



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 02:19 AM UTC

PDB ID : 6LKX / pdb_00006lkx
Title : The structure of PRRSV helicase
Authors : Shi, Y.J.; Tong, X.H.; Peng, G.Q.
Deposited on : 2019-12-20
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
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

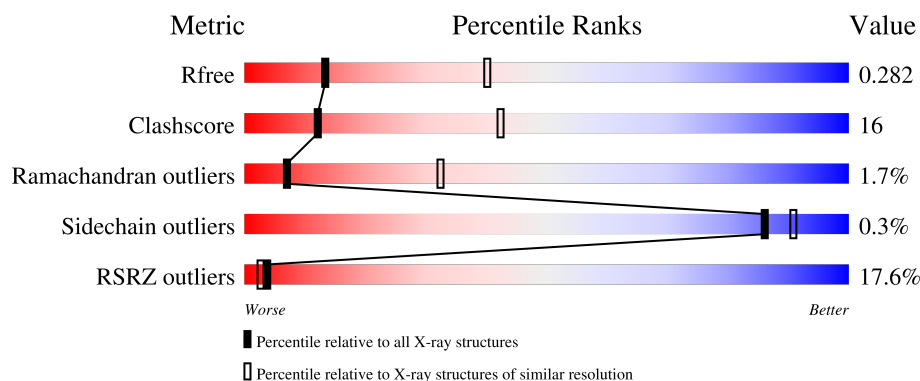
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	499	
1	B	499	

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
2	ZN	B	501	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7061 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 RNA-dependent RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	441	Total	C	N	O	S	0	0	0
			3438	2160	625	628	25			
1	B	441	Total	C	N	O	S	0	0	0
			3439	2160	626	628	25			

