



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 13, 2026 – 06:45 AM UTC

PDB ID : 8CX9 / pdb_00008cx9
Title : Structure of the SARS-COV2 PLpro (C111S) in complex with a dimeric Ubv
that inhibits activity by an unusual allosteric mechanism
Authors : Singer, A.U.; Slater, C.L.; Patel, A.; Russel, R.; Mark, B.L.; Sidhu, S.S.
Deposited on : 2022-05-20
Resolution : 3.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

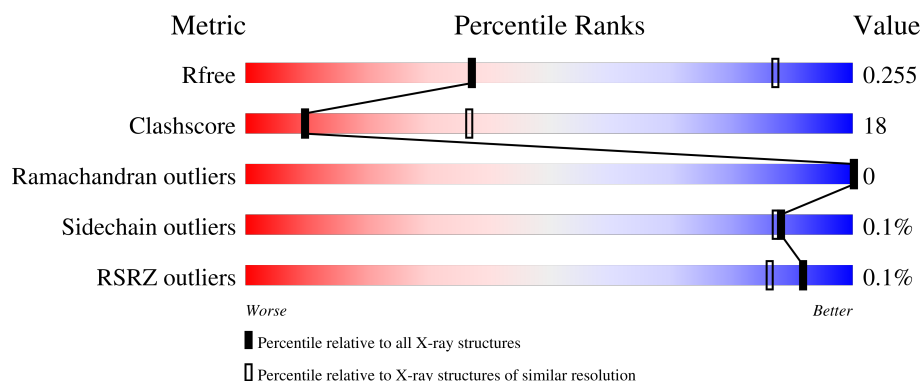
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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.



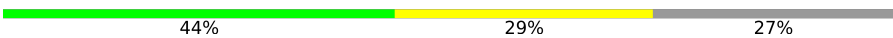
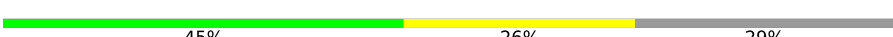
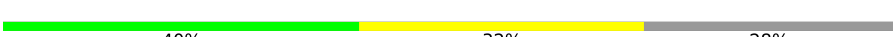
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	320	
1	B	320	
1	C	320	
1	D	320	
2	E	103	

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Mol	Chain	Length	Quality of chain
2	F	103	
2	G	103	
2	H	103	
2	I	103	
2	J	103	
2	K	103	
2	L	103	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BR	A	402	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13989 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 Papain-like protease nsp3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	314	Total	C	N	O	S	0	0	0
			2430	1542	399	470	19			
1	A	314	Total	C	N	O	S	0	0	0
			2450	1555	402	474	19			
1	C	312	Total	C	N	O	S	0	0	0
			2387	1514	392	462	19			
1	D	310	Total	C	N	O	S	0	0	0
			2365	1503	385	458	19			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLY	-	expression tag	UNP P0DTC1
B	-3	PRO	-	expression tag	UNP P0DTC1
B	-2	LEU	-	expression tag	UNP P0DTC1
B	-1	GLY	-	expression tag	UNP P0DTC1
B	0	SER	-	expression tag	UNP P0DTC1
A	-4	GLY	-	expression tag	UNP P0DTC1
A	-3	PRO	-	expression tag	UNP P0DTC1
A	-2	LEU	-	expression tag	UNP P0DTC1
A	-1	GLY	-	expression tag	UNP P0DTC1
A	0	SER	-	expression tag	UNP P0DTC1
C	-4	GLY	-	expression tag	UNP P0DTC1
C	-3	PRO	-	expression tag	UNP P0DTC1
C	-2	LEU	-	expression tag	UNP P0DTC1
C	-1	GLY	-	expression tag	UNP P0DTC1
C	0	SER	-	expression tag	UNP P0DTC1
D	-4	GLY	-	expression tag	UNP P0DTC1
D	-3	PRO	-	expression tag	UNP P0DTC1
D	-2	LEU	-	expression tag	UNP P0DTC1
D	-1	GLY	-	expression tag	UNP P0DTC1
D	0	SER	-	expression tag	UNP P0DTC1

- Molecule 2 is a protein called Ubiquitin variant UbV.CV2.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	74	Total	C	N	O	S	0	0	0
			571	358	97	113	3			
2	I	75	Total	C	N	O	S	0	0	0
			551	349	95	105	2			
2	F	75	Total	C	N	O	S	0	0	0
			580	365	100	112	3			
2	G	75	Total	C	N	O	S	0	0	0
			545	343	93	106	3			
2	K	73	Total	C	N	O	S	0	0	0
			505	316	86	101	2			
2	L	74	Total	C	N	O	S	0	0	0
			517	322	90	102	3			
2	H	74	Total	C	N	O	S	0	0	0
			545	344	94	104	3			
2	J	74	Total	C	N	O	S	0	0	0
			530	333	91	103	3			

There are 320 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-24	HIS	-	expression tag	UNP P62987
E	-23	HIS	-	expression tag	UNP P62987
E	-22	HIS	-	expression tag	UNP P62987
E	-21	HIS	-	expression tag	UNP P62987
E	-20	HIS	-	expression tag	UNP P62987
E	-19	HIS	-	expression tag	UNP P62987
E	-18	VAL	-	expression tag	UNP P62987
E	-17	THR	-	expression tag	UNP P62987
E	-16	SER	-	expression tag	UNP P62987
E	-15	LEU	-	expression tag	UNP P62987
E	-14	TYR	-	expression tag	UNP P62987
E	-13	LYS	-	expression tag	UNP P62987
E	-12	LYS	-	expression tag	UNP P62987
E	-11	ALA	-	expression tag	UNP P62987
E	-10	GLY	-	expression tag	UNP P62987
E	-9	SER	-	expression tag	UNP P62987
E	-8	THR	-	expression tag	UNP P62987
E	-7	ASP	-	expression tag	UNP P62987
E	-6	TYR	-	expression tag	UNP P62987
E	-5	LYS	-	expression tag	UNP P62987
E	-4	ASP	-	expression tag	UNP P62987
E	-3	ASP	-	expression tag	UNP P62987

