Full wwPDB X-ray Structure Validation Report ⓘ

Apr 9, 2024 – 12:08 PM JST

PDB ID	:	8YJX
Title	:	Crystal structure of penicillin-binding protein 2 (PBP2) from Campylobacter jejuni
Authors	:	Choi, H.J.; Ki, D.W.; Yoon, S.I.
Deposited on	:	2024-03-03
Resolution	:	2.95 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:

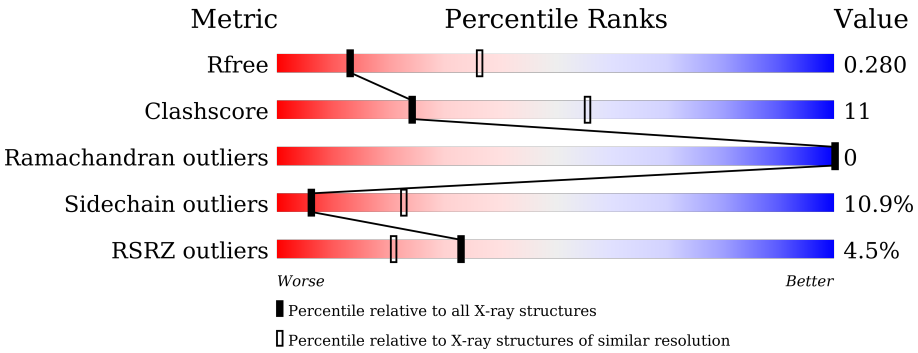
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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 <=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	568	4% 70% 25%
1	B	568	4% 64% 21% 14%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7642 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 Penicillin-binding protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	558	Total	C	N	O	S	0	0	0
			4126	2634	689	794	9			
1	B	490	Total	C	N	O	S	0	0	0
			3508	2242	592	666	8			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	GLY	-	expression tag	UNP A0A3X8PTV6
A	35	SER	-	expression tag	UNP A0A3X8PTV6
A	36	ALA	-	expression tag	UNP A0A3X8PTV6
A	37	LYS	-	expression tag	UNP A0A3X8PTV6
A	38	ASP	-	expression tag	UNP A0A3X8PTV6
A	39	PRO	-	expression tag	UNP A0A3X8PTV6
B	34	GLY	-	expression tag	UNP A0A3X8PTV6
B	35	SER	-	expression tag	UNP A0A3X8PTV6
B	36	ALA	-	expression tag	UNP A0A3X8PTV6
B	37	LYS	-	expression tag	UNP A0A3X8PTV6
B	38	ASP	-	expression tag	UNP A0A3X8PTV6
B	39	PRO	-	expression tag	UNP A0A3X8PTV6

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

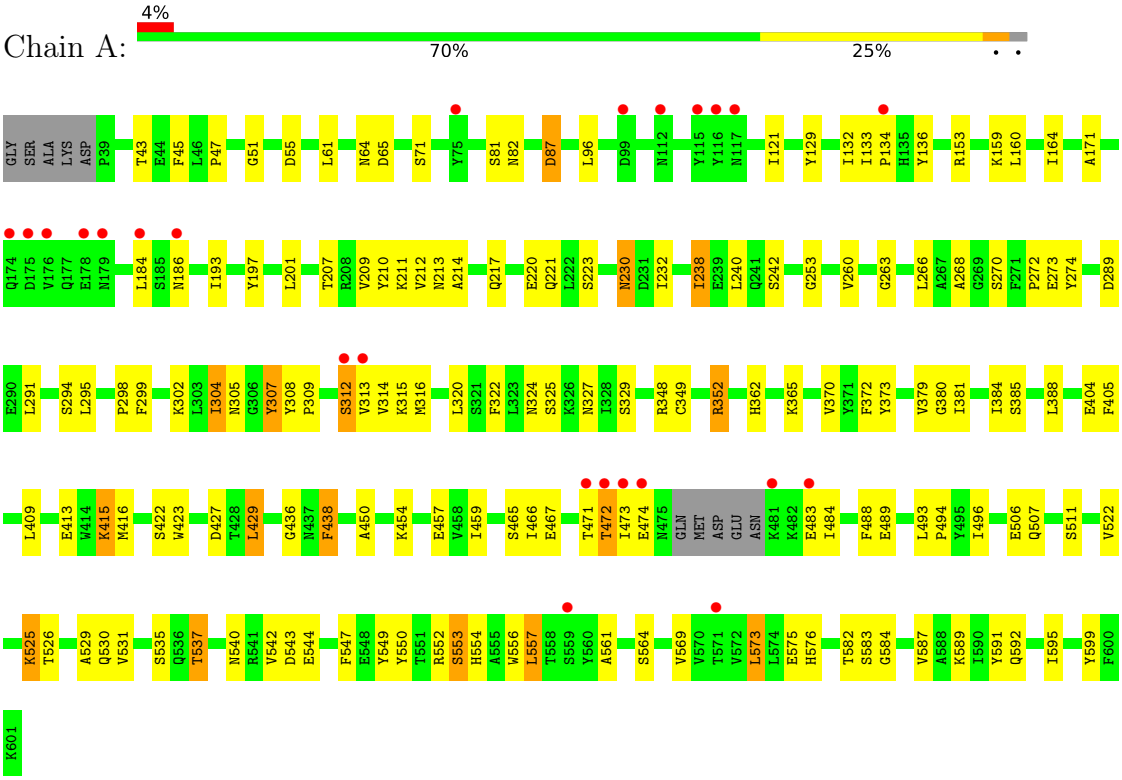
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	5	Total O 5 5	0	0
3	B	1	Total O 1 1	0	0