There are 116 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-49	MET	-	initiating methionine	UNP D2CSC7
A	-48	HIS	-	expression tag	UNP D2CSC7
A	-47	HIS	-	expression tag	UNP D2CSC7
A	-46	HIS	-	expression tag	UNP D2CSC7
A	-45	HIS	-	expression tag	UNP D2CSC7
A	-44	HIS	-	expression tag	UNP D2CSC7
A	-43	HIS	-	expression tag	UNP D2CSC7
A	-42	SER	-	expression tag	UNP D2CSC7
A	-41	SER	-	expression tag	UNP D2CSC7
A	-40	GLY	-	expression tag	UNP D2CSC7
A	-39	LEU	-	expression tag	UNP D2CSC7
A	-38	VAL	-	expression tag	UNP D2CSC7
A	-37	PRO	-	expression tag	UNP D2CSC7
A	-36	ARG	-	expression tag	UNP D2CSC7
A	-35	GLY	-	expression tag	UNP D2CSC7
A	-34	SER	-	expression tag	UNP D2CSC7
A	-33	GLY	-	expression tag	UNP D2CSC7
A	-32	MET	-	expression tag	UNP D2CSC7
A	-31	LYS	-	expression tag	UNP D2CSC7
A	-30	GLU	-	expression tag	UNP D2CSC7
A	-29	THR	-	expression tag	UNP D2CSC7
A	-28	ALA	-	expression tag	UNP D2CSC7
A	-27	ALA	-	expression tag	UNP D2CSC7
A	-26	ALA	-	expression tag	UNP D2CSC7
A	-25	LYS	-	expression tag	UNP D2CSC7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	PHE	-	expression tag	UNP D2CSC7
A	-23	GLU	-	expression tag	UNP D2CSC7
A	-22	ARG	-	expression tag	UNP D2CSC7
A	-21	GLN	-	expression tag	UNP D2CSC7
A	-20	HIS	-	expression tag	UNP D2CSC7
A	-19	MET	-	expression tag	UNP D2CSC7
A	-18	ASP	-	expression tag	UNP D2CSC7
A	-17	SER	-	expression tag	UNP D2CSC7
A	-16	PRO	-	expression tag	UNP D2CSC7
A	-15	ASP	-	expression tag	UNP D2CSC7
A	-14	LEU	-	expression tag	UNP D2CSC7
A	-13	GLY	-	expression tag	UNP D2CSC7
A	-12	THR	-	expression tag	UNP D2CSC7
A	-11	ASP	-	expression tag	UNP D2CSC7
A	-10	ASP	-	expression tag	UNP D2CSC7
A	-9	ASP	-	expression tag	UNP D2CSC7
A	-8	ASP	-	expression tag	UNP D2CSC7
A	-7	LYS	-	expression tag	UNP D2CSC7
A	-6	ALA	-	expression tag	UNP D2CSC7
A	-5	MET	-	expression tag	UNP D2CSC7
A	-4	ALA	-	expression tag	UNP D2CSC7
A	-3	ASP	-	expression tag	UNP D2CSC7
A	-2	ILE	-	expression tag	UNP D2CSC7
A	-1	GLY	-	expression tag	UNP D2CSC7
A	0	SER	-	expression tag	UNP D2CSC7
A	442	LEU	-	expression tag	UNP D2CSC7
A	443	GLU	-	expression tag	UNP D2CSC7
A	444	HIS	-	expression tag	UNP D2CSC7
A	445	HIS	-	expression tag	UNP D2CSC7
A	446	HIS	-	expression tag	UNP D2CSC7
A	447	HIS	-	expression tag	UNP D2CSC7
A	448	HIS	-	expression tag	UNP D2CSC7
A	449	HIS	-	expression tag	UNP D2CSC7
B	-49	MET	-	initiating methionine	UNP D2CSC7
B	-48	HIS	-	expression tag	UNP D2CSC7
B	-47	HIS	-	expression tag	UNP D2CSC7
B	-46	HIS	-	expression tag	UNP D2CSC7
B	-45	HIS	-	expression tag	UNP D2CSC7
B	-44	HIS	-	expression tag	UNP D2CSC7
B	-43	HIS	-	expression tag	UNP D2CSC7
B	-42	SER	-	expression tag	UNP D2CSC7
B	-41	SER	-	expression tag	UNP D2CSC7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-40	GLY	-	expression tag	UNP D2CSC7
B	-39	LEU	-	expression tag	UNP D2CSC7
B	-38	VAL	-	expression tag	UNP D2CSC7
B	-37	PRO	-	expression tag	UNP D2CSC7
B	-36	ARG	-	expression tag	UNP D2CSC7
B	-35	GLY	-	expression tag	UNP D2CSC7
B	-34	SER	-	expression tag	UNP D2CSC7
B	-33	GLY	-	expression tag	UNP D2CSC7
B	-32	MET	-	expression tag	UNP D2CSC7
B	-31	LYS	-	expression tag	UNP D2CSC7
B	-30	GLU	-	expression tag	UNP D2CSC7
B	-29	THR	-	expression tag	UNP D2CSC7
B	-28	ALA	-	expression tag	UNP D2CSC7
B	-27	ALA	-	expression tag	UNP D2CSC7
B	-26	ALA	-	expression tag	UNP D2CSC7
B	-25	LYS	-	expression tag	UNP D2CSC7
B	-24	PHE	-	expression tag	UNP D2CSC7
B	-23	GLU	-	expression tag	UNP D2CSC7
B	-22	ARG	-	expression tag	UNP D2CSC7
B	-21	GLN	-	expression tag	UNP D2CSC7
B	-20	HIS	-	expression tag	UNP D2CSC7
B	-19	MET	-	expression tag	UNP D2CSC7
B	-18	ASP	-	expression tag	UNP D2CSC7
B	-17	SER	-	expression tag	UNP D2CSC7
B	-16	PRO	-	expression tag	UNP D2CSC7
B	-15	ASP	-	expression tag	UNP D2CSC7
B	-14	LEU	-	expression tag	UNP D2CSC7
B	-13	GLY	-	expression tag	UNP D2CSC7
B	-12	THR	-	expression tag	UNP D2CSC7
B	-11	ASP	-	expression tag	UNP D2CSC7
B	-10	ASP	-	expression tag	UNP D2CSC7
B	-9	ASP	-	expression tag	UNP D2CSC7
B	-8	ASP	-	expression tag	UNP D2CSC7
B	-7	LYS	-	expression tag	UNP D2CSC7
B	-6	ALA	-	expression tag	UNP D2CSC7
B	-5	MET	-	expression tag	UNP D2CSC7
B	-4	ALA	-	expression tag	UNP D2CSC7
B	-3	ASP	-	expression tag	UNP D2CSC7
B	-2	ILE	-	expression tag	UNP D2CSC7
B	-1	GLY	-	expression tag	UNP D2CSC7
B	0	SER	-	expression tag	UNP D2CSC7
B	442	LEU	-	expression tag	UNP D2CSC7

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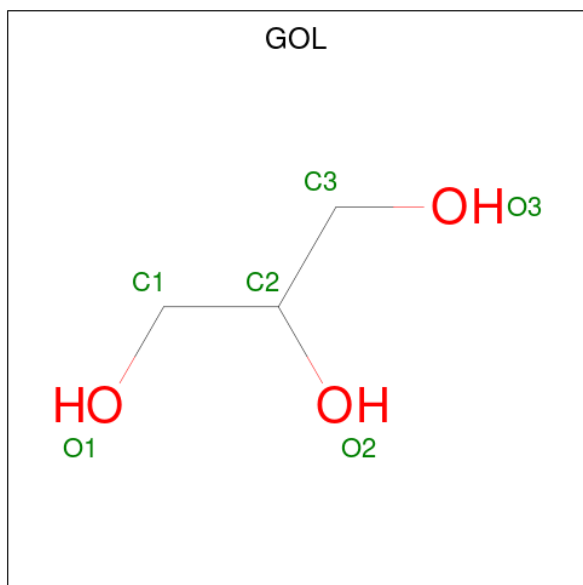
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Chain	Residue	Modelled	Actual	Comment	Reference
B	443	GLU	-	expression tag	UNP D2CSC7
B	444	HIS	-	expression tag	UNP D2CSC7
B	445	HIS	-	expression tag	UNP D2CSC7
B	446	HIS	-	expression tag	UNP D2CSC7
B	447	HIS	-	expression tag	UNP D2CSC7
B	448	HIS	-	expression tag	UNP D2CSC7
B	449	HIS	-	expression tag	UNP D2CSC7

