



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:26 PM UTC

PDB ID : 8ITN / pdb_00008itn
Title : Crystal structure of USP47apo catalytic domain
Authors : Kim, E.E.; Shin, S.C.
Deposited on : 2023-03-22
Resolution : 2.60 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
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

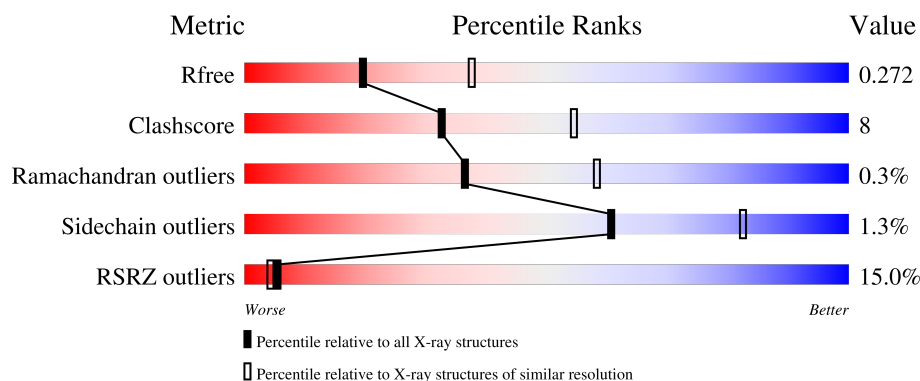
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

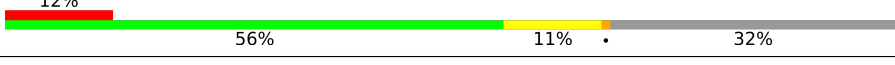
The reported resolution of this entry is 2.60 Å.

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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	508	
1	B	508	
1	C	508	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8432 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 Ubiquitin carboxyl-terminal hydrolase 47.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	0	0	0
			2846	1807	481	539	19			
1	B	329	Total	C	N	O	S	0	0	0
			2678	1708	451	503	16			
1	C	345	Total	C	N	O	S	0	0	0
			2802	1779	472	532	19			

- Molecule 2 is ZINC ION (CCD ID: 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	C	1	Total	Zn	0	0
			1	1		

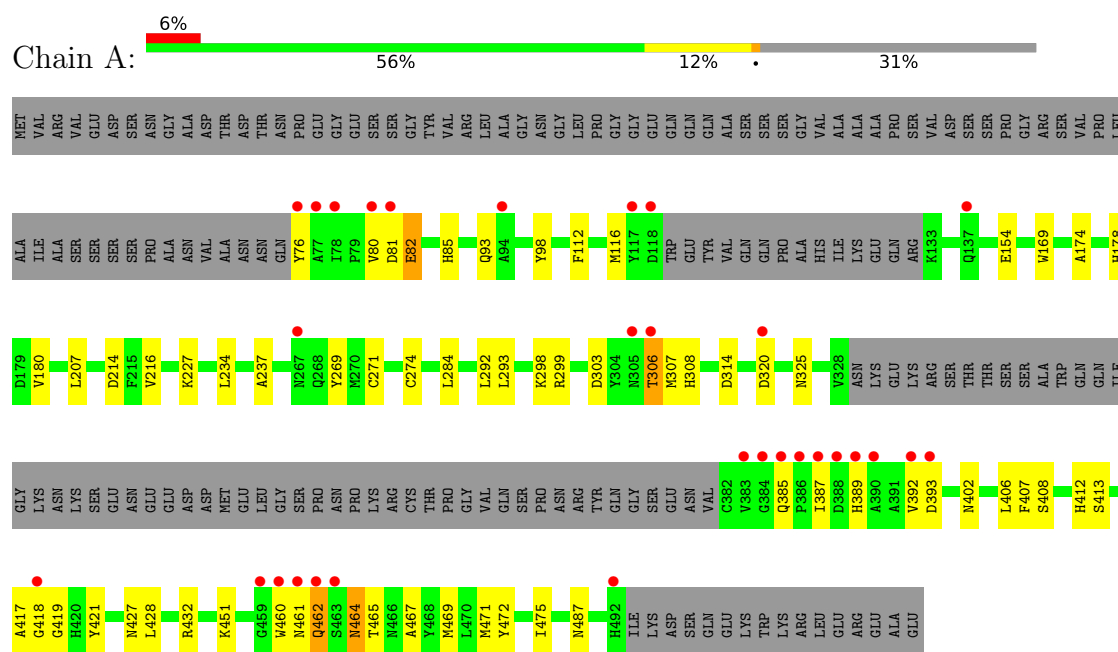
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	76	Total	O	0	0
			76	76		
3	B	11	Total	O	0	0
			11	11		
3	C	17	Total	O	0	0
			17	17		