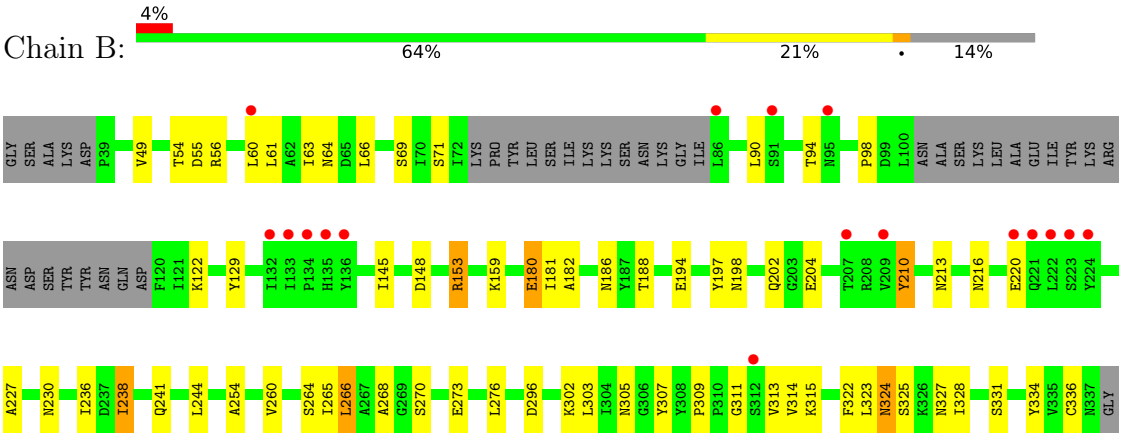
3 Residue-property plots (i)

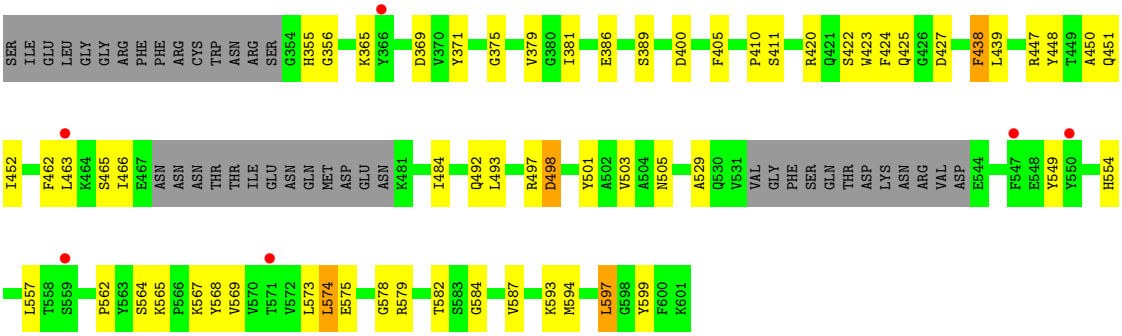
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Penicillin-binding protein 2



• Molecule 1: Penicillin-binding protein 2




SER ILE GLU LEU GLY GLY ARG PHE PHE ARG CYS TRP ASN ARG SER G354 H355 G356 K365 Y366 D369 V370 Y371 G375 V379 G380 I381 E386 S389 D400 F405 P410 S411 R420 Q421 S422 W423 F424 Q425 G426 D427 F438 L439 R447 Y448 T449 A450 Q451
I452 F462 L463 K464 S465 I466 E467 ASN ASN ASN THR THR ILE GLU ASN GLN MET ASP GLU ASN K481 I484 Q492 L493 R497 D498 Y501 A502 V503 A504 N505 A529 Q530 V531 VAL GLY PHE SER GLN THR ASP LYS ASN ARG VAL ASP E544 F547 E548 Y549 Y550 H554
L557 T558 S559 P562 Y563 S564 K565 P566 K567 Y568 V569 V570 T571 V572 L573 L574 E575 G578 R579 T582 S583 G584 V587 K593 M594 L597 G598 Y599 F600 K601

