASP:OD2	2.29	0.80
1:A:335:ARG:HD3	1:A:340:GLU:HB2	1.68	0.76
1:B:292:ASP:OD1	1:B:295:ARG:NE	2.18	0.76
1:B:404:LYS:CE	1:B:411:GLU:OE1	2.35	0.74
1:A:405:GLN:H	1:A:405:GLN:CD	1.96	0.74
1:B:539:LYS:HZ2	1:B:541:TYR:HB2	1.53	0.73
1:B:291:LYS:HA	1:B:294:MET:HE2	1.74	0.69
1:B:384:GLY:HA2	1:B:387:LYS:HD3	1.75	0.69
1:B:508:ILE:HD12	1:B:510:LYS:HD2	1.75	0.68
1:A:334:TYR:CE1	1:A:341:ILE:HB	2.28	0.68
1:A:330:ASN:ND2	1:A:332:VAL:HG23	2.09	0.66
1:A:330:ASN:C	1:A:330:ASN:HD22	2.04	0.66
1:A:489:TYR:HA	1:A:566:ASP:OD1	1.95	0.66
1:B:539:LYS:NZ	1:B:541:TYR:HB2	2.11	0.65
1:B:336:ILE:HD11	1:B:369:LEU:HD11	1.78	0.65
1:B:183:ASN:HD21	1:B:189:ILE:CG2	2.10	0.64
1:A:520:PRO:HB2	1:A:566:ASP:OD2	1.99	0.62
1:A:271:GLU:CD	1:A:449:VAL:HG22	2.24	0.62
1:B:352:LEU:HG	1:B:470:MET:HE1	1.82	0.61
1:B:404:LYS:HE3	1:B:411:GLU:OE1	2.01	0.61
1:B:311:PRO:O	1:B:315:MET:HG3	2.01	0.60
1:B:296:ASN:O	1:B:300:THR:OG1	2.13	0.59
1:A:488:GLY:HA2	1:A:567:ALA:HB3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:THR:HG22	1:B:395:GLY:O	2.03	0.59
1:B:402:PRO:HB2	1:B:407:TRP:CZ2	2.38	0.58
1:B:71:ARG:NH2	1:B:200:LEU:HD12	2.18	0.58
1:B:183:ASN:ND2	1:B:189:ILE:HG21	2.14	0.56
1:A:292:ASP:OD1	1:A:295:ARG:NH1	2.39	0.55
1:B:332:VAL:HG12	1:B:333:PRO:HD2	1.88	0.55
1:A:330:ASN:HD21	1:A:332:VAL:HG23	1.72	0.55
1:B:202:GLY:HA2	3:B:731:HOH:O	2.07	0.54
1:B:183:ASN:ND2	1:B:189:ILE:HD13	2.23	0.54
1:B:380:TYR:HB2	1:B:401:TYR:OH	2.08	0.54
1:A:235:SER:HB2	1:A:271:GLU:HB3	1.90	0.54
1:B:304:GLU:OE1	2:B:601:JXJ:N10	2.41	0.53
1:B:201:THR:O	1:B:201:THR:HG22	2.09	0.53
1:A:330:ASN:ND2	1:A:332:VAL:H	2.06	0.52
1:A:330:ASN:ND2	1:A:330:ASN:C	2.66	0.52
1:A:488:GLY:C	1:A:567:ALA:HB2	2.35	0.52
1:B:360:SER:O	1:B:364:VAL:HG22	2.10	0.51
1:B:490:ARG:H	1:B:566:ASP:HB3	1.75	0.51
1:A:520:PRO:HG3	1:A:563:ILE:HG21	1.92	0.51
1:A:508:ILE:HD12	1:A:510:LYS:HD2	1.92	0.51
1:B:438:TYR:HA	1:B:464:VAL:HG11	1.92	0.51
1:B:281:TYR:OH	3:B:701:HOH:O	2.20	0.51
1:B:335:ARG:HG2	1:B:340:GLU:HA	1.93	0.50
1:B:351:THR:O	1:B:355:VAL:HG23	2.10	0.50
1:B:373:SER:O	1:B:377:VAL:HG23	2.10	0.50
1:B:316:THR:HG22	1:B:371:MET:SD	2.51	0.50
1:B:438:TYR:HA	1:B:464:VAL:CG1	2.41	0.50
1:A:419:TYR:OH	1:A:499:LYS:HE2	2.12	0.49
1:B:397:ARG:HE	1:B:398:SER:H	1.60	0.49
1:A:451:PRO:HB2	1:A:452:PRO:HD3	1.95	0.49
1:A:334:TYR:HE1	1:A:341:ILE:HB	1.73	0.49
1:B:310:LYS:HE2	1:B:417:PHE:HB3	1.95	0.49
1:B:335:ARG:HA	1:B:339:HIS:O	2.12	0.49
1:A:315:MET:HE1	1:A:435:ILE:HG12	1.95	0.49
1:B:332:VAL:CG1	1:B:333:PRO:HD2	2.43	0.48
1:B:405:GLN:HG3	1:B:406:ARG:N	2.28	0.48
1:B:320:ARG:NH2	1:B:375:ALA:HA	2.28	0.48