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	ASP	-	expression tag	UNP P62987
E	-1	ASP	-	expression tag	UNP P62987
E	0	LYS	-	expression tag	UNP P62987
E	4	SER	PHE	variant	UNP P62987
E	9	MET	THR	variant	UNP P62987
E	10	ARG	GLY	variant	UNP P62987
E	12	ARG	THR	variant	UNP P62987
E	46	SER	ALA	variant	UNP P62987
E	48	MET	LYS	variant	UNP P62987
E	49	LEU	GLN	variant	UNP P62987
E	64	GLY	GLU	variant	UNP P62987
E	68	THR	HIS	variant	UNP P62987
E	70	GLY	VAL	variant	UNP P62987
E	72	ILE	ARG	variant	UNP P62987
E	75	ALA	GLY	variant	UNP P62987
E	76	ASN	GLY	variant	UNP P62987
E	77	GLY	-	insertion	UNP P62987
E	78	VAL	ILE	variant	UNP P62987
I	-24	HIS	-	expression tag	UNP P62987
I	-23	HIS	-	expression tag	UNP P62987
I	-22	HIS	-	expression tag	UNP P62987
I	-21	HIS	-	expression tag	UNP P62987
I	-20	HIS	-	expression tag	UNP P62987
I	-19	HIS	-	expression tag	UNP P62987
I	-18	VAL	-	expression tag	UNP P62987
I	-17	THR	-	expression tag	UNP P62987
I	-16	SER	-	expression tag	UNP P62987
I	-15	LEU	-	expression tag	UNP P62987
I	-14	TYR	-	expression tag	UNP P62987
I	-13	LYS	-	expression tag	UNP P62987
I	-12	LYS	-	expression tag	UNP P62987
I	-11	ALA	-	expression tag	UNP P62987
I	-10	GLY	-	expression tag	UNP P62987
I	-9	SER	-	expression tag	UNP P62987
I	-8	THR	-	expression tag	UNP P62987
I	-7	ASP	-	expression tag	UNP P62987
I	-6	TYR	-	expression tag	UNP P62987
I	-5	LYS	-	expression tag	UNP P62987
I	-4	ASP	-	expression tag	UNP P62987
I	-3	ASP	-	expression tag	UNP P62987
I	-2	ASP	-	expression tag	UNP P62987
I	-1	ASP	-	expression tag	UNP P62987

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Chain	Residue	Modelled	Actual	Comment	Reference
I	0	LYS	-	expression tag	UNP P62987
I	4	SER	PHE	variant	UNP P62987
I	9	MET	THR	variant	UNP P62987
I	10	ARG	GLY	variant	UNP P62987
I	12	ARG	THR	variant	UNP P62987
I	46	SER	ALA	variant	UNP P62987
I	48	MET	LYS	variant	UNP P62987
I	49	LEU	GLN	variant	UNP P62987
I	64	GLY	GLU	variant	UNP P62987
I	68	THR	HIS	variant	UNP P62987
I	70	GLY	VAL	variant	UNP P62987
I	72	ILE	ARG	variant	UNP P62987
I	75	ALA	GLY	variant	UNP P62987
I	76	ASN	GLY	variant	UNP P62987
I	77	GLY	-	insertion	UNP P62987
I	78	VAL	ILE	variant	UNP P62987
F	-24	HIS	-	expression tag	UNP P62987
F	-23	HIS	-	expression tag	UNP P62987
F	-22	HIS	-	expression tag	UNP P62987
F	-21	HIS	-	expression tag	UNP P62987
F	-20	HIS	-	expression tag	UNP P62987
F	-19	HIS	-	expression tag	UNP P62987
F	-18	VAL	-	expression tag	UNP P62987
F	-17	THR	-	expression tag	UNP P62987
F	-16	SER	-	expression tag	UNP P62987
F	-15	LEU	-	expression tag	UNP P62987
F	-14	TYR	-	expression tag	UNP P62987
F	-13	LYS	-	expression tag	UNP P62987
F	-12	LYS	-	expression tag	UNP P62987
F	-11	ALA	-	expression tag	UNP P62987
F	-10	GLY	-	expression tag	UNP P62987
F	-9	SER	-	expression tag	UNP P62987
F	-8	THR	-	expression tag	UNP P62987
F	-7	ASP	-	expression tag	UNP P62987
F	-6	TYR	-	expression tag	UNP P62987
F	-5	LYS	-	expression tag	UNP P62987
F	-4	ASP	-	expression tag	UNP P62987
F	-3	ASP	-	expression tag	UNP P62987
F	-2	ASP	-	expression tag	UNP P62987
F	-1	ASP	-	expression tag	UNP P62987
F	0	LYS	-	expression tag	UNP P62987
F	4	SER	PHE	variant	UNP P62987

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Chain	Residue	Modelled	Actual	Comment	Reference
F	9	MET	THR	variant	UNP P62987
F	10	ARG	GLY	variant	UNP P62987
F	12	ARG	THR	variant	UNP P62987
F	46	SER	ALA	variant	UNP P62987
F	48	MET	LYS	variant	UNP P62987
F	49	LEU	GLN	variant	UNP P62987
F	64	GLY	GLU	variant	UNP P62987
F	68	THR	HIS	variant	UNP P62987
F	70	GLY	VAL	variant	UNP P62987
F	72	ILE	ARG	variant	UNP P62987
F	75	ALA	GLY	variant	UNP P62987
F	76	ASN	GLY	variant	UNP P62987
F	77	GLY	-	insertion	UNP P62987
F	78	VAL	ILE	variant	UNP P62987
G	-24	HIS	-	expression tag	UNP P62987
G	-23	HIS	-	expression tag	UNP P62987
G	-22	HIS	-	expression tag	UNP P62987
G	-21	HIS	-	expression tag	UNP P62987
G	-20	HIS	-	expression tag	UNP P62987
G	-19	HIS	-	expression tag	UNP P62987
G	-18	VAL	-	expression tag	UNP P62987
G	-17	THR	-	expression tag	UNP P62987
G	-16	SER	-	expression tag	UNP P62987
G	-15	LEU	-	expression tag	UNP P62987
G	-14	TYR	-	expression tag	UNP P62987
G	-13	LYS	-	expression tag	UNP P62987
G	-12	LYS	-	expression tag	UNP P62987
G	-11	ALA	-	expression tag	UNP P62987
G	-10	GLY	-	expression tag	UNP P62987
G	-9	SER	-	expression tag	UNP P62987
G	-8	THR	-	expression tag	UNP P62987
G	-7	ASP	-	expression tag	UNP P62987
G	-6	TYR	-	expression tag	UNP P62987
G	-5	LYS	-	expression tag	UNP P62987
G	-4	ASP	-	expression tag	UNP P62987
G	-3	ASP	-	expression tag	UNP P62987
G	-2	ASP	-	expression tag	UNP P62987
G	-1	ASP	-	expression tag	UNP P62987
G	0	LYS	-	expression tag	UNP P62987
G	4	SER	PHE	variant	UNP P62987
G	9	MET	THR	variant	UNP P62987
G	10	ARG	GLY	variant	UNP P62987