- 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	3	Total Zn 3 3	0	0
2	B	3	Total Zn 3 3	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



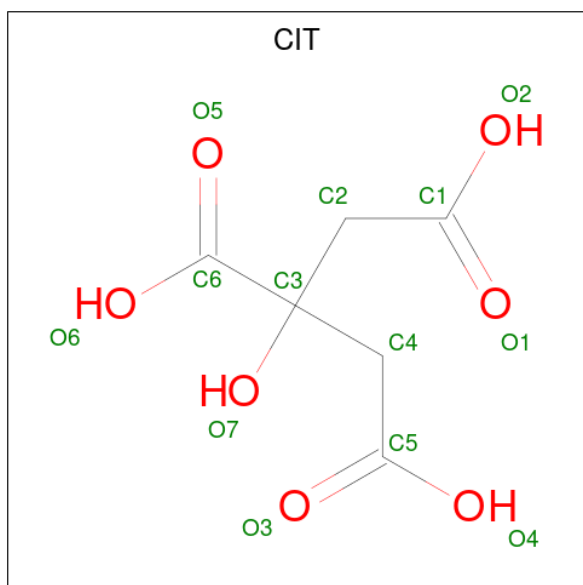
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	6	7		
4	B	1	Total	C	O	0	0
			13	6	7		
4	B	1	Total	C	O	0	0
			13	6	7		

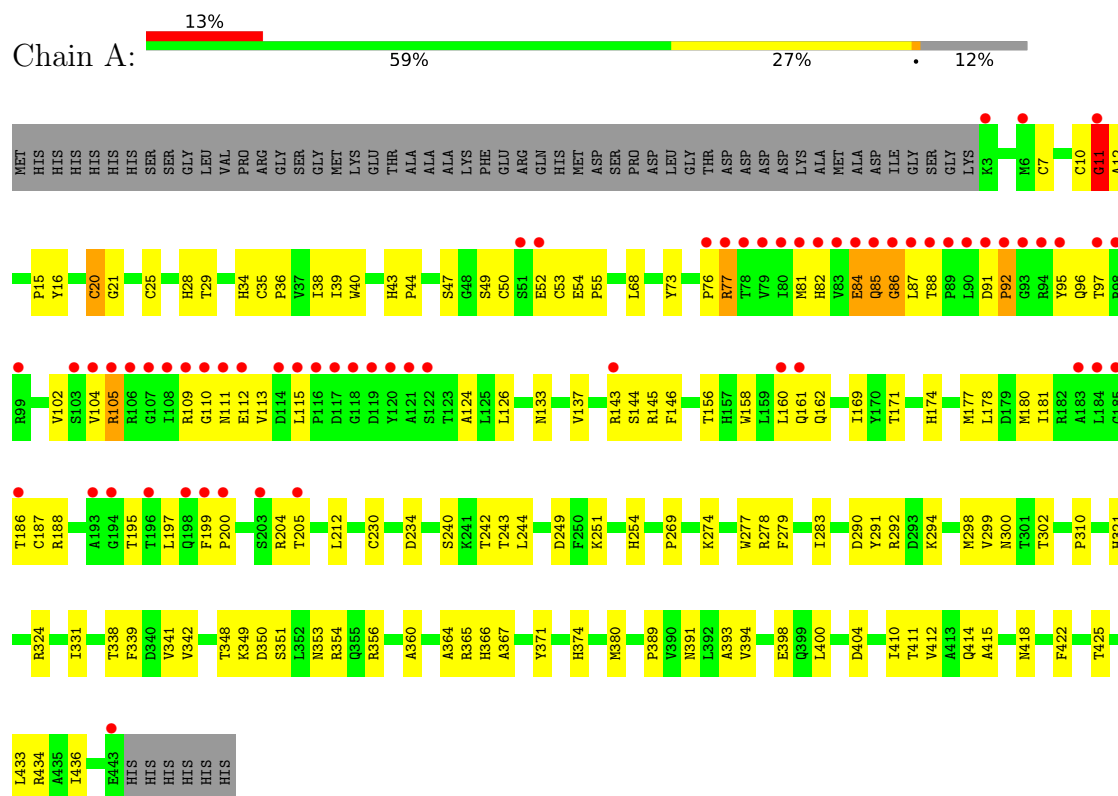
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	46	Total	O	0	0
			46	46		
5	B	63	Total	O	0	0
			63	63		