1:B:457:ARG:HG3	1:B:457:ARG:HH11	1.78	0.48
1:A:459:PHE:CD2	1:A:460:PRO:HD2	2.49	0.47
1:B:397:ARG:NE	1:B:398:SER:H	2.12	0.47
1:A:488:GLY:C	1:A:567:ALA:CB	2.86	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:LYS:HE3	1:B:394:VAL:HG11	1.96	0.47
1:A:300:THR:HG22	1:A:395:GLY:O	2.15	0.47
1:B:404:LYS:NZ	1:B:411:GLU:HB3	2.30	0.47
1:B:402:PRO:HB2	1:B:407:TRP:HZ2	1.80	0.46
1:A:286:PHE:O	1:A:286:PHE:CD2	2.69	0.46
1:B:297:ARG:O	1:B:301:ASP:HB2	2.15	0.46
1:A:336:ILE:O	1:A:336:ILE:HG13	2.15	0.45
1:A:310:LYS:HE2	1:A:364:VAL:HG21	1.98	0.45
1:B:414:THR:HB	1:B:419:TYR:HB2	1.98	0.45
1:B:73:MET:H	1:B:231:ASN:ND2	2.01	0.45
1:A:343:ASP:OD1	1:A:362:VAL:HG23	2.17	0.45
1:B:240:LEU:O	1:B:244:VAL:HG23	2.16	0.44
1:A:331:THR:HG21	1:A:350:LEU:HD12	1.98	0.44
1:B:314:VAL:HG11	1:B:470:MET:HE1	1.99	0.44
1:B:405:GLN:CG	1:B:406:ARG:N	2.81	0.44
1:A:86:VAL:O	1:A:165:SER:HB2	2.18	0.44
1:A:333:PRO:HG3	3:A:722:HOH:O	2.17	0.44
1:A:169:TYR:OH	1:A:181:PHE:HA	2.18	0.43
1:A:334:TYR:CD1	1:A:334:TYR:O	2.71	0.43
1:B:292:ASP:OD1	1:B:295:ARG:CZ	2.66	0.43
1:B:408:SER:HB2	1:B:411:GLU:HG3	2.01	0.43
1:A:334:TYR:CD1	1:A:334:TYR:C	2.97	0.43
1:A:405:GLN:CD	1:A:405:GLN:N	2.71	0.43
1:B:243:LEU:C	1:B:243:LEU:HD12	2.43	0.43
1:B:315:MET:HE1	1:B:435:ILE:HG12	2.00	0.43
1:B:369:LEU:HD23	1:B:369:LEU:HA	1.83	0.42
1:B:393:LEU:O	1:B:396:GLU:HB2	2.20	0.42
1:A:292:ASP:CG	1:A:295:ARG:HH12	2.26	0.42
1:B:295:ARG:O	1:B:295:ARG:HG2	2.19	0.42
1:B:373:SER:CB	1:B:407:TRP:HB2	2.49	0.42
1:A:476:LEU:O	1:A:477:PRO:C	2.60	0.42
1:B:352:LEU:C	1:B:470:MET:HE3	2.44	0.42
1:B:457:ARG:HG3	1:B:457:ARG:NH1	2.35	0.42
1:A:489:TYR:CA	1:A:566:ASP:OD1	2.66	0.41
1:B:315:MET:HG2	1:B:467:VAL:HG21	2.02	0.41
1:B:330:ASN:O	1:B:366:LYS:HE3	2.20	0.41
1:B:281:TYR:CB	1:B:289:THR:HG21	2.51	0.41
1:B:281:TYR:HB3	1:B:289:THR:HG21	2.02	0.41
1:B:352:LEU:HD12	1:B:352:LEU:HA	1.77	0.41
1:B:539:LYS:HD2	1:B:539:LYS:HA	1.44	0.41
1:A:297:ARG:HG3	3:A:707:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:ARG:HD3	1:A:301:ASP:OD2	2.21	0.41
1:A:334:TYR:HE1	1:A:341:ILE:CB	2.34	0.41
1:B:183:ASN:ND2	1:B:189:ILE:CG2	2.79	0.40
1:A:407:TRP:HB3	1:A:412:ARG:HG3	2.03	0.40
1:B:202:GLY:CA	3:B:731:HOH:O	2.68	0.40
1:B:173:GLU:OE1	1:B:173:GLU:N	2.39	0.40
1:B:561:MET:HE1	3:B:737:HOH:O	2.21	0.40
1:A:405:GLN:HG2	1:A:406:ARG:N	2.36	0.40
1:B:181:PHE:HE1	1:B:189:ILE:HD11	1.86	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:405:GLN:NE2	1:B:411:GLU:OE1[2_655]	1.25	0.95
1:B:405:GLN:NE2	1:B:411:GLU:CD[2_655]	1.58	0.62
1:B:405:GLN:NE2	1:B:411:GLU:OE2[2_655]	2.04	0.16