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Chain	Residue	Modelled	Actual	Comment	Reference
G	12	ARG	THR	variant	UNP P62987
G	46	SER	ALA	variant	UNP P62987
G	48	MET	LYS	variant	UNP P62987
G	49	LEU	GLN	variant	UNP P62987
G	64	GLY	GLU	variant	UNP P62987
G	68	THR	HIS	variant	UNP P62987
G	70	GLY	VAL	variant	UNP P62987
G	72	ILE	ARG	variant	UNP P62987
G	75	ALA	GLY	variant	UNP P62987
G	76	ASN	GLY	variant	UNP P62987
G	77	GLY	-	insertion	UNP P62987
G	78	VAL	ILE	variant	UNP P62987
K	-24	HIS	-	expression tag	UNP P62987
K	-23	HIS	-	expression tag	UNP P62987
K	-22	HIS	-	expression tag	UNP P62987
K	-21	HIS	-	expression tag	UNP P62987
K	-20	HIS	-	expression tag	UNP P62987
K	-19	HIS	-	expression tag	UNP P62987
K	-18	VAL	-	expression tag	UNP P62987
K	-17	THR	-	expression tag	UNP P62987
K	-16	SER	-	expression tag	UNP P62987
K	-15	LEU	-	expression tag	UNP P62987
K	-14	TYR	-	expression tag	UNP P62987
K	-13	LYS	-	expression tag	UNP P62987
K	-12	LYS	-	expression tag	UNP P62987
K	-11	ALA	-	expression tag	UNP P62987
K	-10	GLY	-	expression tag	UNP P62987
K	-9	SER	-	expression tag	UNP P62987
K	-8	THR	-	expression tag	UNP P62987
K	-7	ASP	-	expression tag	UNP P62987
K	-6	TYR	-	expression tag	UNP P62987
K	-5	LYS	-	expression tag	UNP P62987
K	-4	ASP	-	expression tag	UNP P62987
K	-3	ASP	-	expression tag	UNP P62987
K	-2	ASP	-	expression tag	UNP P62987
K	-1	ASP	-	expression tag	UNP P62987
K	0	LYS	-	expression tag	UNP P62987
K	4	SER	PHE	variant	UNP P62987
K	9	MET	THR	variant	UNP P62987
K	10	ARG	GLY	variant	UNP P62987
K	12	ARG	THR	variant	UNP P62987
K	46	SER	ALA	variant	UNP P62987

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Chain	Residue	Modelled	Actual	Comment	Reference
K	48	MET	LYS	variant	UNP P62987
K	49	LEU	GLN	variant	UNP P62987
K	64	GLY	GLU	variant	UNP P62987
K	68	THR	HIS	variant	UNP P62987
K	70	GLY	VAL	variant	UNP P62987
K	72	ILE	ARG	variant	UNP P62987
K	75	ALA	GLY	variant	UNP P62987
K	76	ASN	GLY	variant	UNP P62987
K	77	GLY	-	insertion	UNP P62987
K	78	VAL	ILE	variant	UNP P62987
L	-24	HIS	-	expression tag	UNP P62987
L	-23	HIS	-	expression tag	UNP P62987
L	-22	HIS	-	expression tag	UNP P62987
L	-21	HIS	-	expression tag	UNP P62987
L	-20	HIS	-	expression tag	UNP P62987
L	-19	HIS	-	expression tag	UNP P62987
L	-18	VAL	-	expression tag	UNP P62987
L	-17	THR	-	expression tag	UNP P62987
L	-16	SER	-	expression tag	UNP P62987
L	-15	LEU	-	expression tag	UNP P62987
L	-14	TYR	-	expression tag	UNP P62987
L	-13	LYS	-	expression tag	UNP P62987
L	-12	LYS	-	expression tag	UNP P62987
L	-11	ALA	-	expression tag	UNP P62987
L	-10	GLY	-	expression tag	UNP P62987
L	-9	SER	-	expression tag	UNP P62987
L	-8	THR	-	expression tag	UNP P62987
L	-7	ASP	-	expression tag	UNP P62987
L	-6	TYR	-	expression tag	UNP P62987
L	-5	LYS	-	expression tag	UNP P62987
L	-4	ASP	-	expression tag	UNP P62987
L	-3	ASP	-	expression tag	UNP P62987
L	-2	ASP	-	expression tag	UNP P62987
L	-1	ASP	-	expression tag	UNP P62987
L	0	LYS	-	expression tag	UNP P62987
L	4	SER	PHE	variant	UNP P62987
L	9	MET	THR	variant	UNP P62987
L	10	ARG	GLY	variant	UNP P62987
L	12	ARG	THR	variant	UNP P62987
L	46	SER	ALA	variant	UNP P62987
L	48	MET	LYS	variant	UNP P62987
L	49	LEU	GLN	variant	UNP P62987

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Chain	Residue	Modelled	Actual	Comment	Reference
L	64	GLY	GLU	variant	UNP P62987
L	68	THR	HIS	variant	UNP P62987
L	70	GLY	VAL	variant	UNP P62987
L	72	ILE	ARG	variant	UNP P62987
L	75	ALA	GLY	variant	UNP P62987
L	76	ASN	GLY	variant	UNP P62987
L	77	GLY	-	insertion	UNP P62987
L	78	VAL	ILE	variant	UNP P62987
H	-24	HIS	-	expression tag	UNP P62987
H	-23	HIS	-	expression tag	UNP P62987
H	-22	HIS	-	expression tag	UNP P62987
H	-21	HIS	-	expression tag	UNP P62987
H	-20	HIS	-	expression tag	UNP P62987
H	-19	HIS	-	expression tag	UNP P62987
H	-18	VAL	-	expression tag	UNP P62987
H	-17	THR	-	expression tag	UNP P62987
H	-16	SER	-	expression tag	UNP P62987
H	-15	LEU	-	expression tag	UNP P62987
H	-14	TYR	-	expression tag	UNP P62987
H	-13	LYS	-	expression tag	UNP P62987
H	-12	LYS	-	expression tag	UNP P62987
H	-11	ALA	-	expression tag	UNP P62987
H	-10	GLY	-	expression tag	UNP P62987
H	-9	SER	-	expression tag	UNP P62987
H	-8	THR	-	expression tag	UNP P62987
H	-7	ASP	-	expression tag	UNP P62987
H	-6	TYR	-	expression tag	UNP P62987
H	-5	LYS	-	expression tag	UNP P62987
H	-4	ASP	-	expression tag	UNP P62987
H	-3	ASP	-	expression tag	UNP P62987
H	-2	ASP	-	expression tag	UNP P62987
H	-1	ASP	-	expression tag	UNP P62987
H	0	LYS	-	expression tag	UNP P62987
H	4	SER	PHE	variant	UNP P62987
H	9	MET	THR	variant	UNP P62987
H	10	ARG	GLY	variant	UNP P62987
H	12	ARG	THR	variant	UNP P62987
H	46	SER	ALA	variant	UNP P62987
H	48	MET	LYS	variant	UNP P62987
H	49	LEU	GLN	variant	UNP P62987
H	64	GLY	GLU	variant	UNP P62987
H	68	THR	HIS	variant	UNP P62987