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	119.87Å 119.87Å 274.06Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.79 – 2.95 29.79 – 2.94	Depositor EDS
% Data completeness (in resolution range)	99.0 (29.79-2.95) 99.4 (29.79-2.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 2.95Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.235 , 0.279 0.235 , 0.280	Depositor DCC
R_{free} test set	2340 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å^2)	79.2	Xtriage
Anisotropy	0.505	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 79.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.37$	Xtriage
Estimated twinning fraction	0.001 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7642	wwPDB-VP
Average B, all atoms (Å^2)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.43	0/4225	0.61	1/5770 (0.0%)
1	B	0.39	0/3588	0.57	0/4904
All	All	0.41	0/7813	0.59	1/10674 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	312	SER	CB-CA-C	5.19	119.96	110.10

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	4126	0	3734	84	0
1	B	3508	0	3103	78	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	0	0
3	B	1	0	0	0	0
All	All	7642	0	6837	159	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 11.

All (159) 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:307:TYR:CE2	1:B:422:SER:HA	2.19	0.77
1:B:336:CYS:HB3	1:B:356:GLY:H	1.53	0.74
1:A:349:CYS:HB2	1:A:370:VAL:HG23	1.68	0.74
1:A:43:THR:HG22	1:A:209:VAL:HG13	1.70	0.73
1:A:232:ILE:HG22	1:A:466:ILE:HG12	1.71	0.72
1:A:272:PRO:HG2	1:A:298:PRO:HB3	1.70	0.72
1:A:549:TYR:HA	1:A:552:ARG:HD2	1.73	0.71
1:B:323:LEU:HD12	1:B:492:GLN:HB3	1.73	0.70
1:A:291:LEU:HD22	1:A:299:PHE:HB2	1.74	0.70
1:A:307:TYR:H	1:B:422:SER:HB3	1.57	0.69
1:B:254:ALA:HB1	1:B:303:LEU:HD23	1.74	0.68
1:B:309:PRO:HD2	1:B:529:ALA:HB1	1.74	0.68
1:B:241:GLN:HE22	1:B:268:ALA:H	1.38	0.67
1:B:529:ALA:HB3	1:B:554:HIS:HB2	1.75	0.67
1:A:373:TYR:CD1	1:A:429:LEU:HD13	2.30	0.66
1:B:260:VAL:HG13	1:B:450:ALA:HB1	1.78	0.66
1:A:589:LYS:HA	1:A:592:GLN:HE21	1.60	0.65
1:B:61:LEU:HD21	1:B:238:ILE:HG13	1.77	0.65
1:A:193:ILE:HG23	1:A:197:TYR:HD2	1.62	0.65
1:B:241:GLN:NE2	1:B:268:ALA:O	2.31	0.63
1:A:260:VAL:HG12	1:A:454:LYS:HB2	1.82	0.61
1:B:554:HIS:ND1	1:B:575:GLU:HA	2.17	0.59
1:A:465:SER:HA	1:A:474:GLU:HA	1.85	0.57
1:A:209:VAL:HB	1:A:223:SER:H	1.70	0.57
1:A:164:ILE:HD11	1:A:268:ALA:O	2.04	0.57
1:A:305:ASN:HA	1:A:405:PHE:CD2	2.40	0.57
1:A:266:LEU:HD11	1:A:599:TYR:CE1	2.39	0.57
1:B:322:PHE:CD1	1:B:379:VAL:HG21	2.41	0.56
1:B:260:VAL:HG22	1:B:569:VAL:HG23	1.87	0.56
1:A:260:VAL:HG22	1:A:569:VAL:HG23	1.87	0.56
1:A:320:LEU:HD13	1:A:496:ILE:HG13	1.87	0.55
1:B:450:ALA:HB2	1:B:569:VAL:HG21	1.89	0.55
1:B:55:ASP:HB3	1:B:61:LEU:HD11	1.89	0.55
1:A:380:GLY:O	1:A:384:ILE:HG13	2.07	0.54
1:A:415:LYS:HE3	1:A:422:SER:O	2.07	0.54