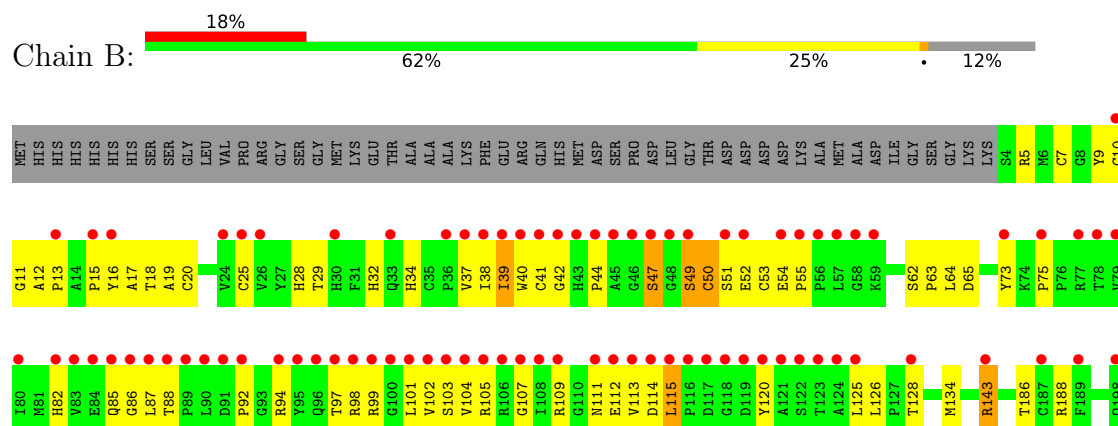
3 Residue-property plots

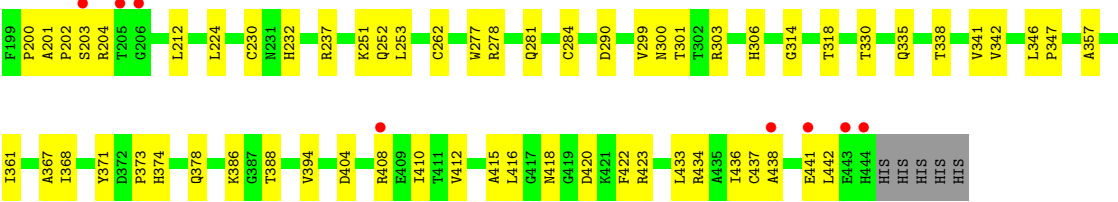
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: RNA-dependent RNA polymerase





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	93.62Å 93.62Å 357.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.81 – 3.00 46.81 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.81-3.00) 99.8 (46.81-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.38 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.225 , 0.281 0.227 , 0.282	Depositor DCC
R_{free} test set	2000 reflections (6.05%)	wwPDB-VP
Wilson B-factor (Å ²)	31.0	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	7061	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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: CIT, ZN, GOL

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	0.47	1/3521 (0.0%)	0.70	2/4794 (0.0%)
1	B	0.45	0/3523	0.70	3/4798 (0.1%)
All	All	0.46	1/7044 (0.0%)	0.70	5/9592 (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	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	389	PRO	N-CA	-5.04	1.43	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	408	ARG	CG-CD-NE	7.30	128.06	112.00
1	B	143	ARG	NE-CZ-NH1	-7.26	114.24	121.50
1	A	77	ARG	CG-CD-NE	5.80	124.75	112.00
1	B	143	ARG	NH1-CZ-NH2	5.13	125.97	119.30
1	A	425	THR	N-CA-C	-5.12	108.78	114.62

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	11	GLY	Peptide
1	A	20	CYS	Peptide

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	3438	0	3405	109	1
1	B	3439	0	3400	110	1
2	A	3	0	0	0	0
2	B	3	0	0	2	0
3	A	18	0	24	2	0
3	B	12	0	16	2	0
4	A	13	0	5	1	0
4	B	26	0	10	1	0
5	A	46	0	0	4	0
5	B	63	0	0	2	0
All	All	7061	0	6860	214	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 16.