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Chain	Residue	Modelled	Actual	Comment	Reference
H	70	GLY	VAL	variant	UNP P62987
H	72	ILE	ARG	variant	UNP P62987
H	75	ALA	GLY	variant	UNP P62987
H	76	ASN	GLY	variant	UNP P62987
H	77	GLY	-	insertion	UNP P62987
H	78	VAL	ILE	variant	UNP P62987
J	-24	HIS	-	expression tag	UNP P62987
J	-23	HIS	-	expression tag	UNP P62987
J	-22	HIS	-	expression tag	UNP P62987
J	-21	HIS	-	expression tag	UNP P62987
J	-20	HIS	-	expression tag	UNP P62987
J	-19	HIS	-	expression tag	UNP P62987
J	-18	VAL	-	expression tag	UNP P62987
J	-17	THR	-	expression tag	UNP P62987
J	-16	SER	-	expression tag	UNP P62987
J	-15	LEU	-	expression tag	UNP P62987
J	-14	TYR	-	expression tag	UNP P62987
J	-13	LYS	-	expression tag	UNP P62987
J	-12	LYS	-	expression tag	UNP P62987
J	-11	ALA	-	expression tag	UNP P62987
J	-10	GLY	-	expression tag	UNP P62987
J	-9	SER	-	expression tag	UNP P62987
J	-8	THR	-	expression tag	UNP P62987
J	-7	ASP	-	expression tag	UNP P62987
J	-6	TYR	-	expression tag	UNP P62987
J	-5	LYS	-	expression tag	UNP P62987
J	-4	ASP	-	expression tag	UNP P62987
J	-3	ASP	-	expression tag	UNP P62987
J	-2	ASP	-	expression tag	UNP P62987
J	-1	ASP	-	expression tag	UNP P62987
J	0	LYS	-	expression tag	UNP P62987
J	4	SER	PHE	variant	UNP P62987
J	9	MET	THR	variant	UNP P62987
J	10	ARG	GLY	variant	UNP P62987
J	12	ARG	THR	variant	UNP P62987
J	46	SER	ALA	variant	UNP P62987
J	48	MET	LYS	variant	UNP P62987
J	49	LEU	GLN	variant	UNP P62987
J	64	GLY	GLU	variant	UNP P62987
J	68	THR	HIS	variant	UNP P62987
J	70	GLY	VAL	variant	UNP P62987
J	72	ILE	ARG	variant	UNP P62987

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Chain	Residue	Modelled	Actual	Comment	Reference
J	75	ALA	GLY	variant	UNP P62987
J	76	ASN	GLY	variant	UNP P62987
J	77	GLY	-	insertion	UNP P62987
J	78	VAL	ILE	variant	UNP P62987

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

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

- Molecule 4 is BROMIDE ION (CCD ID: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Br	0	0
			1	1		
4	A	2	Total	Br	0	0
			2	2		
4	D	1	Total	Br	0	0
			1	1		
4	E	1	Total	Br	0	0
			1	1		
4	F	1	Total	Br	0	0
			1	1		

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Na	0	0
			1	1		
5	C	1	Total	Na	0	0
			1	1		

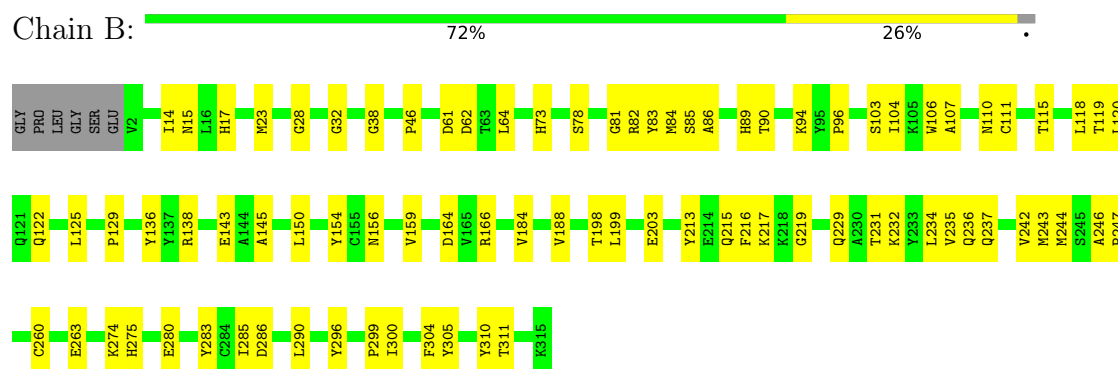
- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total 1	Cl 1	0	0

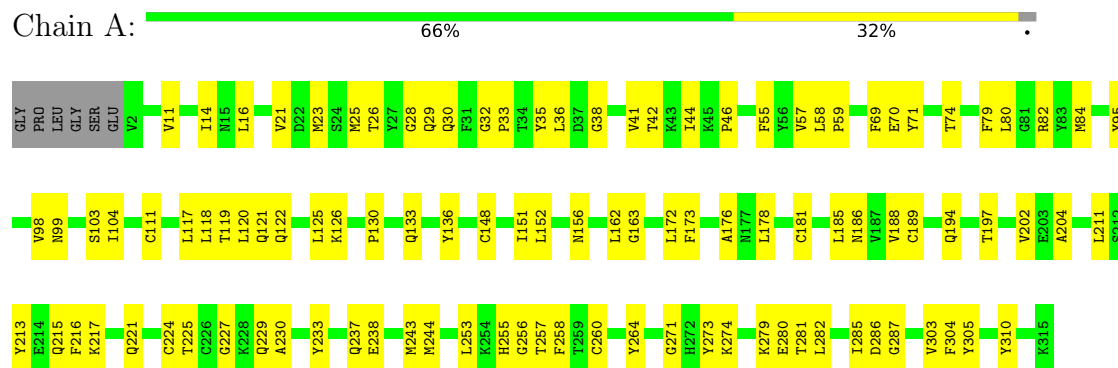
3 Residue-property plots [i](#)

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.