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	393/410 (96%)	384 (98%)	9 (2%)	0	100	100
1	B	387/410 (94%)	376 (97%)	11 (3%)	0	100	100
All	All	780/820 (95%)	760 (97%)	20 (3%)	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	319/324 (98%)	315 (99%)	4 (1%)	61	62
1	B	317/324 (98%)	316 (100%)	1 (0%)	86	89
All	All	636/648 (98%)	631 (99%)	5 (1%)	73	77

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	330	ASN
1	A	334	TYR
1	A	451	PRO
1	A	568	LEU
1	B	295	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	249	ASN
1	A	330	ASN
1	A	357	GLN
1	B	183	ASN
1	B	230	HIS
1	B	231	ASN
1	B	319	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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
2	JXJ	A	601	1	25,31,31	4.31	12 (48%)	28,47,47	7.18	9 (32%)
2	JXJ	B	601	1	25,31,31	4.66	13 (52%)	28,47,47	7.91	5 (17%)

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
2	JXJ	A	601	1	-	5/24/43/43	0/2/2/2
2	JXJ	B	601	1	-	5/24/43/43	0/2/2/2

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	JXJ	C07-S08	-13.10	1.56	1.74
2	A	601	JXJ	C07-S08	-12.01	1.58	1.74
2	B	601	JXJ	C05-N06	8.71	1.57	1.38
2	A	601	JXJ	C05-N06	7.99	1.55	1.38
2	B	601	JXJ	C09-S08	-7.44	1.53	1.71
2	A	601	JXJ	C09-S08	-7.36	1.53	1.71
2	B	601	JXJ	C07-N06	7.33	1.42	1.31
2	A	601	JXJ	C07-N06	6.91	1.41	1.31
2	B	601	JXJ	C01-N12	6.48	1.47	1.34
2	B	601	JXJ	C07-N10	5.99	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	JXJ	C01-N12	5.87	1.46	1.34
2	A	601	JXJ	C07-N10	5.38	1.45	1.34
2	B	601	JXJ	C09-C05	5.19	1.45	1.36
2	A	601	JXJ	C09-C05	4.83	1.45	1.36
2	B	601	JXJ	C02-C05	4.29	1.54	1.46
2	A	601	JXJ	C27-C25	3.77	1.55	1.50
2	A	601	JXJ	C26-C25	3.44	1.55	1.50
2	A	601	JXJ	C02-C05	3.43	1.53	1.46
2	B	601	JXJ	C02-C01	3.42	1.55	1.48
2	B	601	JXJ	C26-C25	3.06	1.54	1.50
2	B	601	JXJ	C24-C16	2.96	1.56	1.53
2	B	601	JXJ	C27-C25	2.86	1.54	1.50
2	B	601	JXJ	C23-C16	2.68	1.55	1.53
2	A	601	JXJ	O11-C01	-2.49	1.18	1.23
2	A	601	JXJ	C02-C01	2.37	1.53	1.48

