



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 9, 2026 – 01:19 AM JST

PDB ID : 9VVV / pdb_00009vvv
Title : Crystal structure of USP15 catalytic domain in complex with Ub-PA
Authors : Liu, B.; Xu, X.
Deposited on : 2025-07-16
Resolution : 2.30 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

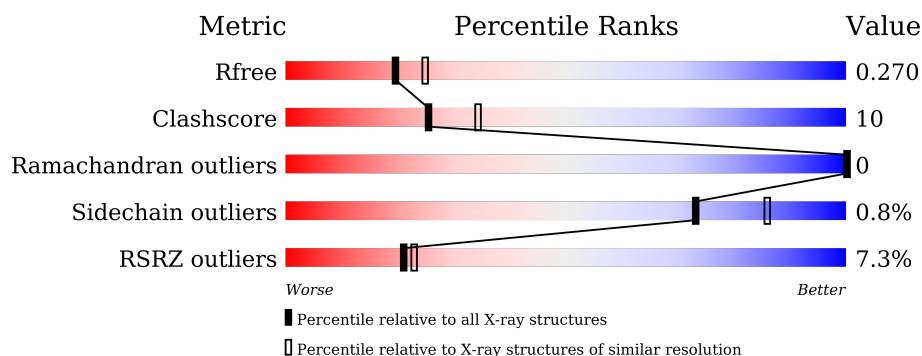
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	347	6% 78% 19% • •
1	B	347	11% 74% 20% • 5%
2	C	76	87% 13%
2	D	76	4% 74% 25% •

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 13112 atoms, of which 6408 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 15.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	338	Total	C	H	N	O	S	0	0	0
			5303	1729	2602	447	508	17			
1	B	331	Total	C	H	N	O	S	0	0	0
			5194	1692	2549	436	501	16			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	283	SER	-	expression tag	UNP Q9Y4E8
A	469	ALA	-	linker	UNP Q9Y4E8
A	470	SER	-	linker	UNP Q9Y4E8
A	783	THR	-	linker	UNP Q9Y4E8
A	784	SER	-	linker	UNP Q9Y4E8
A	785	LYS	-	linker	UNP Q9Y4E8
B	283	SER	-	expression tag	UNP Q9Y4E8
B	469	ALA	-	linker	UNP Q9Y4E8
B	470	SER	-	linker	UNP Q9Y4E8
B	783	THR	-	linker	UNP Q9Y4E8
B	784	SER	-	linker	UNP Q9Y4E8
B	785	LYS	-	linker	UNP Q9Y4E8

- Molecule 2 is a protein called Polyubiquitin-C.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	76	Total	C	H	N	O	S	0	0	0
			1227	379	626	105	116	1			
2	D	76	Total	C	H	N	O	S	0	0	0
			1227	379	626	105	116	1			

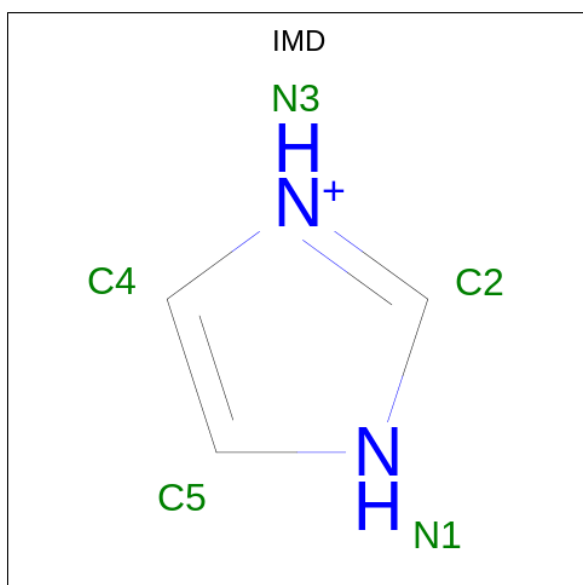
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	76	AYE	GLY	engineered mutation	UNP P0CG48
D	76	AYE	GLY	engineered mutation	UNP P0CG48

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 4 is IMIDAZOLE (CCD ID: IMD) (formula: C₃H₅N₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C H N 10 3 5 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	75	Total O 75 75	0	0
5	C	21	Total O 21 21	0	0
5	B	45	Total O 45 45	0	0