1:B:438:PHE:O	1:B:439:LEU:HG	2.08	0.54
1:A:370:VAL:HA	1:A:373:TYR:CD2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:365:LYS:HA	1:B:503:VAL:HG22	1.91	0.53
1:A:415:LYS:HE2	1:A:427:ASP:OD2	2.08	0.53
1:B:593:LYS:O	1:B:597:LEU:HD12	2.09	0.53
1:B:325:SER:C	1:B:327:ASN:H	2.11	0.52
1:B:375:GLY:O	1:B:379:VAL:HG23	2.09	0.52
1:A:45:PHE:CD1	1:A:207:THR:HG22	2.45	0.52
1:A:160:LEU:HD21	1:A:242:SER:HB2	1.91	0.52
1:B:381:ILE:HG12	1:B:423:TRP:CZ2	2.45	0.52
1:B:557:LEU:HD13	1:B:587:VAL:HG21	1.92	0.52
1:A:467:GLU:HA	1:A:472:THR:HA	1.92	0.51
1:B:266:LEU:HD11	1:B:599:TYR:CE1	2.45	0.51
1:A:322:PHE:HA	1:A:379:VAL:HG21	1.93	0.51
1:A:457:GLU:HA	1:A:484:ILE:HD13	1.93	0.51
1:A:557:LEU:HD12	1:A:584:GLY:HA2	1.92	0.51
1:A:550:TYR:HA	1:A:576:HIS:CD2	2.46	0.50
1:B:60:LEU:HD13	1:B:63:ILE:HG21	1.93	0.50
1:B:305:ASN:HA	1:B:405:PHE:CD2	2.46	0.50
1:B:424:PHE:O	1:B:427:ASP:HB2	2.12	0.50
1:A:436:GLY:O	1:B:420:ARG:HD2	2.12	0.49
1:B:241:GLN:NE2	1:B:268:ALA:H	2.09	0.49
1:A:325:SER:C	1:A:327:ASN:H	2.15	0.49
1:B:498:ASP:HA	1:B:501:TYR:CD2	2.47	0.49
1:A:55:ASP:HB3	1:A:61:LEU:HD11	1.93	0.49
1:A:522:VAL:HG22	1:A:561:ALA:HB2	1.94	0.49
1:B:265:ILE:HG21	1:B:268:ALA:HB2	1.93	0.49
1:B:197:TYR:CZ	1:B:463:LEU:HD22	2.48	0.49
1:B:71:SER:HA	1:B:122:LYS:HA	1.94	0.49
1:B:334:TYR:HD2	1:B:371:TYR:CD2	2.30	0.49
1:B:69:SER:N	1:B:148:ASP:O	2.42	0.48
1:B:557:LEU:HD22	1:B:587:VAL:HG21	1.95	0.48
1:A:240:LEU:HD12	1:A:240:LEU:HA	1.68	0.48
1:A:370:VAL:HA	1:A:373:TYR:HD2	1.79	0.48
1:B:198:ASN:O	1:B:202:GLN:HB2	2.13	0.48
1:B:311:GLY:O	1:B:314:VAL:HG22	2.13	0.48
1:A:544:GLU:HA	1:A:547:PHE:CD1	2.48	0.48
1:A:270:SER:O	1:A:273:GLU:HG3	2.14	0.47
1:A:544:GLU:HA	1:A:547:PHE:CE1	2.49	0.47
1:A:554:HIS:CE1	1:A:576:HIS:ND1	2.82	0.47
1:B:324:ASN:OD1	1:B:324:ASN:N	2.48	0.47
1:B:204:GLU:O	1:B:227:ALA:HB1	2.13	0.47
1:B:182:ALA:O	1:B:186:ASN:N	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:GLU:H	1:A:413:GLU:CD	2.17	0.47
1:A:159:LYS:HA	1:A:274:TYR:O	2.15	0.47
1:A:313:VAL:O	1:A:316:MET:HE2	2.14	0.47
1:A:525:LYS:HE3	1:A:526:THR:O	2.15	0.47
1:B:322:PHE:CE2	1:B:375:GLY:HA3	2.49	0.47
1:B:270:SER:OG	1:B:302:LYS:HG3	2.15	0.46
1:B:465:SER:O	1:B:466:ILE:HD13	2.15	0.46
1:A:554:HIS:CE1	1:A:576:HIS:CE1	3.03	0.46
1:A:530:GLN:HA	1:A:553:SER:HB3	1.98	0.46
1:A:212:VAL:HA	1:A:217:GLN:O	2.14	0.46
1:A:324:ASN:HB3	1:A:488:PHE:CE1	2.50	0.46
1:A:129:TYR:OH	1:A:133:ILE:HD12	2.16	0.46
1:B:549:TYR:CE2	1:B:579:ARG:HG3	2.52	0.45
1:A:47:PRO:HB3	1:A:184:LEU:HB2	1.97	0.45
1:B:71:SER:O	1:B:145:ILE:HA	2.17	0.45
1:A:213:ASN:OD1	1:A:214:ALA:N	2.49	0.45
1:B:447:ARG:O	1:B:451:GLN:HG2	2.16	0.45
1:B:497:ARG:O	1:B:501:TYR:HD2	2.00	0.45
1:A:211:LYS:N	1:A:220:GLU:O	2.44	0.45
1:B:94:THR:O	1:B:98:PRO:HB3	2.17	0.45
1:A:542:VAL:HG12	1:A:543:ASP:H	1.82	0.45
1:B:498:ASP:O	1:B:501:TYR:HB2	2.17	0.45
1:B:153:ARG:NH2	1:B:194:GLU:OE1	2.49	0.45