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	JXJ	C09-S08-C07	39.83	106.00	88.84
2	A	601	JXJ	C09-S08-C07	36.00	104.36	88.84
2	B	601	JXJ	S08-C07-N06	-6.97	109.04	114.54
2	A	601	JXJ	S08-C07-N10	6.86	128.97	120.99
2	B	601	JXJ	O04-N03-C02	5.56	120.43	111.76
2	B	601	JXJ	S08-C07-N10	5.51	127.40	120.99
2	A	601	JXJ	S08-C07-N06	-5.23	110.42	114.54
2	B	601	JXJ	C09-C05-N06	-5.08	108.44	115.43
2	A	601	JXJ	C09-C05-N06	-3.98	109.95	115.43
2	A	601	JXJ	O04-N03-C02	3.19	116.73	111.76
2	A	601	JXJ	N10-C07-N06	-2.96	120.61	124.05
2	A	601	JXJ	C07-N06-C05	-2.46	106.96	110.57
2	A	601	JXJ	O17-C14-C13	-2.32	117.66	124.21
2	A	601	JXJ	O04-C25-C26	2.18	120.58	115.63

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	JXJ	O04-C25-C28-O29
2	B	601	JXJ	C14-C13-C16-C23
2	B	601	JXJ	C14-C13-C16-C24
2	B	601	JXJ	N12-C13-C16-C23

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Mol	Chain	Res	Type	Atoms
2	B	601	JXJ	N12-C13-C16-C24
2	A	601	JXJ	C27-C25-C28-O30
2	A	601	JXJ	C27-C25-C28-O29
2	A	601	JXJ	N12-C01-C02-N03
2	A	601	JXJ	O11-C01-C02-N03
2	B	601	JXJ	O11-C01-C02-N03