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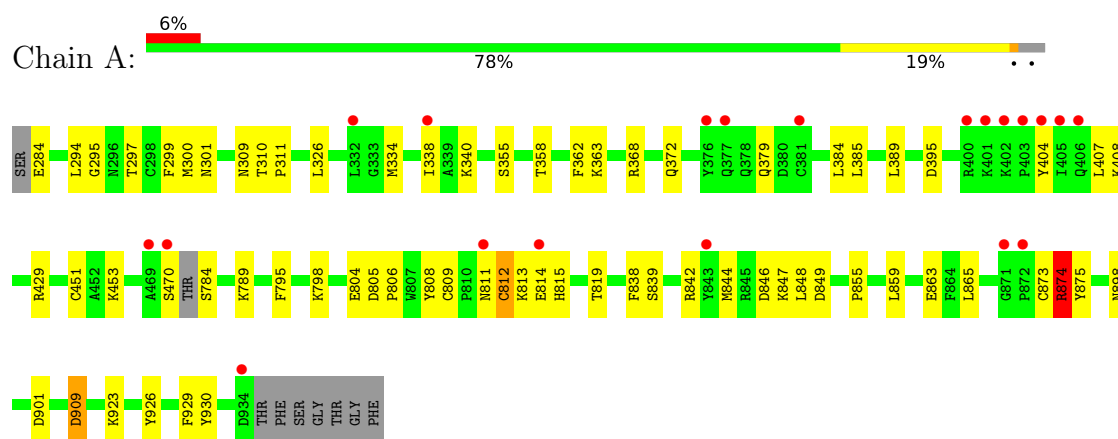
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	8	Total	O	0	0
			8	8		

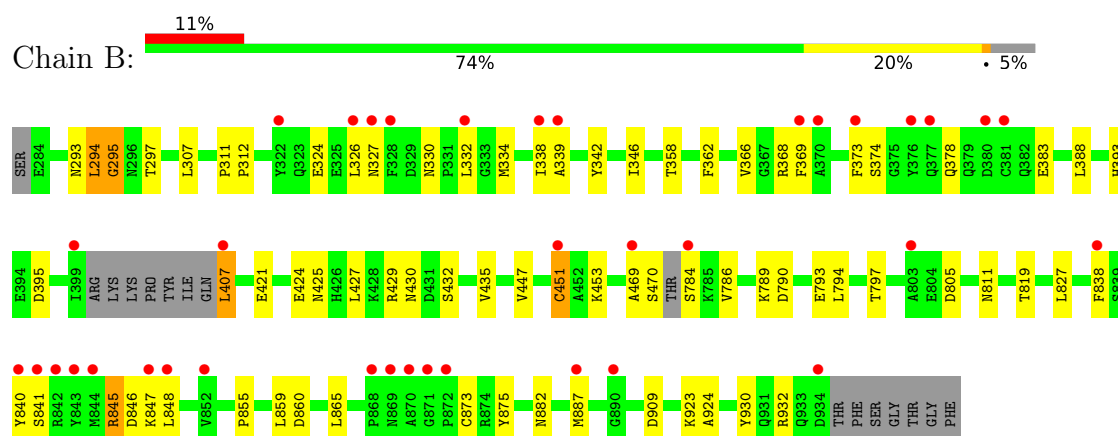
3 Residue-property plots

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.

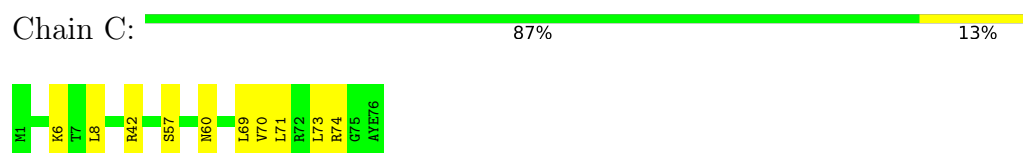
- Molecule 1: Ubiquitin carboxyl-terminal hydrolase 15