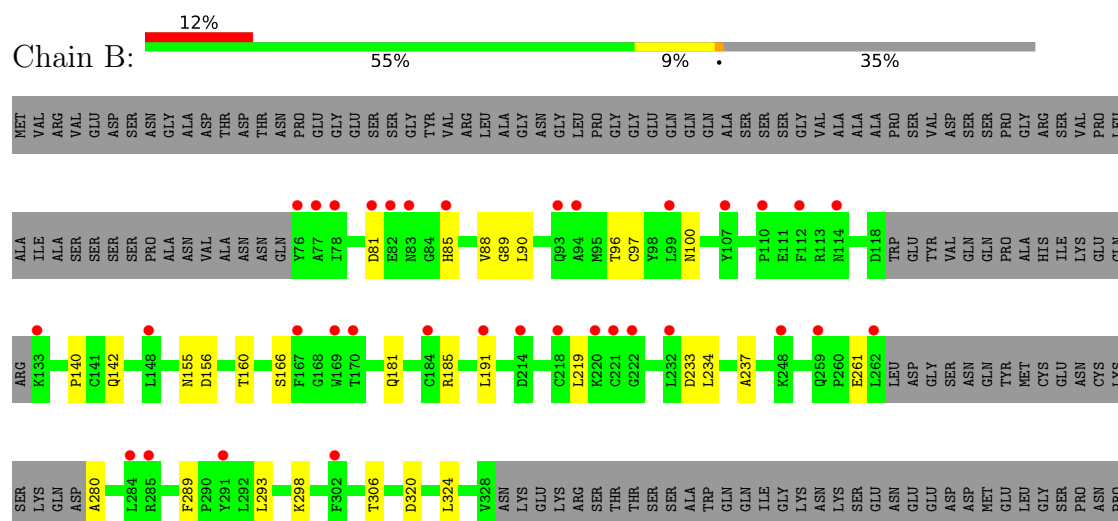
3 Residue-property plots

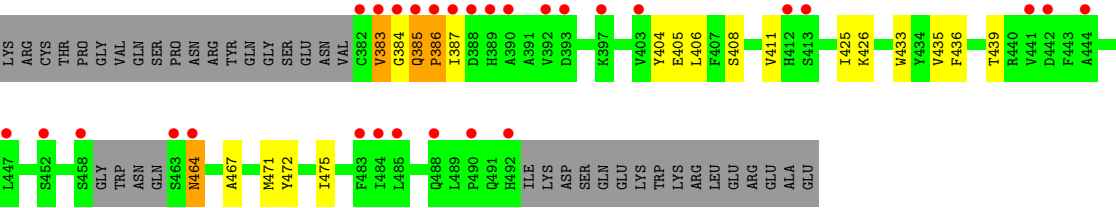
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Ubiquitin carboxyl-terminal hydrolase 47