All (214) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:CYS:HG	2:B:501:ZN:ZN	0.75	0.96
1:A:10:CYS:O	1:A:12:ALA:N	2.01	0.93
1:B:10:CYS:O	1:B:12:ALA:N	2.01	0.92
1:B:39:ILE:HG22	1:B:40:TRP:H	1.38	0.86
1:B:10:CYS:HB3	1:B:28:HIS:HE1	1.43	0.81
1:B:98:ARG:HH11	1:B:120:TYR:HD1	1.25	0.81
1:B:50:CYS:SG	1:B:51:SER:N	2.54	0.81
1:B:9:TYR:OH	1:B:65:ASP:OD1	2.02	0.77
1:B:10:CYS:SG	1:B:28:HIS:ND1	2.61	0.74
1:B:50:CYS:HB3	1:B:53:CYS:SG	2.27	0.73
1:A:87:LEU:HD22	1:A:110:GLY:HA3	1.71	0.73
1:A:91:ASP:CG	1:A:92:PRO:HD2	2.15	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:CYS:HB3	1:B:28:HIS:CE1	2.25	0.71
1:B:278:ARG:HH21	4:B:505:CIT:H21	1.55	0.71
1:A:109:ARG:H	1:A:109:ARG:HD2	1.57	0.69
1:A:10:CYS:HB3	1:A:28:HIS:CE1	2.28	0.69
1:A:391:ASN:HD21	1:A:418:ASN:HD21	1.39	0.68
1:A:15:PRO:HG2	1:A:16:TYR:CD2	2.29	0.68
1:B:188:ARG:HG2	1:B:204:ARG:HA	1.74	0.67
1:A:331:ILE:HD13	1:A:360:ALA:HB2	1.76	0.67
1:A:339:PHE:HB3	3:A:506:GOL:H2	1.76	0.66
1:B:87:LEU:HD22	1:B:112:GLU:H	1.61	0.66
1:B:97:THR:HG23	1:B:102:VAL:HG21	1.77	0.66
1:B:10:CYS:SG	1:B:28:HIS:CE1	2.88	0.65
1:A:349:LYS:HD3	1:A:374:HIS:HB3	1.78	0.65
1:A:171:THR:HG21	1:A:177:MET:HA	1.79	0.65
1:B:252:GLN:HB3	1:B:335:GLN:NE2	2.12	0.65
1:B:64:LEU:HB2	1:B:134:MET:HE2	1.80	0.64
1:A:77:ARG:HD2	1:A:77:ARG:N	2.14	0.63
1:B:87:LEU:HD11	1:B:109:ARG:HB3	1.80	0.63
1:B:303:ARG:HE	1:B:388:THR:HG1	1.45	0.63
1:A:156:THR:HG22	4:A:505:CIT:O2	1.82	0.62
1:A:95:TYR:CD2	1:A:124:ALA:HA	2.34	0.62
1:B:88:THR:HG22	1:B:113:VAL:HG21	1.80	0.62
1:B:85:GLN:HB3	1:B:109:ARG:HH12	1.65	0.61
1:A:169:ILE:HG21	1:A:180:MET:SD	2.41	0.61
1:A:354:ARG:NH2	1:A:380:MET:O	2.33	0.61
1:A:404:ASP:HB3	1:A:410:ILE:HD13	1.81	0.61
1:A:97:THR:HG23	1:A:102:VAL:HG21	1.81	0.61
1:B:252:GLN:HB3	1:B:335:GLN:HE21	1.65	0.60
1:B:47:SER:C	1:B:49:SER:H	2.09	0.60
1:A:212:LEU:HG	1:A:234:ASP:HB3	1.83	0.59
1:B:306:HIS:CE1	3:B:506:GOL:H2	2.38	0.59
1:B:412:VAL:HG21	1:B:436:ILE:HG21	1.83	0.59
1:A:249:ASP:OD2	1:A:291:TYR:OH	2.19	0.59
1:A:10:CYS:HB3	1:A:28:HIS:HE1	1.66	0.59
1:B:10:CYS:SG	2:B:501:ZN:ZN	1.87	0.59
1:B:15:PRO:HG2	1:B:16:TYR:CE2	2.39	0.57
1:A:81:MET:HE3	1:A:115:LEU:HD11	1.87	0.56
1:B:412:VAL:HG21	1:B:436:ILE:CG2	2.35	0.56
1:A:254:HIS:HB2	5:A:635:HOH:O	2.04	0.56
1:B:97:THR:OG1	1:B:98:ARG:N	2.39	0.56
1:A:49:SER:HB2	1:A:53:CYS:SG	2.46	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:LEU:HA	1:A:111:ASN:O	2.07	0.55
1:A:434:ARG:HG2	1:B:277:TRP:CE2	2.41	0.55
1:B:41:CYS:HB3	1:B:52:GLU:OE2	2.07	0.55
1:B:92:PRO:HA	1:B:104:VAL:HG12	1.88	0.55
1:B:422:PHE:CG	1:B:433:LEU:HD21	2.42	0.55
1:B:303:ARG:NE	1:B:388:THR:OG1	2.31	0.55
1:B:342:VAL:HG23	1:B:368:ILE:HG13	1.89	0.55
1:B:44:PRO:O	1:B:47:SER:OG	2.24	0.55
1:A:212:LEU:CD2	1:A:230:CYS:HB3	2.37	0.54
1:B:252:GLN:HE21	1:B:335:GLN:NE2	2.04	0.54
1:B:5:ARG:HH11	1:B:94:ARG:NH1	2.06	0.54
1:A:299:VAL:HG12	1:A:300:ASN:H	1.72	0.54
1:A:144:SER:HB3	1:A:244:LEU:O	2.08	0.54
1:B:101:LEU:H	1:B:101:LEU:HD23	1.72	0.54
1:A:38:ILE:HB	1:A:96:GLN:NE2	2.23	0.53
1:A:84:GLU:HB2	1:A:87:LEU:O	2.08	0.53
1:A:411:THR:OG1	1:A:414:GLN:HG3	2.08	0.53