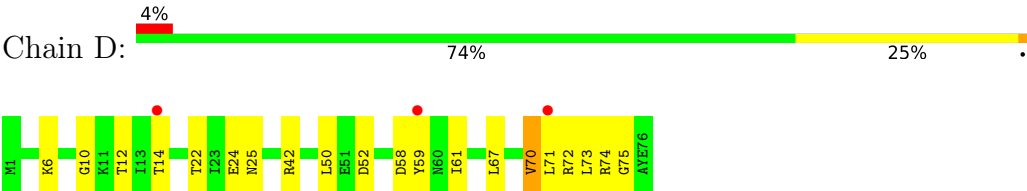
- Molecule 1: Ubiquitin carboxyl-terminal hydrolase 15



- Molecule 2: Polyubiquitin-C



- Molecule 2: Polyubiquitin-C



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	130.87Å 131.85Å 139.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.68 – 2.30 38.68 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (38.68-2.30) 99.6 (38.68-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 2.31Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.222 , 0.273 0.225 , 0.270	Depositor DCC
R_{free} test set	2660 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	47.0	Xtriage
Anisotropy	0.329	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 28.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13112	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% 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: AYE, IMD, 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	0.75	2/2770 (0.1%)	0.89	5/3753 (0.1%)
1	B	0.73	3/2711 (0.1%)	0.86	2/3671 (0.1%)
2	C	0.78	1/603 (0.2%)	0.86	0/811
2	D	0.63	1/603 (0.2%)	0.74	0/811
All	All	0.73	7/6687 (0.1%)	0.86	7/9046 (0.1%)

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
All	All	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	294	LEU	C-N	-6.92	1.23	1.33
1	A	310	THR	C-O	6.41	1.32	1.24
2	C	69	LEU	C-O	-6.09	1.16	1.24
1	B	841	SER	C-N	5.49	1.42	1.33
1	B	909	ASP	C-O	-5.23	1.19	1.24
1	A	909	ASP	C-O	-5.17	1.19	1.24
2	D	70	VAL	C-O	-5.14	1.18	1.24

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	812	CYS	N-CA-C	-7.88	100.10	110.43
1	B	294	LEU	O-C-N	-7.28	113.31	122.26
1	B	374	SER	N-CA-C	-6.46	100.27	109.96
1	A	812	CYS	N-CA-CB	6.11	119.00	110.26
1	A	812	CYS	CA-C-N	-5.76	114.59	123.17
1	A	812	CYS	C-N-CA	-5.76	114.59	123.17
1	A	874	ARG	CB-CA-C	5.68	120.22	109.37

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	874	ARG	Sidechain
1	B	295	GLY	Mainchain

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	2701	2602	2605	58	0
1	B	2645	2549	2549	59	0
2	C	601	626	630	13	0
2	D	601	626	631	16	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	5	5	5	0	0
5	A	75	0	0	0	0
5	B	45	0	0	2	0
5	C	21	0	0	0	0
5	D	8	0	0	0	0
All	All	6704	6408	6420	125	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 10.