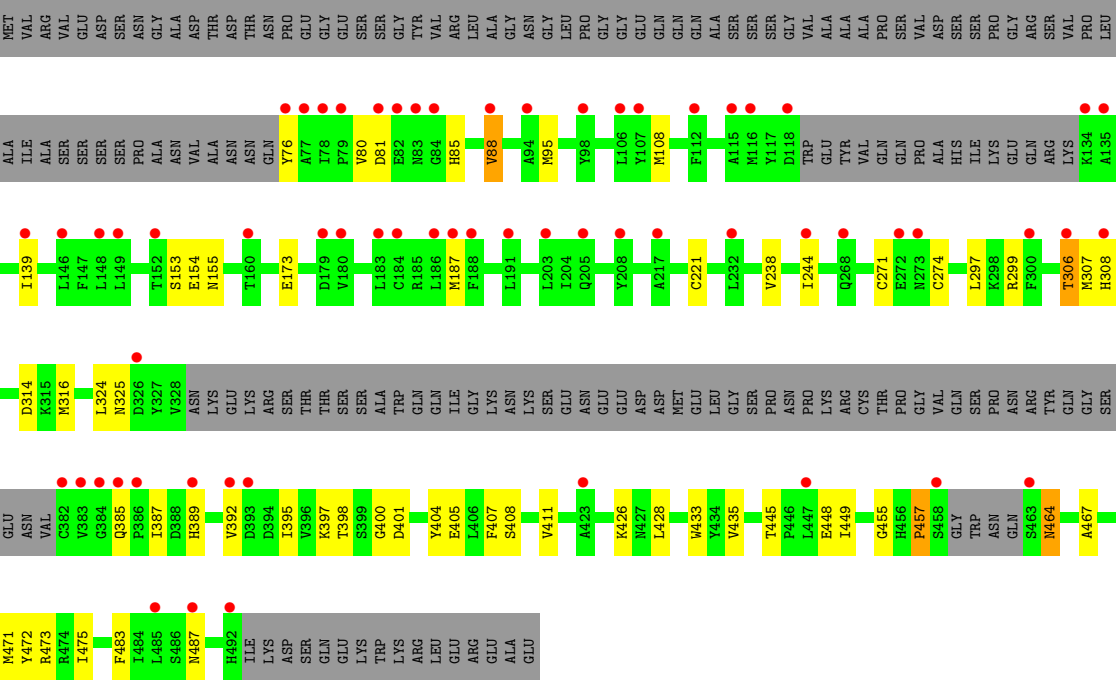


• Molecule 1: Ubiquitin carboxyl-terminal hydrolase 47





● Molecule 1: Ubiquitin carboxyl-terminal hydrolase 47



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	94.08Å 58.91Å 251.93Å 90.00° 96.69° 90.00°	Depositor
Resolution (Å)	35.50 – 2.60 35.50 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.0 (35.50-2.60) 96.2 (35.50-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.66 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.20.1-4487	Depositor
R, R_{free}	0.258 , 0.269 0.259 , 0.272	Depositor DCC
R_{free} test set	2000 reflections (4.64%)	wwPDB-VP
Wilson B-factor (Å ²)	43.2	Xtriage
Anisotropy	0.471	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	8432	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% 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

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	0.18	0/2913	0.33	1/3941 (0.0%)
1	B	0.18	0/2740	0.39	5/3706 (0.1%)
1	C	0.09	0/2866	0.30	2/3876 (0.1%)
All	All	0.15	0/8519	0.34	8/11523 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	383	VAL	CB-CA-C	-7.64	99.73	110.12
1	B	383	VAL	N-CA-C	6.54	117.52	107.78
1	C	306	THR	CA-C-N	6.21	132.87	121.70
1	C	306	THR	C-N-CA	6.21	132.87	121.70
1	B	306	THR	CA-C-N	5.99	132.47	121.70
1	B	306	THR	C-N-CA	5.99	132.47	121.70
1	A	417	ALA	N-CA-C	-5.76	105.35	112.38
1	B	97	CYS	CB-CA-C	-5.42	109.86	117.23

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	2846	0	2732	58	0
1	B	2678	0	2587	35	0
1	C	2802	0	2691	44	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
3	A	76	0	0	2	0
3	B	11	0	0	0	0
3	C	17	0	0	0	0
All	All	8432	0	8010	129	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 8.