1:B:15:PRO:HG2	1:B:16:TYR:CD2	2.43	0.52
1:A:20:CYS:N	1:A:21:GLY:HA2	2.24	0.52
1:A:178:LEU:HD12	1:A:197:LEU:HD22	1.92	0.52
1:B:114:ASP:O	1:B:115:LEU:HB3	2.08	0.52
1:B:418:ASN:ND2	1:B:420:ASP:HB2	2.25	0.52
1:A:274:LYS:HB3	1:A:294:LYS:O	2.09	0.52
1:A:400:LEU:HD23	1:A:436:ILE:HD12	1.91	0.51
1:A:195:THR:OG1	1:A:199:PHE:HE1	1.92	0.51
1:A:292:ARG:NH2	5:A:601:HOH:O	2.09	0.51
1:A:40:TRP:HE1	1:A:52:GLU:HB3	1.76	0.51
1:B:113:VAL:HG12	1:B:114:ASP:O	2.11	0.51
1:B:10:CYS:CB	1:B:28:HIS:CE1	2.93	0.51
1:A:178:LEU:HD21	1:A:199:PHE:HA	1.93	0.50
1:B:281:GLN:HA	1:B:284:CYS:HB2	1.93	0.50
1:A:10:CYS:O	1:A:10:CYS:SG	2.69	0.50
1:A:54:GLU:N	1:A:55:PRO:HD2	2.26	0.50
1:A:349:LYS:CD	1:A:350:ASP:H	2.25	0.50
1:A:299:VAL:HG12	1:A:300:ASN:N	2.26	0.50
1:B:378:GLN:OE1	3:B:506:GOL:H12	2.11	0.50
1:A:279:PHE:CD1	1:A:283:ILE:HB	2.47	0.50
1:A:181:ILE:HG23	1:A:187:CYS:SG	2.52	0.50
1:A:310:PRO:HD3	1:A:371:TYR:CZ	2.47	0.50
1:B:232:HIS:CE1	1:B:262:CYS:HA	2.46	0.50
1:B:39:ILE:HG22	1:B:40:TRP:N	2.18	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:GLU:HB2	1:A:87:LEU:H	1.76	0.49
1:B:299:VAL:HG11	5:B:623:HOH:O	2.12	0.49
1:B:423:ARG:NH1	5:B:605:HOH:O	2.45	0.49
1:A:144:SER:O	1:A:269:PRO:HD2	2.12	0.49
1:B:418:ASN:HD21	1:B:420:ASP:HB2	1.76	0.49
1:A:73:TYR:HE1	1:A:126:LEU:HD23	1.77	0.48
1:B:17:ALA:O	1:B:37:VAL:HG23	2.13	0.48
1:A:20:CYS:H	1:A:21:GLY:HA2	1.78	0.48
1:B:314:GLY:HA2	1:B:394:VAL:HG21	1.95	0.48
1:B:38:ILE:C	1:B:39:ILE:HD13	2.39	0.48
1:B:86:GLY:O	1:B:87:LEU:HD23	2.13	0.48
1:A:393:ALA:HB1	1:A:400:LEU:HD11	1.95	0.48
1:A:278:ARG:HD3	1:A:338:THR:HG23	1.96	0.48
1:A:412:VAL:HG21	1:A:436:ILE:HG21	1.96	0.48
1:B:416:LEU:HD11	1:B:437:CYS:SG	2.54	0.47
1:B:404:ASP:HB3	1:B:410:ILE:HD13	1.95	0.47
1:A:274:LYS:H	1:B:441:GLU:CD	2.23	0.47
1:B:301:THR:HG21	1:B:386:LYS:HG2	1.96	0.47
1:B:73:TYR:CE2	1:B:75:PRO:HB3	2.50	0.47
1:B:303:ARG:NE	1:B:388:THR:HG1	2.10	0.47
1:B:20:CYS:HB2	1:B:128:THR:OG1	2.15	0.47
1:A:82:HIS:O	1:A:88:THR:HG23	2.15	0.46
1:A:321:HIS:HA	1:A:324:ARG:HD3	1.97	0.46
1:A:143:ARG:HB3	1:A:243:THR:HG21	1.98	0.46
1:B:94:ARG:HB2	1:B:125:LEU:HD12	1.98	0.46
1:A:44:PRO:O	1:A:47:SER:OG	2.28	0.46
1:B:32:HIS:NE2	1:B:34:HIS:HB3	2.31	0.46
1:B:128:THR:O	1:B:237:ARG:NH1	2.35	0.46
1:A:174:HIS:O	1:A:177:MET:HB3	2.16	0.46
1:B:73:TYR:HE1	1:B:126:LEU:HD13	1.81	0.46
1:B:251:LYS:HD2	1:B:290:ASP:OD1	2.16	0.46
1:B:299:VAL:HG12	1:B:300:ASN:N	2.30	0.46
1:A:43:HIS:CE1	1:A:50:CYS:HB3	2.51	0.45
1:A:145:ARG:HG2	1:A:146:PHE:N	2.30	0.45
1:B:423:ARG:HD3	1:B:423:ARG:HA	1.77	0.45
1:B:188:ARG:HB3	1:B:204:ARG:HD3	1.99	0.45
1:A:10:CYS:C	1:A:12:ALA:N	2.74	0.45
1:A:277:TRP:CH2	1:A:298:MET:HE2	2.52	0.45
1:B:202:PRO:O	1:B:204:ARG:HG2	2.17	0.45
1:A:158:TRP:NE1	1:B:442:LEU:HD12	2.31	0.45
1:A:7:CYS:N	1:A:11:GLY:HA2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ARG:HG2	1:A:204:ARG:HA	1.98	0.45
1:B:18:THR:HG21	1:B:32:HIS:ND1	2.32	0.45
1:B:62:SER:OG	1:B:63:PRO:HD2	2.17	0.45
1:B:107:GLY:HA2	1:B:112:GLU:HG3	1.97	0.45
1:A:133:ASN:O	1:A:137:VAL:HG23	2.17	0.45
1:A:212:LEU:HD22	1:A:230:CYS:HB3	1.99	0.45