All (125) 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:470:SER:HG	1:A:784:SER:N	1.37	1.18
1:A:838:PHE:CE1	2:C:73:LEU:HD13	2.07	0.90
1:A:844:MET:HE1	1:B:845:ARG:HH22	1.44	0.82
1:A:798:LYS:HD2	1:A:819:THR:HG21	1.63	0.78
1:A:470:SER:OG	1:A:784:SER:N	2.17	0.78
1:A:338:ILE:HG12	1:A:395:ASP:OD2	1.84	0.77
1:B:447:VAL:HB	1:B:819:THR:HG22	1.67	0.77
1:B:326:LEU:HD23	1:B:395:ASP:O	1.84	0.76
1:A:838:PHE:HE1	2:C:73:LEU:HD13	1.49	0.74
1:A:844:MET:HE1	1:B:845:ARG:NH2	2.02	0.73
1:B:827:LEU:O	1:B:932:ARG:NH1	2.22	0.72
1:A:301:ASN:ND2	1:A:909:ASP:OD1	2.17	0.71
1:B:793:GLU:O	1:B:797:THR:HG23	1.93	0.69
1:A:326:LEU:HD13	1:A:340:LYS:HD2	1.77	0.66
1:A:846:ASP:OD2	1:B:845:ARG:HD3	1.95	0.66
1:B:805:ASP:HB3	2:D:14:THR:HG22	1.78	0.65
1:B:378:GLN:O	2:D:74:ARG:NH1	2.30	0.64
1:A:814:GLU:CD	1:A:815:HIS:H	2.06	0.63
1:B:427:LEU:HD23	1:B:430:ASN:O	1.98	0.62
1:B:838:PHE:HB3	2:D:71:LEU:HD12	1.80	0.62
1:A:798:LYS:HD2	1:A:819:THR:CG2	2.28	0.62
1:A:838:PHE:CE1	2:C:73:LEU:CD1	2.81	0.61
2:D:61:ILE:HD13	2:D:67:LEU:HD21	1.83	0.61
1:B:887:MET:HE3	2:D:72:ARG:O	2.00	0.61
1:B:427:LEU:HD21	1:B:435:VAL:HG11	1.81	0.61
1:A:470:SER:OG	1:A:470:SER:O	2.17	0.61
1:B:432:SER:HG	1:B:435:VAL:H	1.48	0.60
1:B:429:ARG:NH2	2:D:58:ASP:O	2.35	0.60
1:B:327:ASN:OD1	1:B:330:ASN:HB2	2.02	0.60
1:B:294:LEU:HD21	1:B:358:THR:HG23	1.84	0.59
1:A:379:GLN:OE1	2:C:74:ARG:NH1	2.36	0.59
1:B:469:ALA:HB2	1:B:794:LEU:HD22	1.84	0.59
1:A:300:MET:HE1	1:A:363:LYS:HA	1.84	0.59
1:B:819:THR:HG23	5:B:1125:HOH:O	2.03	0.58
1:A:926:TYR:CE1	2:C:73:LEU:HD22	2.38	0.58
1:A:295:GLY:O	1:A:297:THR:HG23	2.03	0.58
1:B:421:GLU:HA	1:B:424:GLU:HG2	1.84	0.57
1:A:865:LEU:HD11	1:A:873:CYS:SG	2.44	0.57
1:B:326:LEU:HD21	1:B:339:ALA:HB3	1.86	0.57
2:C:8:LEU:HD21	2:C:71:LEU:HD13	1.86	0.57
1:A:849:ASP:O	1:A:923:LYS:HG2	2.05	0.57
1:B:295:GLY:O	1:B:297:THR:HG23	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:447:VAL:HB	1:B:819:THR:CG2	2.34	0.56
1:B:789:LYS:NZ	1:B:860:ASP:O	2.39	0.56
1:A:842:ARG:HG2	1:A:842:ARG:HH11	1.69	0.56
1:B:882:ASN:HB3	1:B:924:ALA:HB1	1.87	0.56
2:D:24:GLU:HB3	2:D:52:ASP:OD2	2.06	0.55
2:D:50:LEU:HD22	2:D:59:TYR:CD2	2.43	0.53
1:B:334:MET:HG3	1:B:369:PHE:HB2	1.90	0.53
1:A:806:PRO:HB2	1:A:815:HIS:HB3	1.90	0.53
1:A:404:TYR:CG	1:A:404:TYR:O	2.59	0.53
1:B:451:CYS:HB3	1:B:453:LYS:H	1.73	0.52
1:B:847:LYS:HG3	2:D:73:LEU:HD11	1.92	0.52
1:B:840:TYR:HD1	1:B:840:TYR:O	1.93	0.52
1:B:847:LYS:CG	2:D:73:LEU:HD11	2.40	0.51
1:B:330:ASN:OD1	1:B:332:LEU:HB2	2.10	0.51
1:A:309:ASN:O	1:A:311:PRO:HD3	2.11	0.51
1:B:786:VAL:HG12	1:B:790:ASP:HB2	1.92	0.51
1:A:875:TYR:HB3	1:A:930:TYR:HB3	1.93	0.50
1:B:855:PRO:HG2	1:B:859:LEU:HB2	1.94	0.50
1:B:362:PHE:O	1:B:366:VAL:HG13	2.13	0.49
1:A:804:GLU:C	1:A:806:PRO:HD3	2.37	0.49
1:B:334:MET:HE1	1:B:368:ARG:HB2	1.95	0.49
1:A:898:ASN:HB3	1:A:901:ASP:OD1	2.13	0.49
2:D:6:LYS:HD2	2:D:12:THR:OG1	2.13	0.49
1:B:427:LEU:CD2	1:B:430:ASN:O	2.60	0.48
1:A:404:TYR:O	1:A:404:TYR:CD2	2.67	0.48
1:B:865:LEU:HD11	1:B:873:CYS:SG	2.53	0.48
1:B:451:CYS:SG	1:B:811:ASN:ND2	2.68	0.47