All (129) 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:462:GLN:HG2	1:A:462:GLN:O	1.64	0.93
1:A:408:SER:HB3	1:A:471:MET:HB2	1.61	0.81
1:B:320:ASP:CG	1:B:384:GLY:O	2.25	0.79
1:B:408:SER:HB3	1:B:471:MET:HB2	1.64	0.78
1:A:461:ASN:HB2	1:A:462:GLN:HA	1.68	0.76
1:A:299:ARG:NH2	1:A:314:ASP:O	2.21	0.73
1:C:408:SER:HB3	1:C:471:MET:HB2	1.69	0.72
1:B:90:LEU:O	1:B:439:THR:HG22	1.89	0.72
1:A:413:SER:HB3	1:A:465:THR:HG22	1.75	0.69
1:B:88:VAL:HG22	1:B:155:ASN:O	1.93	0.68
1:A:306:THR:CB	1:A:308:HIS:H	2.06	0.67
1:C:85:HIS:NE2	1:C:153:SER:O	2.27	0.67
1:C:306:THR:HB	1:C:308:HIS:H	1.61	0.65
1:B:88:VAL:HG12	1:B:89:GLY:N	2.12	0.64
1:C:457:PRO:CG	1:C:464:ASN:HB3	2.28	0.64
1:C:88:VAL:HG13	1:C:155:ASN:O	1.98	0.64
1:A:76:TYR:HD2	1:C:154:GLU:HG3	1.63	0.63
1:A:214:ASP:HB3	1:A:284:LEU:HD23	1.79	0.63
1:B:81:ASP:N	1:B:85:HIS:O	2.25	0.62
1:A:461:ASN:N	1:A:462:GLN:HB3	2.15	0.62
1:B:234:LEU:HD22	1:B:293:LEU:HD11	1.82	0.62
1:B:88:VAL:HG13	1:B:156:ASP:C	2.25	0.61
1:B:385:GLN:HB2	1:B:386:PRO:HD3	1.82	0.61
1:C:238:VAL:HG21	1:C:299:ARG:HG2	1.83	0.59
1:A:460:TRP:C	1:A:462:GLN:HB3	2.26	0.59
1:B:404:TYR:HB3	1:B:472:TYR:HB3	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:THR:OG1	1:A:307:MET:HA	2.03	0.58
1:C:455:GLY:O	1:C:457:PRO:HD3	2.03	0.58
1:A:93:GLN:NE2	1:A:421:TYR:O	2.37	0.56
1:A:427:ASN:ND2	3:A:706:HOH:O	2.38	0.56
1:B:405:GLU:HB2	1:B:475:ILE:HD11	1.88	0.56
1:B:219:LEU:HG	1:B:280:ALA:HA	1.88	0.55
1:A:306:THR:HB	1:A:308:HIS:N	2.22	0.55
1:A:462:GLN:H	1:A:462:GLN:HE21	1.55	0.54
1:B:88:VAL:CG2	1:B:155:ASN:O	2.54	0.54
1:C:299:ARG:NH2	1:C:314:ASP:O	2.40	0.54
1:C:404:TYR:HB3	1:C:472:TYR:HB3	1.90	0.54
1:A:306:THR:HB	1:A:308:HIS:H	1.71	0.53
1:A:76:TYR:CD2	1:C:154:GLU:HG3	2.42	0.53
1:A:412:HIS:HE2	1:A:419:GLY:HA3	1.74	0.53
1:B:464:ASN:ND2	1:B:464:ASN:O	2.42	0.53
1:A:462:GLN:O	1:A:462:GLN:CG	2.46	0.53
1:A:464:ASN:HD22	1:A:464:ASN:N	2.04	0.53
1:C:457:PRO:HG3	1:C:464:ASN:HB3	1.91	0.53
1:A:234:LEU:HD22	1:A:293:LEU:HD11	1.90	0.53
1:B:320:ASP:HA	1:B:406:LEU:HB3	1.89	0.53
1:C:389:HIS:HB2	1:C:392:VAL:HG12	1.90	0.52
1:C:81:ASP:N	1:C:85:HIS:O	2.38	0.52
1:A:412:HIS:NE2	1:A:419:GLY:HA3	2.25	0.52
1:A:81:ASP:N	1:A:85:HIS:O	2.35	0.52
1:B:90:LEU:O	1:B:439:THR:CG2	2.58	0.52
1:C:221:CYS:HB3	1:C:274:CYS:SG	2.49	0.52
1:A:303:ASP:HB3	1:A:306:THR:HG1	1.73	0.52
1:A:325:ASN:ND2	1:A:402:ASN:H	2.08	0.52
1:A:214:ASP:OD2	1:A:227:LYS:NZ	2.38	0.51
1:C:405:GLU:HB2	1:C:475:ILE:HD11	1.91	0.51
1:B:387:ILE:HD12	1:B:387:ILE:H	1.77	0.50
1:B:185:ARG:HD3	1:C:307:MET:HE3	1.93	0.50
1:C:385:GLN:HG3	1:C:449:ILE:HB	1.94	0.50
1:A:81:ASP:HB3	1:A:82:GLU:OE1	2.12	0.50
1:C:95:MET:HE1	1:C:173:GLU:HG3	1.94	0.50
1:C:395:ILE:O	1:C:398:THR:OG1	2.29	0.49
1:B:90:LEU:HD22	1:B:100:ASN:HA	1.94	0.49
1:A:487:ASN:HB2	1:C:387:ILE:HG12	1.94	0.49
1:A:325:ASN:HD21	1:A:402:ASN:H	1.60	0.49
1:A:464:ASN:O	1:A:464:ASN:ND2	2.45	0.49
1:B:237:ALA:HA	1:B:298:LYS:HB3	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:411:VAL:HA	1:C:467:ALA:HA	1.93	0.49