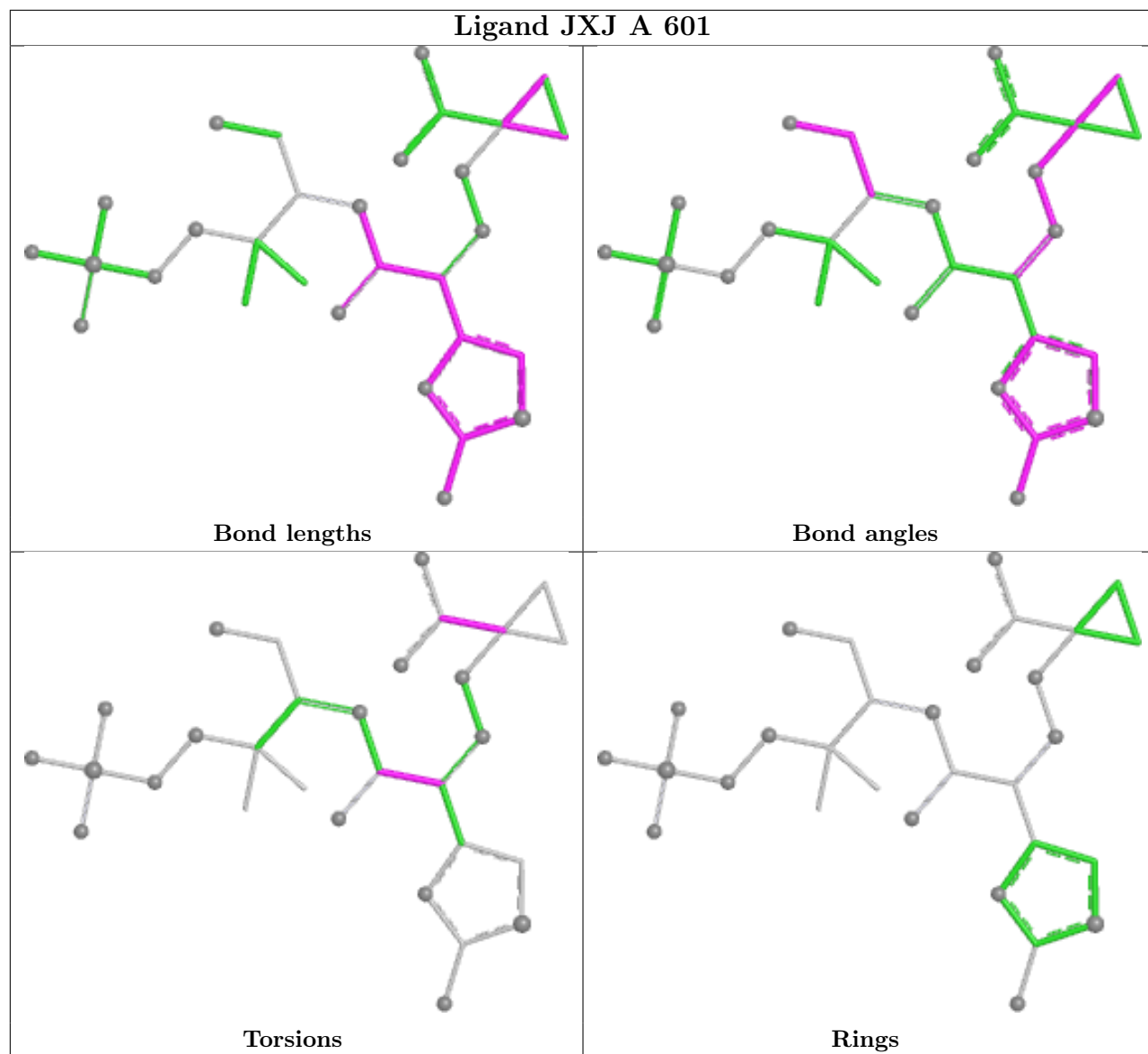
There are no ring outliers.