1:A:284:GLU:OE1	1:A:355:SER:OG	2.31	0.47
1:B:334:MET:N	5:B:1105:HOH:O	2.47	0.47
1:A:789:LYS:NZ	1:A:863:GLU:OE2	2.43	0.47
1:B:393:HIS:HD1	1:B:432:SER:CB	2.27	0.47
1:A:805:ASP:N	1:A:806:PRO:HD3	2.30	0.47
1:A:926:TYR:CZ	2:C:73:LEU:HD22	2.49	0.47
2:D:6:LYS:HE2	2:D:10:GLY:O	2.15	0.46
1:A:846:ASP:OD1	1:A:847:LYS:N	2.48	0.46
1:A:798:LYS:CG	1:A:819:THR:HG23	2.46	0.45
1:B:427:LEU:CD2	1:B:435:VAL:HG11	2.47	0.45
1:A:855:PRO:HG2	1:A:859:LEU:HB2	1.99	0.45
1:A:839:SER:HB2	1:A:848:LEU:HD21	1.99	0.44
1:A:795:PHE:O	2:C:6:LYS:NZ	2.50	0.44
1:A:326:LEU:CD1	1:A:340:LYS:HD2	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:SER:CB	1:A:784:SER:N	2.80	0.44
1:B:838:PHE:O	1:B:848:LEU:HD12	2.18	0.44
1:A:294:LEU:HD21	1:A:358:THR:HG23	2.00	0.44
1:A:407:LEU:HG	1:A:408:LYS:N	2.31	0.44
1:A:811:ASN:C	1:A:812:CYS:O	2.59	0.44
1:A:300:MET:HA	1:A:384:LEU:HD22	1.98	0.44
1:B:451:CYS:SG	1:B:811:ASN:HB3	2.58	0.44
1:A:838:PHE:HE1	2:C:73:LEU:CD1	2.21	0.43
1:B:840:TYR:O	1:B:840:TYR:CD1	2.70	0.43
1:A:372:GLN:CD	1:A:372:GLN:H	2.26	0.43
1:A:429:ARG:HH22	2:C:60:ASN:HB2	1.84	0.43
1:A:798:LYS:HG3	1:A:819:THR:HG23	2.01	0.43
1:A:808:TYR:OH	1:A:813:LYS:HG3	2.19	0.43
1:A:300:MET:HE2	1:A:362:PHE:CD2	2.54	0.42
1:A:451:CYS:SG	1:A:453:LYS:HB2	2.59	0.42
1:A:809:CYS:O	1:A:812:CYS:O	2.37	0.42
1:B:373:PHE:HZ	1:B:383:GLU:HG2	1.84	0.42
1:B:324:GLU:OE1	1:B:324:GLU:N	2.51	0.42
1:B:882:ASN:HB3	1:B:924:ALA:CB	2.49	0.42
2:D:73:LEU:HD12	2:D:73:LEU:HA	1.93	0.42
1:B:338:ILE:C	1:B:338:ILE:HD12	2.44	0.42
1:B:887:MET:HE2	1:B:887:MET:HB3	1.89	0.42
1:A:385:LEU:HD11	1:A:929:PHE:HZ	1.85	0.42
1:B:388:LEU:C	1:B:388:LEU:HD13	2.44	0.42
1:B:875:TYR:HB3	1:B:930:TYR:HB3	2.02	0.42
2:C:42:ARG:HB2	2:C:70:VAL:HG23	2.02	0.42
1:B:342:TYR:CE2	1:B:346:ILE:HG13	2.55	0.42
1:A:926:TYR:CD1	2:C:73:LEU:HD22	2.55	0.41
1:B:311:PRO:N	1:B:312:PRO:CD	2.83	0.41
1:B:293:ASN:OD1	1:B:294:LEU:N	2.54	0.41
1:A:844:MET:HA	1:A:844:MET:HE2	2.03	0.41
1:B:470:SER:CB	1:B:784:SER:HG	2.34	0.41
1:A:334:MET:HE1	1:A:368:ARG:HB2	2.03	0.41
2:C:57:SER:O	2:C:60:ASN:N	2.35	0.41
1:B:307:LEU:CD1	1:B:388:LEU:HD12	2.51	0.41
1:B:407:LEU:HD21	1:B:425:ASN:OD1	2.20	0.41
2:D:42:ARG:HB2	2:D:70:VAL:HG23	2.03	0.41
1:A:299:PHE:CE1	1:A:379:GLN:HB2	2.56	0.41
1:B:827:LEU:HD23	1:B:827:LEU:HA	1.94	0.41
1:A:389:LEU:HD23	1:A:389:LEU:HA	1.86	0.40
1:B:378:GLN:HB3	2:D:75:GLY:C	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:22:THR:HG22	2:D:25:ASN:ND2	2.37	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	334/347 (96%)	316 (95%)	18 (5%)	0	100	100
1	B	325/347 (94%)	309 (95%)	16 (5%)	0	100	100
2	C	73/76 (96%)	70 (96%)	3 (4%)	0	100	100
2	D	73/76 (96%)	68 (93%)	5 (7%)	0	100	100
All	All	805/846 (95%)	763 (95%)	42 (5%)	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	295/306 (96%)	294 (100%)	1 (0%)	86	93
1	B	290/306 (95%)	285 (98%)	5 (2%)	53	72
2	C	68/68 (100%)	68 (100%)	0	100	100
2	D	68/68 (100%)	68 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	721/748 (96%)	715 (99%)	6 (1%)	73 86