1:C:426:LYS:HB2	1:C:433:TRP:CD2	2.48	0.49
1:B:464:ASN:HD22	1:B:464:ASN:N	2.11	0.48
1:A:385:GLN:H	1:A:385:GLN:CD	2.21	0.48
1:A:407:PHE:HB3	1:A:428:LEU:HD21	1.96	0.48
1:A:237:ALA:HA	1:A:298:LYS:HB2	1.96	0.48
1:C:407:PHE:HB3	1:C:428:LEU:HD21	1.94	0.48
1:A:462:GLN:HE21	1:A:462:GLN:N	2.12	0.47
1:C:464:ASN:HD22	1:C:464:ASN:N	2.12	0.47
1:A:180:VAL:HG21	1:A:469:MET:HE1	1.95	0.47
1:A:320:ASP:HA	1:A:406:LEU:HB3	1.97	0.47
1:B:88:VAL:CG1	1:B:89:GLY:N	2.77	0.47
1:B:140:PRO:HG3	1:B:191:LEU:HD23	1.96	0.47
1:C:88:VAL:CG1	1:C:155:ASN:O	2.63	0.46
1:A:464:ASN:HD22	1:A:464:ASN:H	1.63	0.46
1:A:461:ASN:N	1:A:462:GLN:CB	2.79	0.46
1:C:324:LEU:HD13	1:C:404:TYR:CD1	2.51	0.46
1:A:216:VAL:HG11	1:A:269:TYR:CE1	2.51	0.46
1:C:139:ILE:HD12	1:C:187:MET:HG2	1.99	0.45
1:A:387:ILE:HG12	1:C:487:ASN:HB3	1.98	0.45
1:A:393:ASP:OD2	1:A:475:ILE:HG21	2.16	0.45
1:A:464:ASN:N	1:A:464:ASN:ND2	2.64	0.45
1:A:432:ARG:HA	1:A:432:ARG:HD2	1.76	0.44
1:A:234:LEU:HD12	1:A:234:LEU:HA	1.79	0.44
1:B:142:GLN:HG3	1:B:166:SER:HB3	2.00	0.44
1:C:81:ASP:HB2	1:C:85:HIS:H	1.83	0.44
1:C:139:ILE:HD11	1:C:187:MET:HA	2.00	0.44
1:C:457:PRO:HG2	1:C:464:ASN:HB3	1.99	0.44
1:C:428:LEU:HD13	1:C:473:ARG:CZ	2.48	0.44
1:A:169:TRP:HB3	1:A:174:ALA:HB1	2.00	0.43
1:C:271:CYS:HB3	1:C:274:CYS:HB2	2.01	0.43
1:A:306:THR:CB	1:A:308:HIS:N	2.77	0.43
1:C:325:ASN:OD1	1:C:401:ASP:N	2.52	0.43
1:B:261:GLU:HG3	1:C:244:ILE:O	2.18	0.43
1:C:397:LYS:HA	1:C:400:GLY:O	2.19	0.43
1:A:271:CYS:HB3	1:A:274:CYS:HB2	2.01	0.43
1:B:425:ILE:HB	1:B:436:PHE:CE1	2.54	0.43
1:B:426:LYS:HB2	1:B:433:TRP:CD2	2.54	0.43
1:A:80:VAL:HG11	1:C:80:VAL:HG21	2.00	0.43
1:C:108:MET:HA	1:C:483:PHE:HZ	1.84	0.42
1:A:306:THR:CB	1:A:307:MET:HA	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:ARG:HD2	1:A:467:ALA:O	2.19	0.42
1:C:445:THR:HG23	1:C:448:GLU:H	1.84	0.42
1:A:303:ASP:HB3	1:A:306:THR:OG1	2.20	0.41
1:B:289:PHE:CE1	1:B:324:LEU:HD23	2.55	0.41
1:B:406:LEU:HB2	1:B:472:TYR:CE2	2.55	0.41
1:A:451:LYS:NZ	3:A:712:HOH:O	2.50	0.41
1:B:90:LEU:HD23	1:B:160:THR:CG2	2.50	0.41
1:B:411:VAL:HA	1:B:467:ALA:HA	2.02	0.41
1:A:207:LEU:HB3	1:A:292:LEU:HD12	2.03	0.41
1:C:387:ILE:H	1:C:387:ILE:HD12	1.85	0.41
1:B:464:ASN:HD22	1:B:464:ASN:H	1.69	0.41
1:B:181:GLN:NE2	1:B:233:ASP:OD2	2.54	0.41
1:B:405:GLU:OE2	1:B:426:LYS:NZ	2.42	0.41
1:C:405:GLU:OE2	1:C:426:LYS:NZ	2.39	0.41
1:A:389:HIS:HB3	1:A:392:VAL:H	1.85	0.40
1:A:112:PHE:O	1:A:116:MET:HG2	2.21	0.40
1:A:98:TYR:OH	1:A:178:HIS:O	2.37	0.40
1:A:406:LEU:HB2	1:A:472:TYR:CE2	2.57	0.40
1:B:385:GLN:N	1:B:386:PRO:CD	2.84	0.40
1:C:297:LEU:HD13	1:C:316:MET:HE3	2.04	0.40
1:A:154:GLU:HB3	1:C:76:TYR:HD2	1.87	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	344/508 (68%)	323 (94%)	20 (6%)	1 (0%)	36	58
1	B	319/508 (63%)	302 (95%)	16 (5%)	1 (0%)	36	58
1	C	337/508 (66%)	317 (94%)	19 (6%)	1 (0%)	36	58
All	All	1000/1524 (66%)	942 (94%)	55 (6%)	3 (0%)	36	58