1:B:88:THR:O	1:B:111:ASN:ND2	2.50	0.45
1:A:133:ASN:HB3	1:A:240:SER:HB3	1.98	0.44
1:B:5:ARG:NH1	1:B:94:ARG:HD2	2.32	0.44
1:B:54:GLU:N	1:B:55:PRO:HD2	2.33	0.44
1:A:38:ILE:HA	1:A:44:PRO:HA	1.98	0.44
1:A:415:ALA:HA	1:A:418:ASN:OD1	2.17	0.44
1:B:347:PRO:O	1:B:374:HIS:NE2	2.50	0.44
1:B:47:SER:C	1:B:49:SER:N	2.76	0.44
1:B:97:THR:CG2	1:B:102:VAL:HG21	2.46	0.44
1:B:357:ALA:O	1:B:361:ILE:HG12	2.17	0.44
1:B:82:HIS:O	1:B:88:THR:HA	2.18	0.44
1:A:40:TRP:NE1	1:A:52:GLU:HB3	2.33	0.43
1:B:346:LEU:HB2	1:B:371:TYR:O	2.18	0.43
1:A:160:LEU:C	1:A:162:GLN:H	2.26	0.43
1:A:20:CYS:HA	1:A:126:LEU:HB2	1.99	0.43
1:A:178:LEU:HA	1:A:181:ILE:HD12	2.00	0.43
1:A:365:ARG:HD3	5:A:607:HOH:O	2.17	0.43
1:A:86:GLY:O	1:A:112:GLU:HA	2.19	0.43
1:B:278:ARG:HD3	1:B:338:THR:HG23	1.99	0.43
1:B:10:CYS:C	1:B:12:ALA:H	2.12	0.43
1:B:143:ARG:HA	1:B:143:ARG:HD3	1.54	0.43
1:B:422:PHE:CD1	1:B:433:LEU:HD21	2.54	0.43
1:A:25:CYS:O	1:A:29:THR:HG23	2.18	0.43
1:A:34:HIS:CD2	1:A:68:LEU:HB3	2.54	0.43
1:A:158:TRP:CD1	1:B:438:ALA:HB1	2.53	0.43
1:A:186:THR:HG21	1:A:205:THR:HG23	2.01	0.43
1:A:35:CYS:HB2	1:A:36:PRO:HD2	2.00	0.43
1:A:105:ARG:H	1:A:105:ARG:HG2	1.58	0.43
1:A:160:LEU:HD13	1:A:160:LEU:HA	1.85	0.43
1:A:97:THR:HG23	1:A:102:VAL:CG2	2.49	0.42
1:A:353:ASN:HD21	1:A:356:ARG:HG3	1.84	0.42
1:A:394:VAL:HG23	5:A:626:HOH:O	2.18	0.42
1:A:433:LEU:HD12	1:A:433:LEU:HA	1.83	0.42
1:A:278:ARG:HE	3:A:504:GOL:H31	1.84	0.42
1:A:15:PRO:HG2	1:A:16:TYR:CE2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:VAL:HG13	1:A:367:ALA:HB3	2.00	0.42
1:B:371:TYR:CZ	1:B:373:PRO:HG3	2.54	0.42
1:A:277:TRP:CE2	1:B:434:ARG:HG2	2.54	0.42
1:B:186:THR:HG23	1:B:203:SER:OG	2.20	0.42
1:B:25:CYS:O	1:B:29:THR:HG23	2.20	0.42
1:A:84:GLU:HB2	1:A:87:LEU:N	2.34	0.42
1:A:109:ARG:H	1:A:109:ARG:CD	2.29	0.42
1:B:41:CYS:SG	1:B:42:GLY:N	2.91	0.42
1:B:253:LEU:H	1:B:335:GLN:NE2	2.18	0.42
1:A:422:PHE:CG	1:A:433:LEU:HD21	2.55	0.42
1:A:77:ARG:HD2	1:A:77:ARG:H	1.85	0.42
1:A:242:THR:OG1	1:A:243:THR:N	2.53	0.42
1:B:224:LEU:HA	1:B:224:LEU:HD12	1.83	0.41
1:A:104:VAL:HG12	1:A:113:VAL:HB	2.02	0.41
1:B:19:ALA:HB1	1:B:73:TYR:OH	2.20	0.41
1:B:201:ALA:HA	1:B:202:PRO:HD3	1.88	0.41
1:A:342:VAL:HG22	1:A:364:ALA:HB2	2.02	0.41
1:B:341:VAL:HA	1:B:367:ALA:O	2.21	0.41
1:A:87:LEU:HD23	1:A:112:GLU:HG2	2.02	0.41
1:A:348:THR:O	1:A:351:SER:OG	2.27	0.41
1:A:7:CYS:O	1:A:11:GLY:N	2.53	0.41
1:A:85:GLN:HG3	1:A:86:GLY:H	1.86	0.41
1:B:19:ALA:HB1	1:B:73:TYR:CZ	2.55	0.41
1:A:38:ILE:HD13	1:A:44:PRO:HB3	2.01	0.41
1:A:398:GLU:HA	1:A:398:GLU:OE1	2.21	0.41
1:B:10:CYS:O	1:B:10:CYS:SG	2.76	0.41
1:A:76:PRO:HD3	1:A:126:LEU:HD21	2.03	0.41
1:B:7:CYS:HB3	1:B:10:CYS:C	2.46	0.41
1:B:103:SER:OG	1:B:105:ARG:HD3	2.21	0.41
1:B:5:ARG:HH12	1:B:94:ARG:HD2	1.85	0.40
1:B:85:GLN:HB3	1:B:109:ARG:NH1	2.31	0.40
1:B:99:ARG:HD2	1:B:99:ARG:HA	1.89	0.40
1:B:212:LEU:HD22	1:B:230:CYS:HB3	2.02	0.40
1:B:318:THR:O	1:B:330:THR:HA	2.21	0.40
1:B:87:LEU:HD22	1:B:112:GLU:N	2.33	0.40
1:A:251:LYS:HG3	1:A:290:ASP:HB3	2.03	0.40
1:B:415:ALA:HA	1:B:418:ASN:OD1	2.21	0.40
1:A:302:THR:HG23	1:A:366:HIS:C	2.47	0.40