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	874	ARG
1	B	407	LEU
1	B	451	CYS
1	B	845	ARG
1	B	846	ASP
1	B	923	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	348	GLN
1	B	430	ASN
1	B	815	HIS
1	B	834	HIS

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 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	IMD	A	1002	-	5,5,5	0.93	0	5,5,5	0.60	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	IMD	A	1002	-	-	-	0/1/1/1

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 [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	338/347 (97%)	0.32	20 (5%) 28 30	30, 55, 79, 98	0
1	B	331/347 (95%)	0.87	37 (11%) 10 11	45, 68, 99, 118	0
2	C	75/76 (98%)	-0.06	0 100 100	37, 49, 62, 70	0
2	D	75/76 (98%)	0.89	3 (4%) 42 44	48, 71, 89, 99	0
All	All	819/846 (96%)	0.56	60 (7%) 21 23	30, 61, 93, 118	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	407	LEU	6.2
1	A	469	ALA	4.9
1	B	399	ILE	4.4
1	B	872	PRO	4.2
1	A	400	ARG	3.9
1	B	380	ASP	3.8
1	B	842	ARG	3.8
1	A	401	LYS	3.5
1	B	871	GLY	3.5
1	B	848	LEU	3.4
1	B	843	TYR	3.3
1	B	934	ASP	3.3
2	D	14	THR	3.3
1	B	469	ALA	3.3
1	B	326	LEU	3.3
1	B	339	ALA	3.2
1	B	844	MET	3.2
1	B	328	PHE	3.2
1	A	402	LYS	3.1
1	B	377	GLN	3.1
1	A	470	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	868	PRO	3.0
1	B	332	LEU	2.9
1	B	852	VAL	2.9
1	B	451	CYS	2.9
1	A	404	TYR	2.8
1	A	405	ILE	2.7
1	B	870	ALA	2.7
1	B	887	MET	2.7
1	B	373	PHE	2.6
1	A	814	GLU	2.5
1	B	847	LYS	2.5
1	A	843	TYR	2.5
1	B	369	PHE	2.5
1	A	376	TYR	2.5
1	B	840	TYR	2.5
1	A	377	GLN	2.5
1	A	872	PRO	2.4
1	A	871	GLY	2.4
2	D	71	LEU	2.4
1	A	934	ASP	2.3
1	A	406	GLN	2.3
1	B	869	ASN	2.3
1	B	327	ASN	2.2
1	B	381	CYS	2.2
1	B	322	TYR	2.2
1	B	838	PHE	2.2
1	A	811	ASN	2.2
2	D	59	TYR	2.2
1	B	338	ILE	2.2
1	B	370	ALA	2.2
1	A	338	ILE	2.1
1	A	381	CYS	2.1
1	A	332	LEU	2.1
1	B	376	TYR	2.1
1	A	403	PRO	2.1
1	B	784	SER	2.1
1	B	803	ALA	2.1
1	B	890	GLY	2.1
1	B	841	SER	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](#)