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	386	PRO
1	C	457	PRO
1	A	418	GLY

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	312/444 (70%)	308 (99%)	4 (1%)	61	82
1	B	293/444 (66%)	288 (98%)	5 (2%)	53	78
1	C	308/444 (69%)	305 (99%)	3 (1%)	68	86
All	All	913/1332 (68%)	901 (99%)	12 (1%)	61	82

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	GLU
1	A	306	THR
1	A	462	GLN
1	A	464	ASN
1	B	96	THR
1	B	383	VAL
1	B	385	GLN
1	B	435	VAL
1	B	464	ASN
1	C	88	VAL
1	C	435	VAL
1	C	464	ASN

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

Mol	Chain	Res	Type
1	A	181	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	200	HIS
1	A	325	ASN
1	A	462	GLN
1	A	464	ASN
1	B	181	GLN
1	B	200	HIS
1	B	464	ASN
1	C	172	ASN
1	C	181	GLN
1	C	464	ASN
1	C	466	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 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, 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	350/508 (68%)	0.52	30 (8%) 16 12	18, 40, 77, 142	0
1	B	329/508 (64%)	1.33	63 (19%) 3 2	59, 94, 136, 203	0
1	C	345/508 (67%)	1.30	61 (17%) 4 3	61, 87, 135, 176	0
All	All	1024/1524 (67%)	1.05	154 (15%) 5 4	18, 79, 131, 203	0

All (154) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	112	PHE	6.7
1	C	393	ASP	5.9
1	A	385	GLN	5.6
1	A	384	GLY	5.5
1	C	184	CYS	5.0
1	A	81	ASP	5.0
1	B	463	SER	4.9
1	C	383	VAL	4.9
1	A	460	TRP	4.8
1	B	221	CYS	4.7
1	A	388	ASP	4.6
1	B	148	LEU	4.6
1	B	492	HIS	4.5
1	C	115	ALA	4.5
1	C	148	LEU	4.5
1	A	393	ASP	4.4
1	B	387	ILE	4.4
1	C	78	ILE	4.4
1	B	393	ASP	4.2
1	B	285	ARG	4.1
1	C	492	HIS	4.1
1	C	98	TYR	4.0
1	B	85	HIS	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	388	ASP	3.9
1	C	81	ASP	3.9
1	B	184	CYS	3.9
1	C	389	HIS	3.9
1	A	306	THR	3.8
1	B	259	GLN	3.8
1	C	384	GLY	3.8
1	C	146	LEU	3.8
1	B	382	CYS	3.7
1	C	382	CYS	3.7
1	B	302	PHE	3.7
1	B	442	ASP	3.7
1	B	218	CYS	3.6
1	A	462	GLN	3.6
1	C	191	LEU	3.6
1	A	94	ALA	3.6
1	B	81	ASP	3.6
1	A	320	ASP	3.6
1	A	117	TYR	3.5
1	A	76	TYR	3.4
1	C	458	SER	3.4
1	B	82	GLU	3.4
1	B	385	GLN	3.4
1	C	149	LEU	3.3
1	A	461	ASN	3.3
1	B	483	PHE	3.3
1	A	77	ALA	3.3
1	B	78	ILE	3.2
1	C	385	GLN	3.2
1	C	77	ALA	3.1
1	C	485	LEU	3.1
1	B	94	ALA	3.1
1	A	492	HIS	3.1
1	C	423	ALA	3.1
1	C	88	VAL	3.1
1	C	386	PRO	3.0
1	C	272	GLU	3.0
1	A	383	VAL	3.0
1	B	383	VAL	3.0
1	C	487	ASN	2.9
1	A	459	GLY	2.9
1	B	386	PRO	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	305	ASN	2.9
1	B	447	LEU	2.9
1	C	180	VAL	2.9
1	B	464	ASN	2.9
1	C	232	LEU	2.9
1	C	84	GLY	2.8
1	C	244	ILE	2.8
1	B	222	GLY	2.7
1	C	106	LEU	2.7
1	C	183	LEU	2.7
1	C	187	MET	2.7
1	B	412	HIS	2.7
1	B	444	ALA	2.7
1	C	139	ILE	2.6
1	A	390	ALA	2.6
1	B	452	SER	2.6
1	C	160	THR	2.6
1	C	306	THR	2.6
1	A	418	GLY	2.6
1	B	458	SER	2.6
1	B	441	VAL	2.6
1	A	78	ILE	2.5
1	B	262	LEU	2.5
1	C	392	VAL	2.5
1	C	217	ALA	2.5
1	C	152	THR	2.5
1	C	463	SER	2.5
1	C	83	ASN	2.4
1	B	291	TYR	2.4
1	C	107	TYR	2.4
1	B	112	PHE	2.4
1	A	389	HIS	2.4
1	C	179	ASP	2.4
1	A	386	PRO	2.4
1	B	93	GLN	2.4
1	C	208	TYR	2.4
1	B	284	LEU	2.4
1	C	203	LEU	2.3
1	B	83	ASN	2.3
1	B	114	ASN	2.3
1	C	186	LEU	2.3
1	B	488	GLN	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	300	PHE	2.3
1	B	413	SER	2.3
1	C	188	PHE	2.3
1	B	133	LYS	2.3
1	C	134	LYS	2.3
1	C	268	GLN	2.3
1	B	390	ALA	2.2
1	B	76	TYR	2.2
1	B	167	PHE	2.2
1	B	77	ALA	2.2
1	B	107	TYR	2.2
1	A	267	ASN	2.2
1	A	118	ASP	2.2
1	C	118	ASP	2.2
1	B	191	LEU	2.2
1	B	485	LEU	2.2
1	B	169	TRP	2.2
1	B	248	LYS	2.2
1	B	403	VAL	2.2
1	C	76	TYR	2.2
1	B	214	ASP	2.2
1	B	384	GLY	2.2
1	C	94	ALA	2.2
1	C	135	ALA	2.2
1	C	79	PRO	2.2
1	C	447	LEU	2.2
1	A	80	VAL	2.2
1	A	387	ILE	2.2
1	B	110	PRO	2.1
1	A	137	GLN	2.1
1	B	397	LYS	2.1
1	B	99	LEU	2.1
1	B	170	THR	2.1
1	B	484	ILE	2.1
1	C	273	ASN	2.1
1	A	392	VAL	2.1
1	B	392	VAL	2.1
1	C	116	MET	2.1
1	C	205	GLN	2.1
1	C	308	HIS	2.1
1	A	463	SER	2.0
1	B	220	LYS	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	490	PRO	2.0
1	B	232	LEU	2.0
1	C	82	GLU	2.0
1	C	326	ASP	2.0
1	B	389	HIS	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](#)