1:A:362:HIS:HA	1:A:365:LYS:HB3	1.98	0.44
1:B:197:TYR:CE1	1:B:463:LEU:HD22	2.52	0.44
1:B:336:CYS:SG	1:B:355:HIS:HB2	2.56	0.44
1:B:557:LEU:HD13	1:B:584:GLY:HA2	2.00	0.44
1:A:133:ILE:N	1:A:134:PRO:HD2	2.32	0.44
1:B:66:LEU:O	1:B:129:TYR:HB2	2.17	0.44
1:A:51:GLY:HA3	1:A:230:ASN:O	2.16	0.44
1:B:180:GLU:HG3	1:B:181:ILE:HD12	1.99	0.44
1:B:210:TYR:H	1:B:210:TYR:HD2	1.64	0.44
1:A:315:LYS:HB3	1:A:372:PHE:CZ	2.52	0.44
1:A:253:GLY:HA2	1:A:575:GLU:HG3	2.00	0.44
1:A:308:TYR:HB2	1:A:556:TRP:HZ2	1.83	0.43
1:A:554:HIS:HE1	1:A:576:HIS:CE1	2.36	0.43
1:A:556:TRP:CZ2	1:A:573:LEU:HD13	2.53	0.43
1:B:400:ASP:OD1	1:B:400:ASP:N	2.48	0.43
1:B:493:LEU:O	1:B:497:ARG:HG3	2.18	0.43
1:B:562:PRO:HG2	1:B:565:LYS:O	2.19	0.43
1:A:557:LEU:HD13	1:A:587:VAL:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:LEU:N	1:A:494:PRO:CD	2.82	0.42
1:B:254:ALA:HB1	1:B:303:LEU:CD2	2.46	0.42
1:A:238:ILE:HD13	1:A:238:ILE:HA	1.80	0.42
1:A:302:LYS:HE3	1:A:575:GLU:OE1	2.19	0.42
1:B:244:LEU:HD23	1:B:244:LEU:HA	1.66	0.42
1:A:471:THR:HG23	1:A:471:THR:O	2.20	0.42
1:B:410:PRO:HD3	1:B:438:PHE:HA	2.01	0.42
1:A:171:ALA:HB2	1:A:186:ASN:HA	2.00	0.42
1:A:365:LYS:NZ	1:A:506:GLU:HB3	2.34	0.42
1:A:589:LYS:HA	1:A:592:GLN:NE2	2.32	0.42
1:B:159:LYS:HG2	1:B:273:GLU:HB2	2.02	0.42
1:A:320:LEU:HD12	1:A:320:LEU:HA	1.79	0.42
1:B:54:THR:HG22	1:B:60:LEU:HD23	2.02	0.41
1:B:60:LEU:HD23	1:B:60:LEU:HA	1.84	0.41
1:B:265:ILE:HD12	1:B:462:PHE:CZ	2.55	0.41
1:A:263:GLY:HA3	1:A:459:ILE:O	2.20	0.41
1:A:352:ARG:H	1:A:352:ARG:HG2	1.63	0.41
1:A:201:LEU:HD21	1:A:232:ILE:CD1	2.51	0.41
1:B:574:LEU:HD12	1:B:578:GLY:CA	2.51	0.41
1:A:305:ASN:HA	1:A:405:PHE:HD2	1.83	0.41
1:A:537:THR:O	1:A:540:ASN:N	2.54	0.41
1:B:315:LYS:NZ	1:B:369:ASP:OD1	2.39	0.41
1:A:314:VAL:HG11	1:A:438:PHE:CE1	2.56	0.41
1:A:320:LEU:CD2	1:A:489:GLU:HG2	2.50	0.41
1:A:591:TYR:O	1:A:595:ILE:HG13	2.21	0.41
1:A:373:TYR:CG	1:A:429:LEU:HD13	2.56	0.41
1:A:381:ILE:HG12	1:A:423:TRP:CZ2	2.55	0.41
1:A:309:PRO:HD2	1:A:529:ALA:HB1	2.02	0.40
1:B:260:VAL:HG23	1:B:567:LYS:O	2.20	0.40
1:B:452:ILE:HD13	1:B:452:ILE:HA	1.87	0.40
1:B:594:MET:HE2	1:B:594:MET:HB3	1.97	0.40
1:B:55:ASP:HB2	1:B:236:ILE:O	2.21	0.40
1:B:56:ARG:HG2	1:B:236:ILE:O	2.21	0.40
1:B:213:ASN:OD1	1:B:216:ASN:N	2.54	0.40
1:B:493:LEU:HD23	1:B:493:LEU:HA	1.83	0.40
1:B:568:TYR:CE2	1:B:599:TYR:HB3	2.56	0.40
1:A:304:ILE:HB	1:A:404:GLU:HG3	2.03	0.40
1:A:87:ASP:OD1	1:A:87:ASP:N	2.55	0.40
1:A:450:ALA:HB2	1:A:569:VAL:HG21	2.04	0.40
1:B:296:ASP:OD1	1:B:296:ASP:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	554/568 (98%)	509 (92%)	45 (8%)	0	100	100
1	B	478/568 (84%)	449 (94%)	29 (6%)	0	100	100
All	All	1032/1136 (91%)	958 (93%)	74 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	398/491 (81%)	352 (88%)	46 (12%)	5	20
1	B	317/491 (65%)	285 (90%)	32 (10%)	7	26
All	All	715/982 (73%)	637 (89%)	78 (11%)	6	23