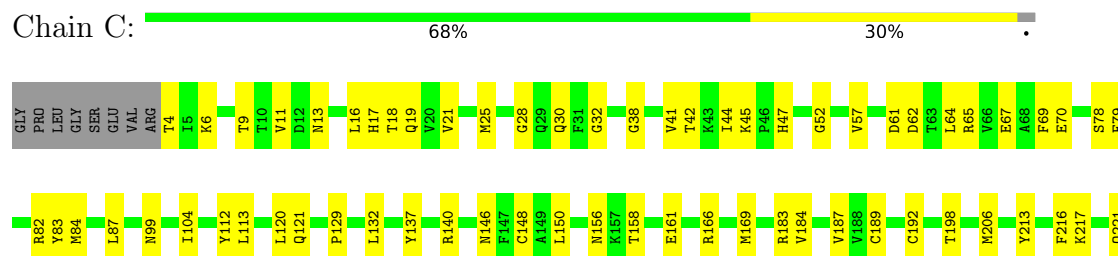
• Molecule 1: Papain-like protease nsp3



• Molecule 1: Papain-like protease nsp3



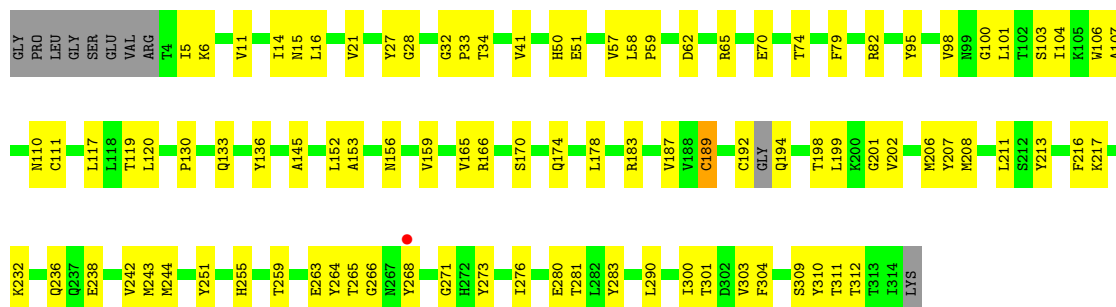
• Molecule 1: Papain-like protease nsp3





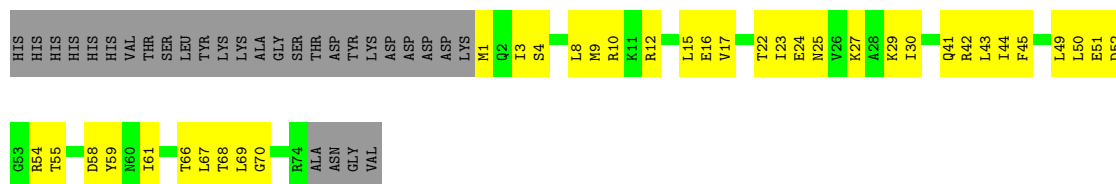
- Molecule 1: Papain-like protease nsp3

Chain D: 67% 29% .



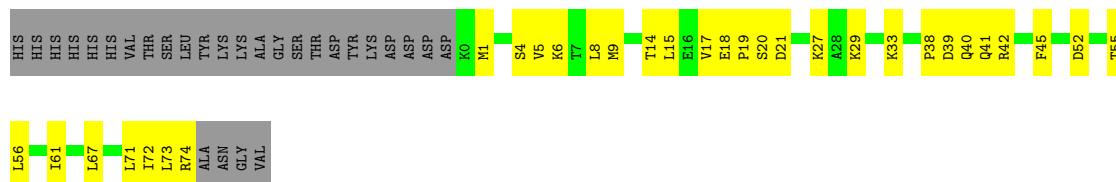
- Molecule 2: Ubiquitin variant UbV.CV2.1

Chain E: 37% 35% 28%



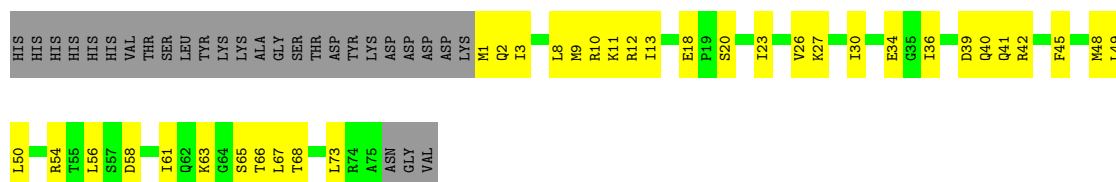
- Molecule 2: Ubiquitin variant UbV.CV2.1

Chain I: 43% 30% 27%



- Molecule 2: Ubiquitin variant UbV.CV2.1

Chain F: 39% 34% 27%



- Molecule 2: Ubiquitin variant UbV.CV2.1

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.58Å 174.86Å 121.56Å 90.00° 95.74° 90.00°	Depositor
Resolution (Å)	47.79 – 3.50 47.79 – 3.50	Depositor EDS
% Data completeness (in resolution range)	81.5 (47.79-3.50) 81.5 (47.79-3.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.225 , 0.270 (Not available) , 0.255	Depositor DCC
R_{free} test set	2000 reflections (6.99%)	wwPDB-VP
Wilson B-factor (Å ²)	61.5	Xtriage
Anisotropy	0.562	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 48.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	13989	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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: ZN, BR, CL, NA

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	0.19	0/2509	0.47	0/3416
1	B	0.19	0/2488	0.46	0/3390
1	C	0.21	0/2445	0.55	0/3338
1	D	0.22	0/2422	0.53	0/3310
2	E	0.23	0/575	0.54	0/775
2	F	0.29	0/584	0.56	0/785
2	G	0.28	0/549	0.62	0/742
2	H	0.29	0/549	0.62	0/741
2	I	0.29	0/555	0.68	0/750
2	J	0.35	1/534 (0.2%)	0.67	0/724
2	K	0.20	0/509	0.59	0/692
2	L	0.28	0/520	0.75	0/707
All	All	0.23	1/14239 (0.0%)	0.55	0/19370

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	23	ILE	CG1-CD1	-5.12	1.31	1.51

There are no bond angle outliers.

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	2450	0	2324	81	0
1	B	2430	0	2295	61	1
1	C	2387	0	2220	82	0
1	D	2365	0	2185	86	0
2	E	571	0	592	48	0
2	F	580	0	615	32	0
2	G	545	0	548	35	0
2	H	545	0	556	20	1
2	I	551	0	566	33	0
2	J	530	0	519	24	0
2	K	505	0	470	27	0
2	L	517	0	490	33	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	2	0	0	3	0
4	B	1	0	0	1	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	1	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	D	1	0	0	1	0
All	All	13989	0	13380	482	1

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 18.