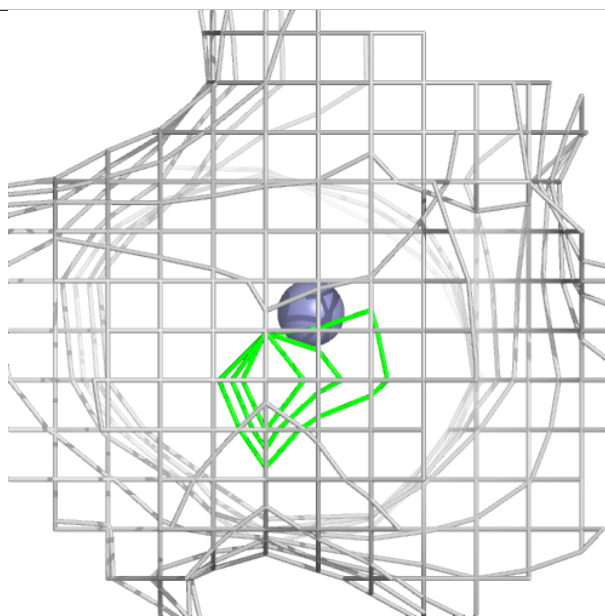
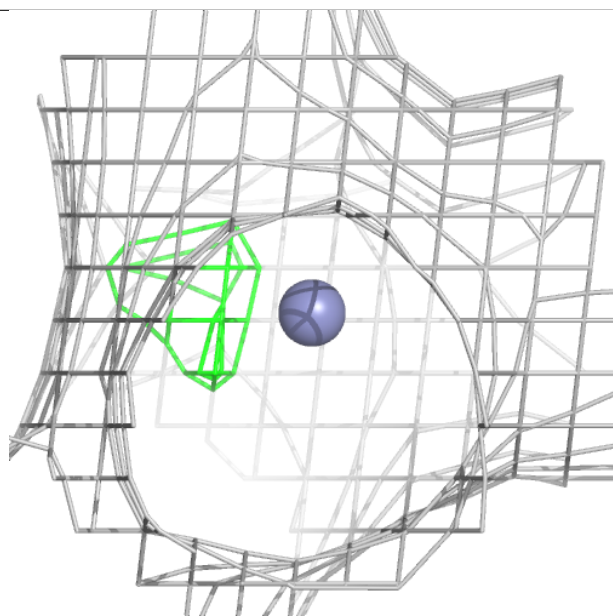
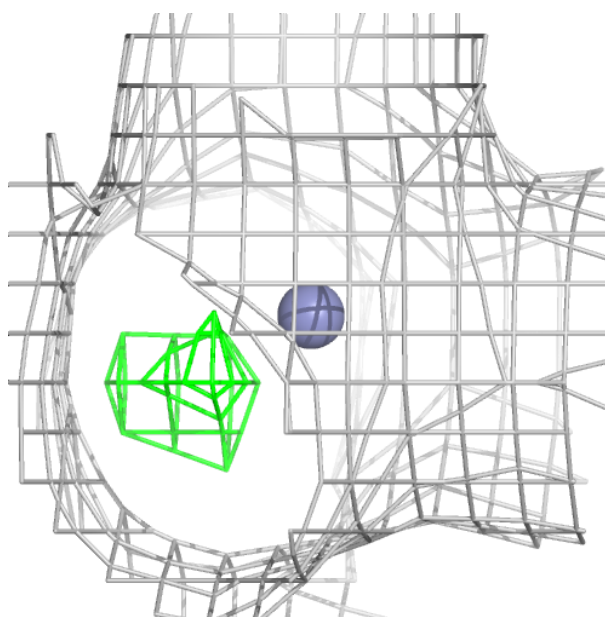
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