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	65	ASP
1	A	71	SER
1	A	81	SER
1	A	82	ASN
1	A	87	ASP
1	A	96	LEU
1	A	121	ILE

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Mol	Chain	Res	Type
1	A	132	ILE
1	A	136	TYR
1	A	153	ARG
1	A	210	TYR
1	A	221	GLN
1	A	230	ASN
1	A	238	ILE
1	A	289	ASP
1	A	294	SER
1	A	295	LEU
1	A	304	ILE
1	A	307	TYR
1	A	312	SER
1	A	329	SER
1	A	348	ARG
1	A	352	ARG
1	A	385	SER
1	A	388	LEU
1	A	409	LEU
1	A	415	LYS
1	A	416	MET
1	A	429	LEU
1	A	438	PHE
1	A	472	THR
1	A	473	ILE
1	A	483	GLU
1	A	507	GLN
1	A	511	SER
1	A	525	LYS
1	A	531	VAL
1	A	535	SER
1	A	537	THR
1	A	553	SER
1	A	557	LEU
1	A	564	SER
1	A	573	LEU
1	A	582	THR
1	A	583	SER
1	B	49	VAL
1	B	64	ASN
1	B	90	LEU
1	B	153	ARG

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Mol	Chain	Res	Type
1	B	180	GLU
1	B	188	THR
1	B	210	TYR
1	B	220	GLU
1	B	230	ASN
1	B	238	ILE
1	B	264	SER
1	B	266	LEU
1	B	276	LEU
1	B	307	TYR
1	B	313	VAL
1	B	324	ASN
1	B	328	ILE
1	B	331	SER
1	B	386	GLU
1	B	389	SER
1	B	411	SER
1	B	425	GLN
1	B	438	PHE
1	B	448	TYR
1	B	484	ILE
1	B	498	ASP
1	B	505	ASN
1	B	564	SER
1	B	573	LEU
1	B	574	LEU
1	B	582	THR
1	B	597	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	ASN
1	A	202	GLN
1	A	297	HIS
1	A	305	ASN
1	A	425	GLN
1	A	592	GLN
1	B	186	ASN
1	B	230	ASN
1	B	241	GLN
1	B	378	GLN