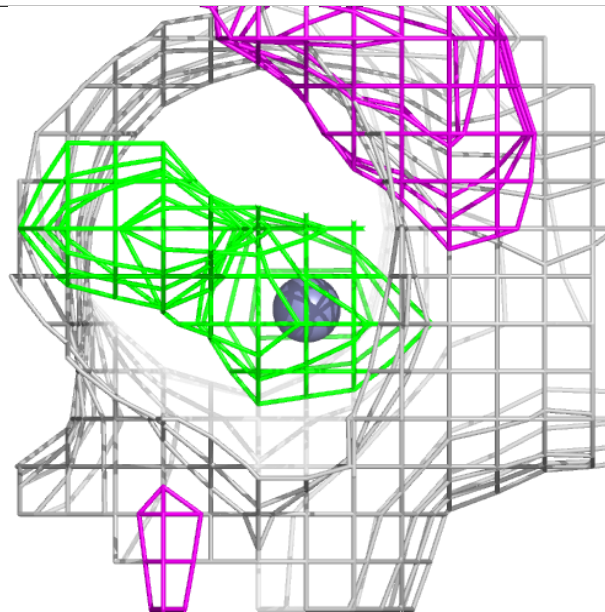
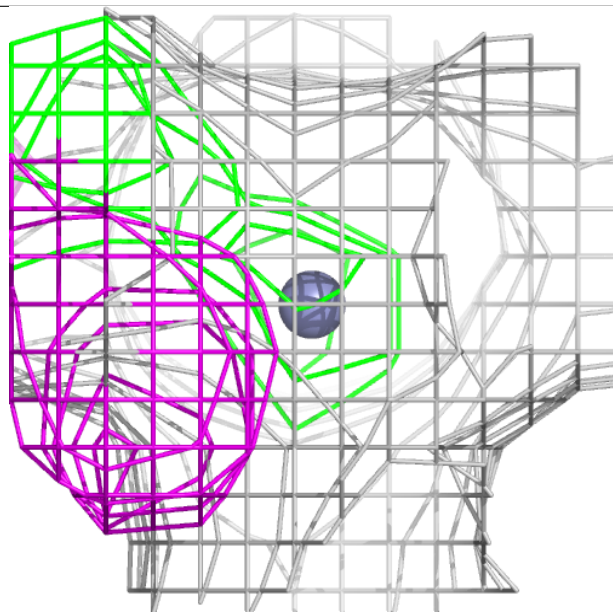
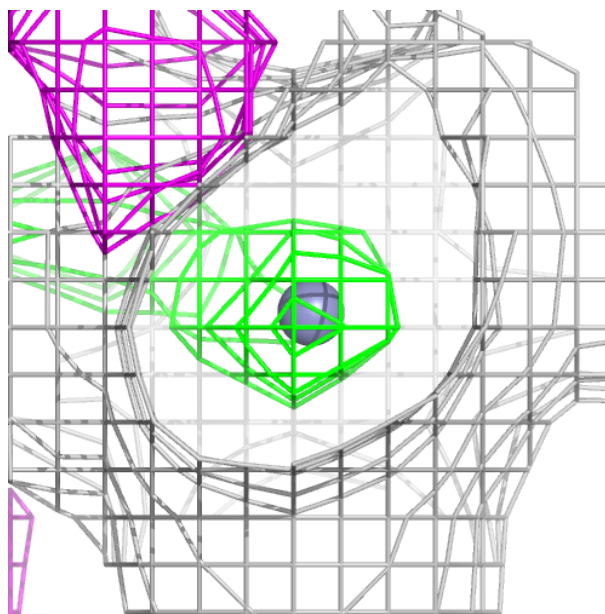
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	IMD	A	1002	5/5	0.70	0.24	47,54,64,65	0
3	ZN	B	1001	1/1	0.99	0.06	65,65,65,65	0
3	ZN	A	1001	1/1	0.99	0.04	40,40,40,40	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.