The worst 5 of 482 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:D:189:CYS:SG	1:D:192:CYS:HB2	1.99	1.02
1:D:283:TYR:HD2	1:D:290:LEU:HD11	1.36	0.91
2:J:23:ILE:HD11	2:J:54:ARG:H	1.36	0.87
1:A:23:MET:HA	1:A:46:PRO:HG2	1.59	0.85
2:I:15:LEU:HD22	2:I:29:LYS:HZ3	1.45	0.81

All (1) 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:215:GLN:OE1	2:H:57:SER:OG[1_554]	2.07	0.13

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	312/320 (98%)	295 (95%)	17 (5%)	0	100	100
1	B	312/320 (98%)	293 (94%)	19 (6%)	0	100	100
1	C	310/320 (97%)	284 (92%)	26 (8%)	0	100	100
1	D	306/320 (96%)	284 (93%)	22 (7%)	0	100	100
2	E	72/103 (70%)	65 (90%)	7 (10%)	0	100	100
2	F	73/103 (71%)	65 (89%)	8 (11%)	0	100	100
2	G	73/103 (71%)	65 (89%)	8 (11%)	0	100	100
2	H	72/103 (70%)	64 (89%)	8 (11%)	0	100	100
2	I	73/103 (71%)	64 (88%)	9 (12%)	0	100	100
2	J	72/103 (70%)	68 (94%)	4 (6%)	0	100	100
2	K	71/103 (69%)	67 (94%)	4 (6%)	0	100	100
2	L	72/103 (70%)	59 (82%)	13 (18%)	0	100	100
All	All	1818/2104 (86%)	1673 (92%)	145 (8%)	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	263/278 (95%)	263 (100%)	0	100	100
1	B	259/278 (93%)	259 (100%)	0	100	100
1	C	250/278 (90%)	250 (100%)	0	100	100
1	D	246/278 (88%)	245 (100%)	1 (0%)	84	81
2	E	65/93 (70%)	65 (100%)	0	100	100
2	F	66/93 (71%)	66 (100%)	0	100	100
2	G	58/93 (62%)	58 (100%)	0	100	100
2	H	58/93 (62%)	58 (100%)	0	100	100
2	I	59/93 (63%)	59 (100%)	0	100	100
2	J	54/93 (58%)	54 (100%)	0	100	100
2	K	48/93 (52%)	48 (100%)	0	100	100
2	L	50/93 (54%)	50 (100%)	0	100	100
All	All	1476/1856 (80%)	1475 (100%)	1 (0%)	88	87

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	189	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	308	ASN
1	D	30	GLN
2	G	41	GLN
2	E	60	ASN
2	F	41	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](#)

Of 13 ligands modelled in this entry, 13 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 [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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	314/320 (98%)	-0.28	0	100	100	26, 49, 89, 107	0
1	B	314/320 (98%)	-0.26	0	100	100	28, 46, 74, 102	0
1	C	312/320 (97%)	-0.15	0	100	100	24, 53, 95, 108	0
1	D	310/320 (96%)	-0.06	1 (0%)	90	76	37, 70, 102, 150	0
2	E	74/103 (71%)	-0.32	0	100	100	35, 50, 77, 93	0
2	F	75/103 (72%)	-0.20	0	100	100	35, 50, 70, 98	0
2	G	75/103 (72%)	-0.08	0	100	100	35, 68, 91, 101	0
2	H	74/103 (71%)	-0.00	0	100	100	44, 67, 99, 107	0
2	I	75/103 (72%)	-0.14	0	100	100	43, 82, 101, 108	0
2	J	74/103 (71%)	0.09	0	100	100	59, 92, 102, 119	0
2	K	73/103 (70%)	0.17	0	100	100	67, 96, 119, 134	0
2	L	74/103 (71%)	0.21	0	100	100	87, 109, 132, 167	0
All	All	1844/2104 (87%)	-0.14	1 (0%)	92	86	24, 59, 105, 167	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	268	TYR	2.8

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

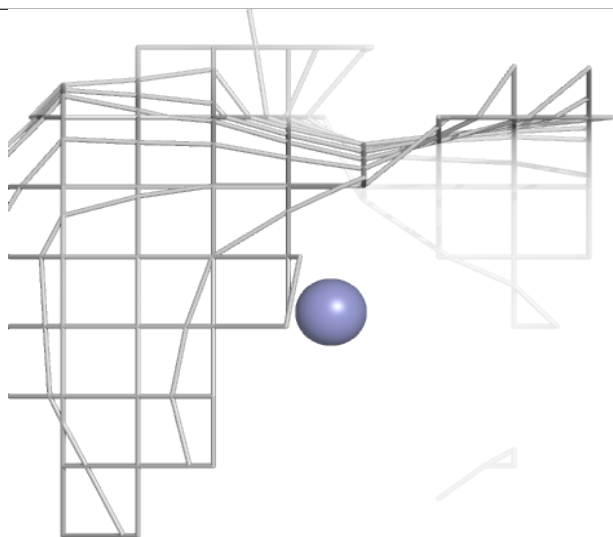
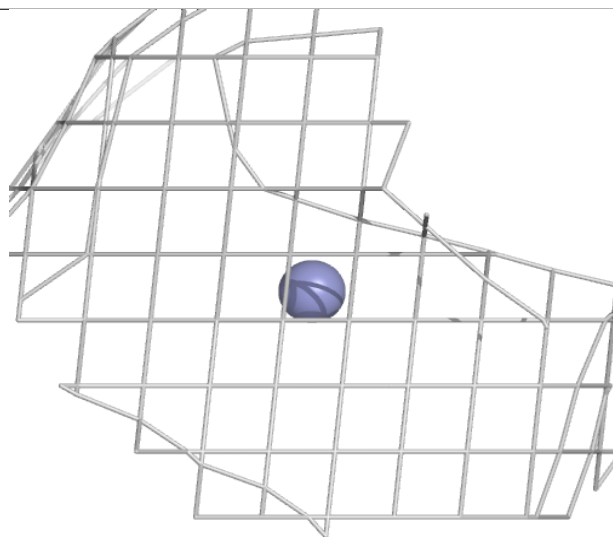
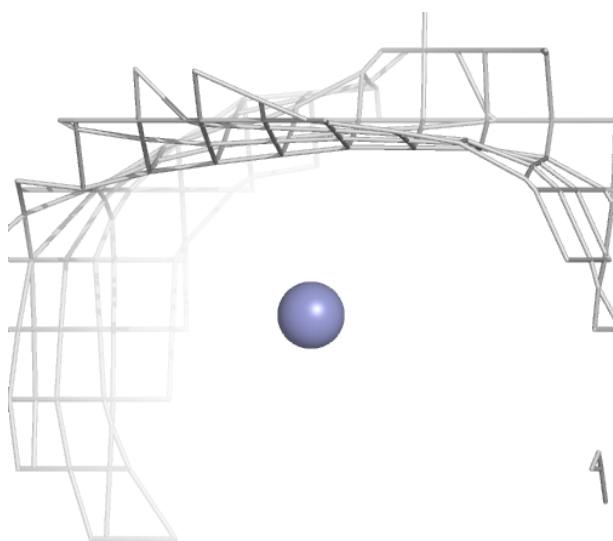
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NA	C	402	1/1	0.73	0.19	36,36,36,36	0
5	NA	A	404	1/1	0.76	0.22	26,26,26,26	0
3	ZN	D	401	1/1	0.86	0.08	185,185,185,185	0
4	BR	D	402	1/1	0.86	0.10	104,104,104,104	0
3	ZN	A	401	1/1	0.88	0.08	57,57,57,57	0
6	CL	D	403	1/1	0.89	0.07	53,53,53,53	0
4	BR	A	402	1/1	0.90	0.08	87,87,87,87	0
4	BR	F	101	1/1	0.93	0.05	82,82,82,82	0
4	BR	E	101	1/1	0.94	0.08	62,62,62,62	0
4	BR	B	402	1/1	0.96	0.07	77,77,77,77	0
3	ZN	B	401	1/1	0.97	0.04	66,66,66,66	0
4	BR	A	403	1/1	0.97	0.09	86,86,86,86	0
3	ZN	C	401	1/1	1.00	0.04	49,49,49,49	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.