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Mol	Chain	Res	Type
1	B	425	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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	558/568 (98%)	0.02	24 (4%)	35	22	52, 93, 147, 178	0
1	B	490/568 (86%)	0.09	23 (4%)	31	20	66, 109, 147, 182	0
All	All	1048/1136 (92%)	0.05	47 (4%)	33	21	52, 102, 147, 182	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	116	TYR	4.4
1	B	135	HIS	3.7
1	B	86	LEU	3.7
1	A	471	THR	3.5
1	B	132	ILE	3.5
1	B	222	LEU	3.3
1	B	221	GLN	3.3
1	B	366	TYR	3.2
1	B	550	TYR	3.2
1	B	223	SER	3.1
1	A	184	LEU	3.1
1	A	134	PRO	3.1
1	B	312	SER	3.0
1	A	178	GLU	2.9
1	A	312	SER	2.9
1	A	99	ASP	2.9
1	B	136	TYR	2.9
1	B	134	PRO	2.8
1	A	176	VAL	2.7
1	A	474	GLU	2.7
1	A	179	ASN	2.7
1	A	117	ASN	2.6
1	A	174	GLN	2.6
1	A	473	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	472	THR	2.5
1	A	175	ASP	2.5
1	A	115	TYR	2.5
1	A	559	SER	2.5
1	B	571	THR	2.5
1	B	207	THR	2.4
1	A	313	VAL	2.4
1	B	209	VAL	2.4
1	A	75	TYR	2.3
1	A	112	ASN	2.2
1	B	224	TYR	2.2
1	B	91	SER	2.2
1	B	547	PHE	2.1
1	B	133	ILE	2.1
1	A	483	GLU	2.1
1	B	463	LEU	2.1
1	A	481	LYS	2.1
1	B	60	LEU	2.1
1	B	220	GLU	2.1
1	A	186	ASN	2.1
1	B	559	SER	2.0
1	A	571	THR	2.0
1	B	95	ASN	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 monosaccharides 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, 95^{th} 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.

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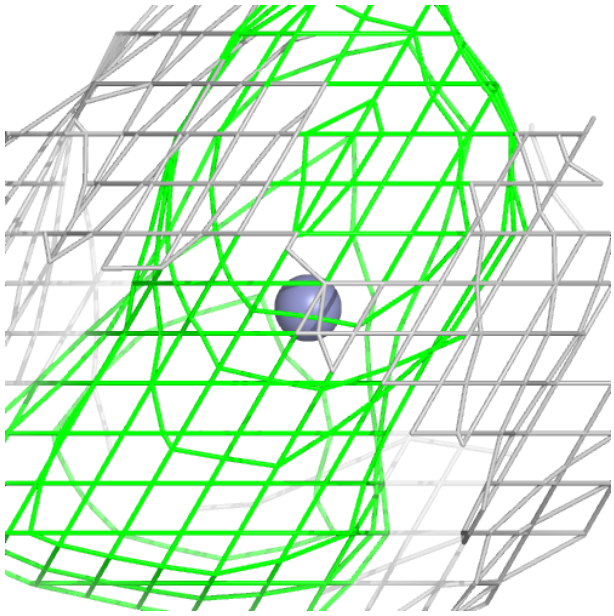
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

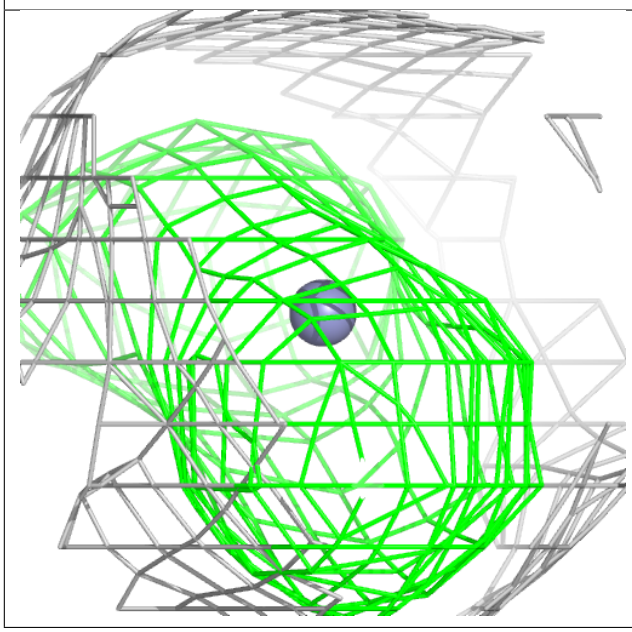
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	B	701	1/1	0.98	0.19	108,108,108,108	0
2	ZN	A	701	1/1	0.99	0.12	68,68,68,68	0

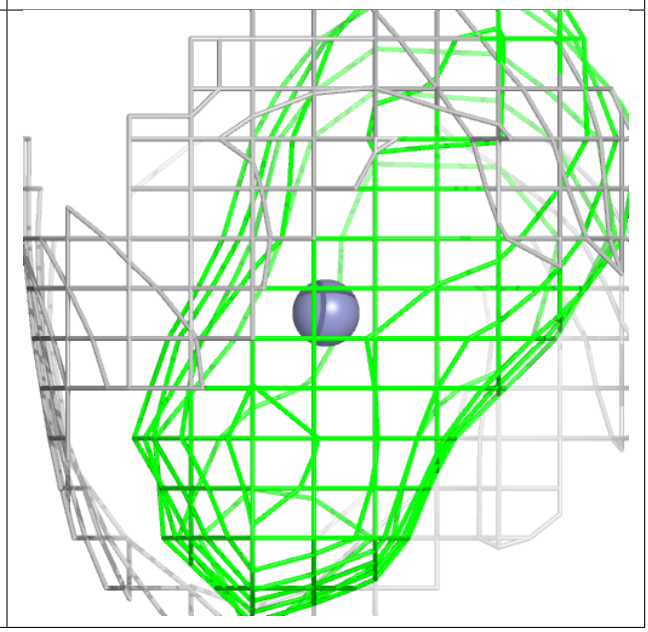
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ZN B 701:

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

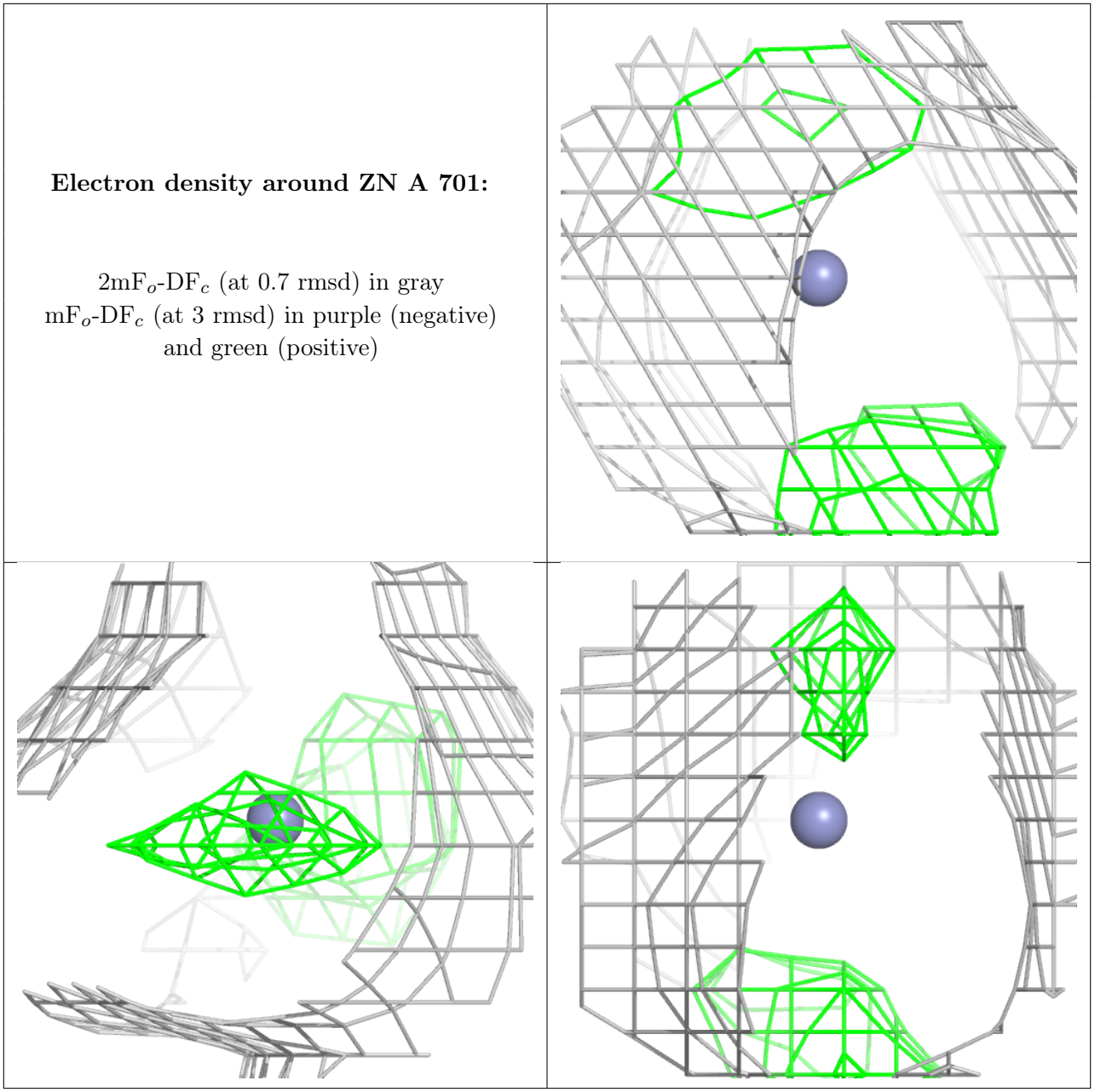






Electron density around ZN A 701:

$2mF_o$-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.