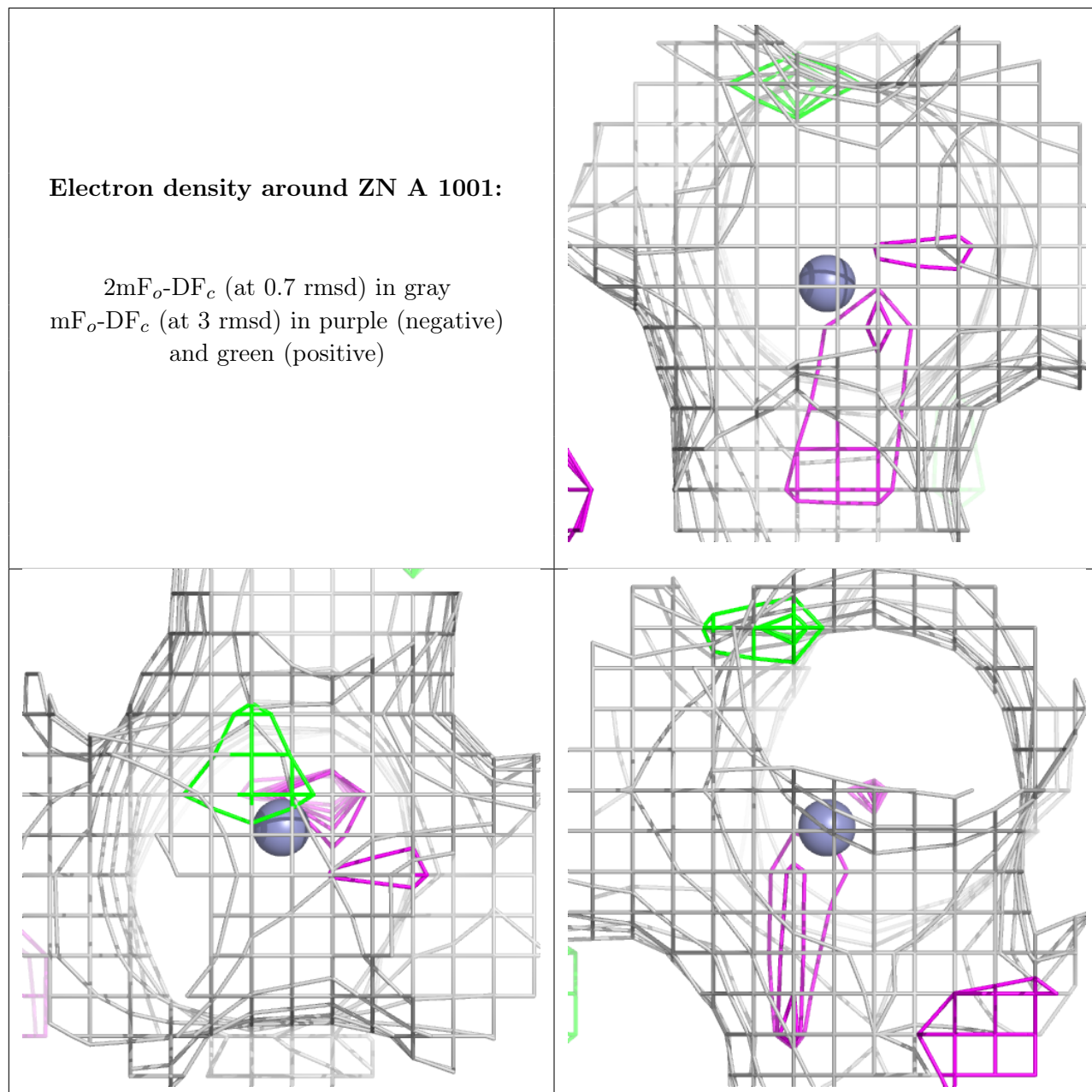
Electron density around ZN B 1001:

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



Electron density around ZN A 1001:

$2mF_o-DF_c$ (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.