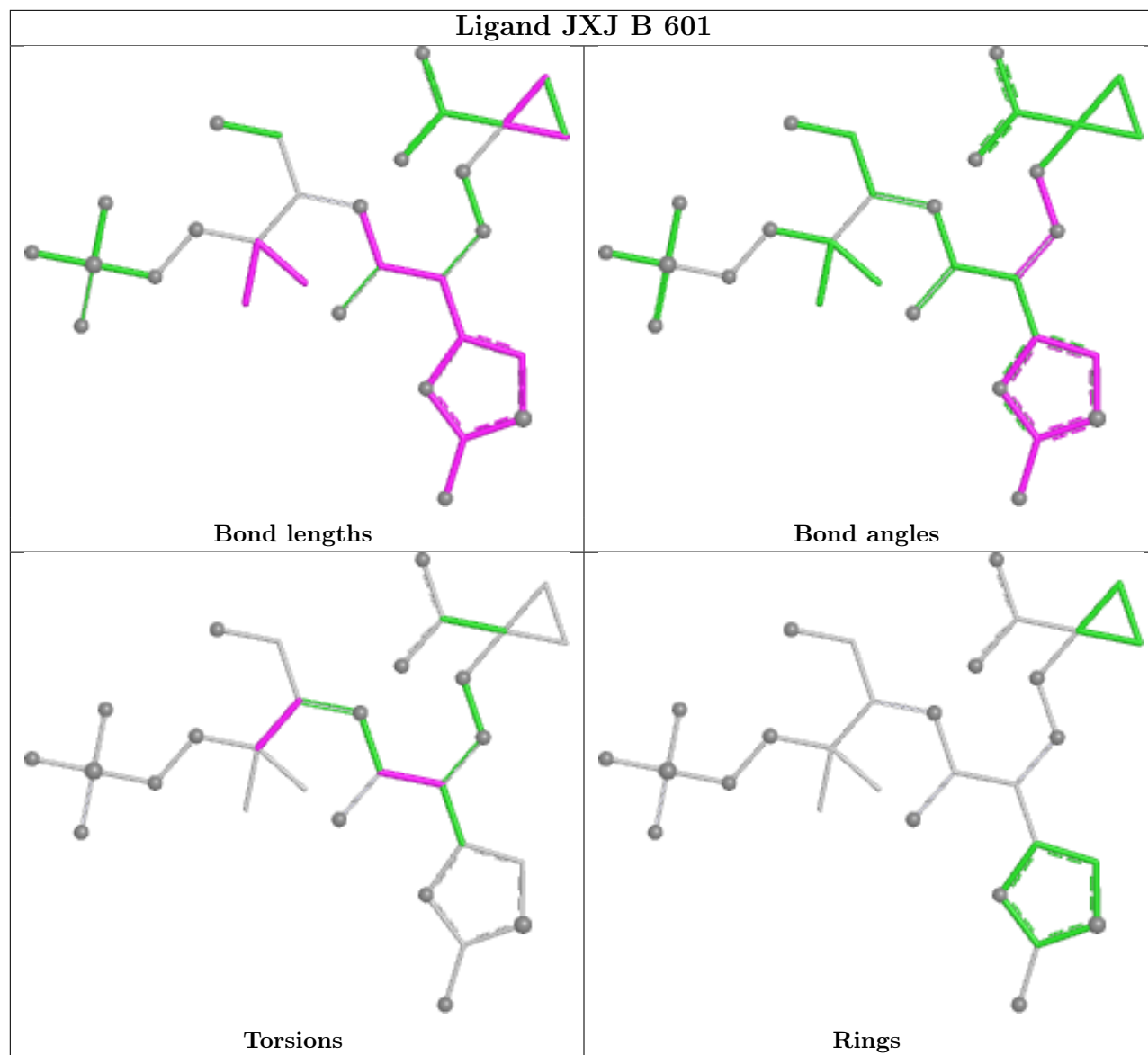
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	JXJ	1	0
2	B	601	JXJ	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.

Ligand JXJ A 601





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	399/410 (97%)	0.06	15 (3%) 44 44	27, 40, 66, 78	0
1	B	395/410 (96%)	0.37	24 (6%) 27 27	28, 48, 82, 108	0
All	All	794/820 (96%)	0.21	39 (4%) 35 35	27, 44, 76, 108	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	204	GLY	7.6
1	B	202	GLY	4.6
1	A	566	ASP	4.5
1	A	567	ALA	4.4
1	A	333	PRO	4.3
1	B	203	GLN	4.2
1	B	295	ARG	4.1
1	B	296	ASN	4.1
1	A	336	ILE	4.1
1	A	227	GLY	4.0
1	A	451	PRO	4.0
1	B	72	GLY	3.9
1	B	407	TRP	3.9
1	A	452	PRO	3.6
1	A	87	PRO	3.6
1	A	334	TYR	3.5
1	A	335	ARG	3.4
1	B	87	PRO	3.4
1	B	200	LEU	3.4
1	B	408	SER	3.2
1	A	287	ALA	3.0
1	A	337	ASN	2.8
1	B	456	GLU	2.6
1	A	186	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	370	ALA	2.5
1	B	446	ILE	2.5
1	B	406	ARG	2.5
1	A	400	LEU	2.5
1	B	336	ILE	2.4
1	B	566	ASP	2.3
1	A	199	TRP	2.3
1	B	165	SER	2.2
1	B	405	GLN	2.2
1	B	303	PHE	2.2
1	B	294	MET	2.2
1	B	410	ILE	2.2
1	B	321	GLY	2.2
1	B	332	VAL	2.1
1	B	344	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](#)