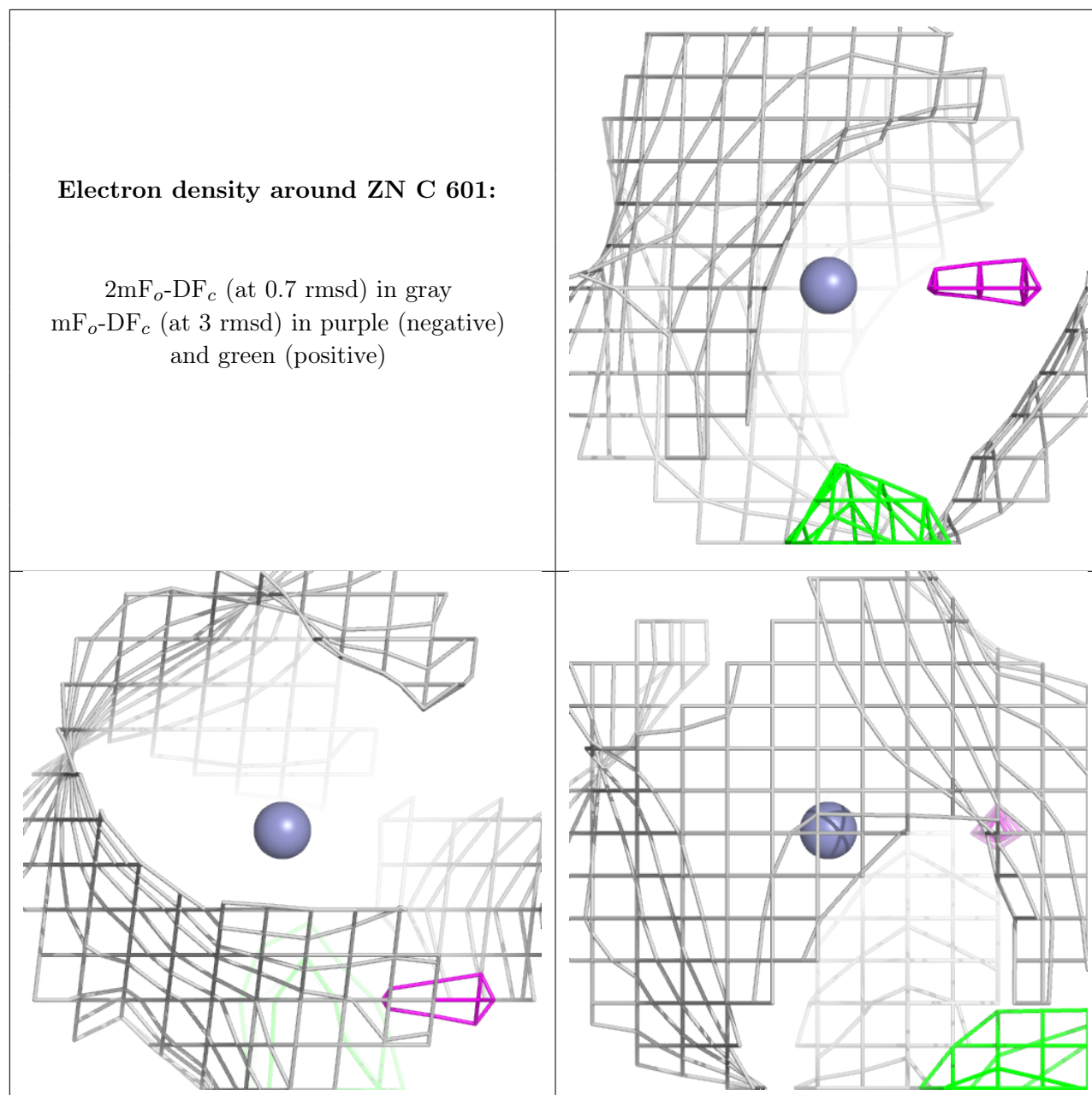
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	A	601	1/1	0.98	0.04	30,30,30,30	0
2	ZN	C	601	1/1	0.99	0.03	71,71,71,71	0

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 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 ⓘ

There are no such residues in this entry.