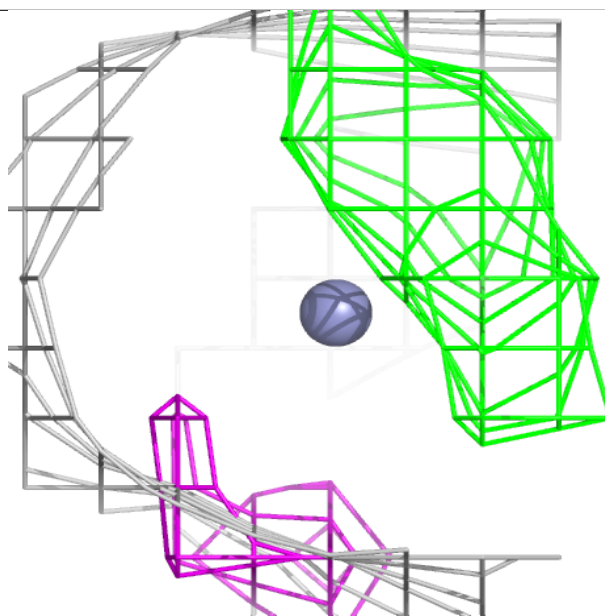
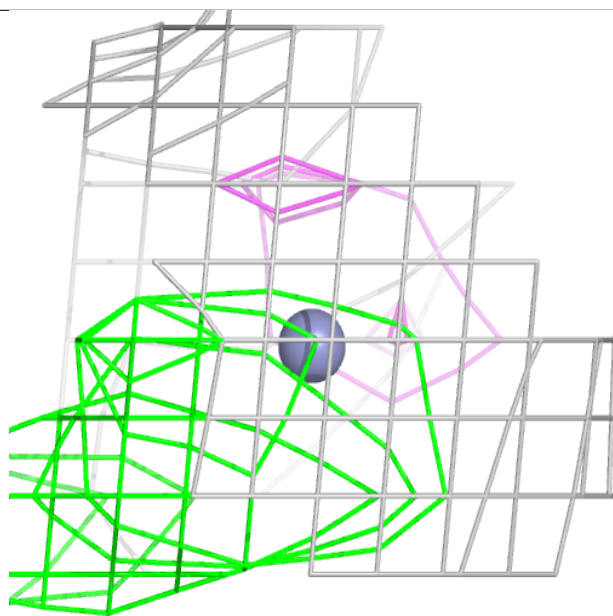
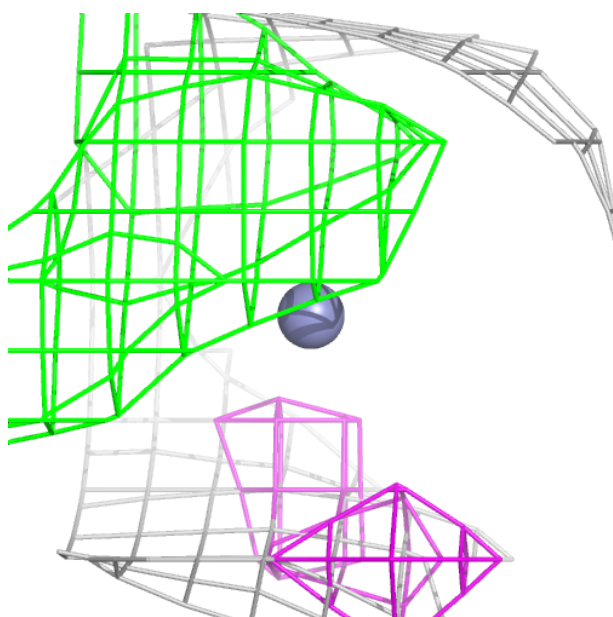
Electron density around ZN D 401:

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



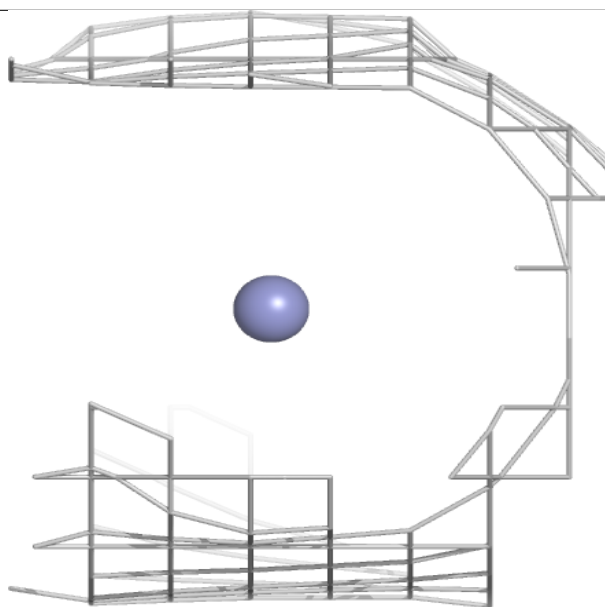
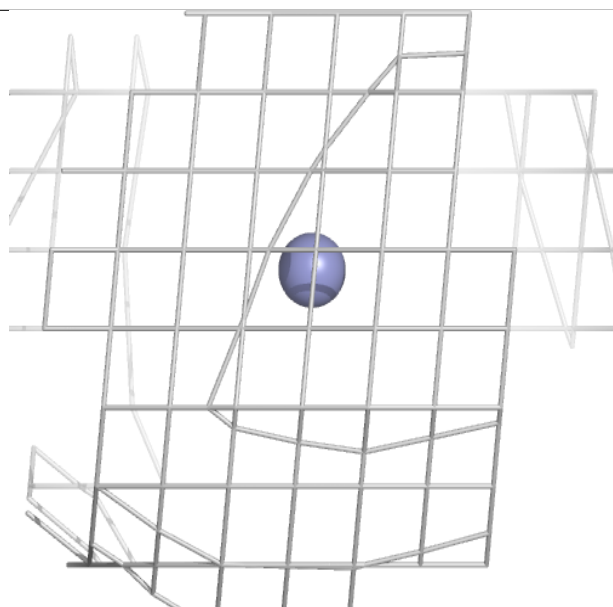
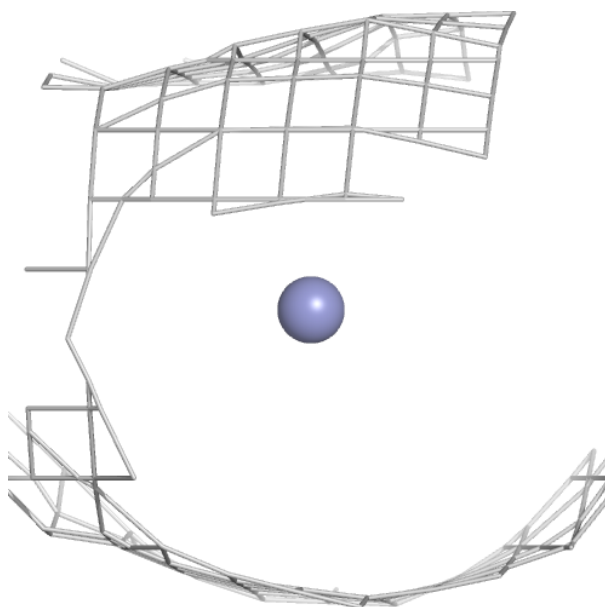
Electron density around ZN A 401:

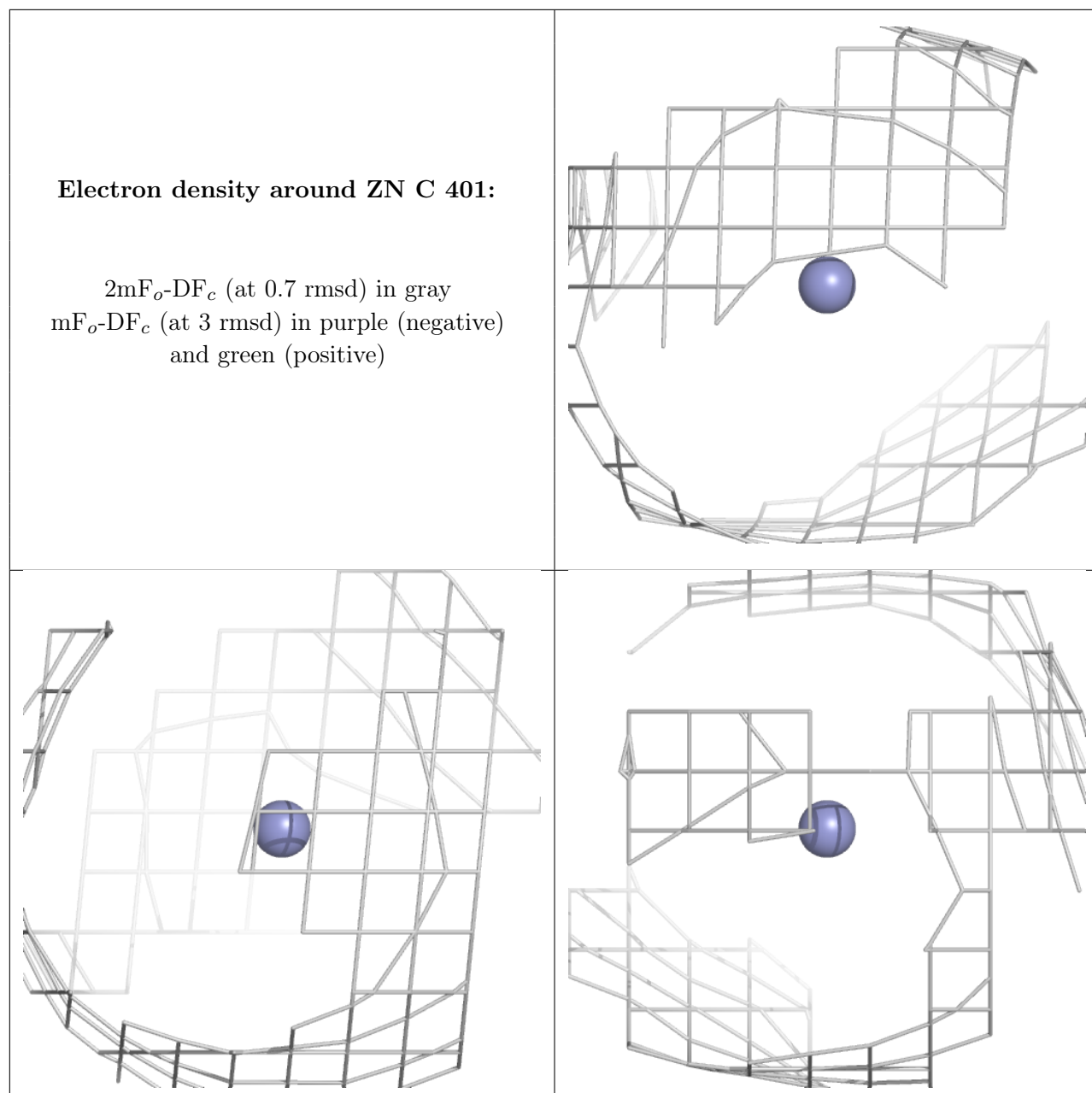
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN B 401:

$2mF_o-DF_c$ (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.