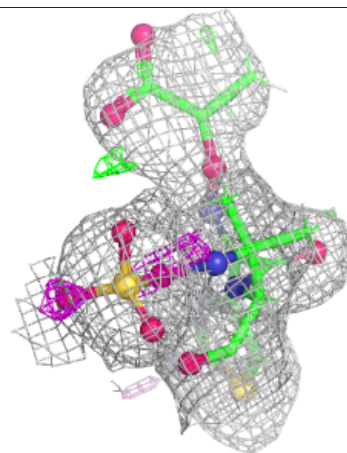
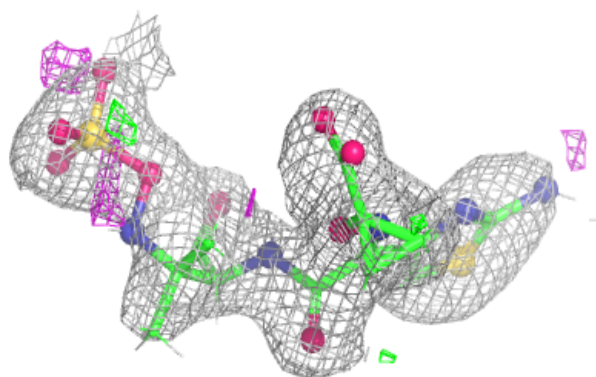
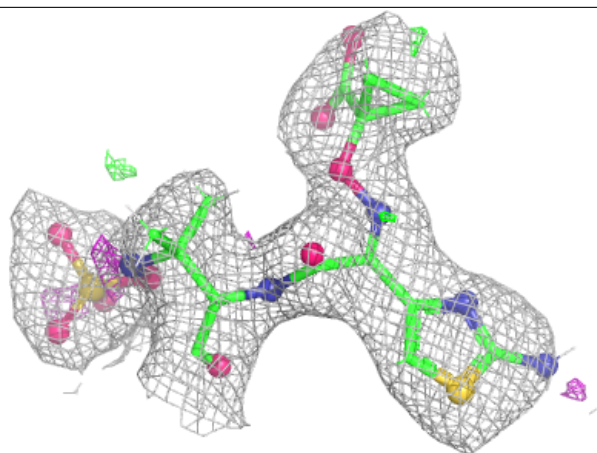
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	JXJ	B	601	30/30	0.87	0.11	58,72,89,91	0
2	JXJ	A	601	30/30	0.89	0.11	38,52,70,86	0

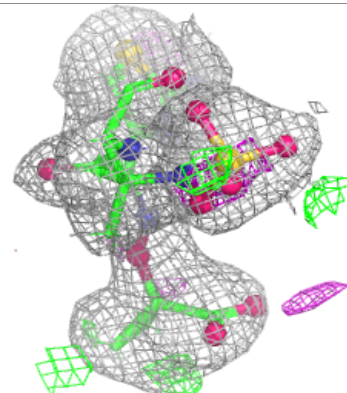
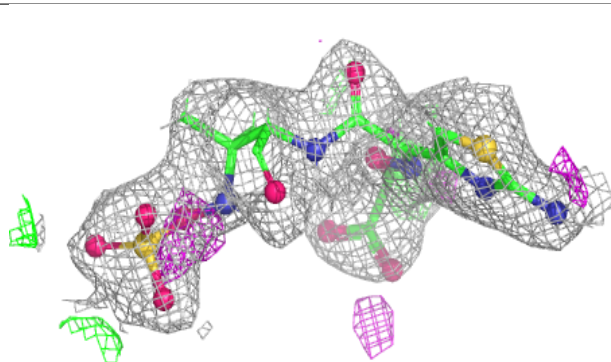
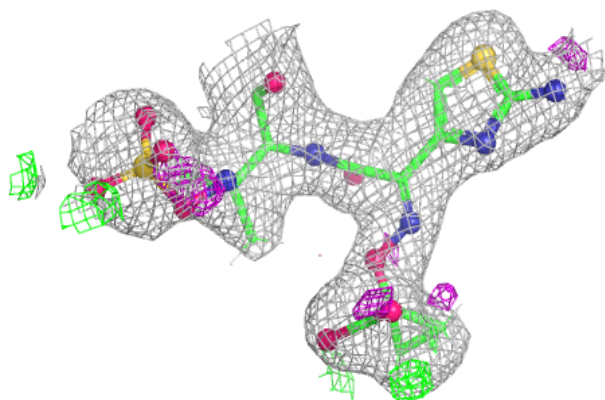
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around JXJ B 601:

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

**Electron density around JXJ A 601:**

$2mF_o-DF_c$ (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.