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:A:10:CYS:O	1:B:143:ARG:NH1[3_555]	1.89	0.31

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	439/499 (88%)	398 (91%)	34 (8%)	7 (2%)	7	34
1	B	439/499 (88%)	387 (88%)	44 (10%)	8 (2%)	6	31
All	All	878/998 (88%)	785 (89%)	78 (9%)	15 (2%)	7	32

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	GLY
1	B	11	GLY
1	A	84	GLU
1	A	92	PRO
1	A	200	PRO
1	B	13	PRO
1	A	161	GLN
1	B	115	LEU
1	B	200	PRO
1	B	47	SER
1	B	49	SER
1	B	50	CYS
1	B	39	ILE
1	A	86	GLY
1	A	39	ILE

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	378/425 (89%)	376 (100%)	2 (0%)	81	89
1	B	378/425 (89%)	378 (100%)	0	100	100
All	All	756/850 (89%)	754 (100%)	2 (0%)	86	91

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	GLN
1	A	105	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	GLN
1	A	157	HIS
1	A	161	GLN
1	A	190	ASN
1	A	221	ASN
1	A	315	GLN
1	A	399	GLN
1	A	406	ASN
1	A	418	ASN
1	B	162	GLN
1	B	175	GLN
1	B	335	GLN
1	B	345	HIS
1	B	391	ASN
1	B	418	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 6 are monoatomic - leaving 8 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	$\# Z > 2$
3	GOL	A	507	-	5,5,5	1.05	0	5,5,5	1.19	1 (20%)
4	CIT	B	504	-	12,12,12	1.10	0	17,17,17	1.91	5 (29%)
3	GOL	B	506	-	5,5,5	1.47	2 (40%)	5,5,5	1.05	0
4	CIT	B	505	-	12,12,12	1.12	0	17,17,17	1.66	3 (17%)
3	GOL	A	506	-	5,5,5	0.97	0	5,5,5	1.40	1 (20%)
3	GOL	A	504	-	5,5,5	1.13	0	5,5,5	0.90	0
4	CIT	A	505	-	12,12,12	1.37	1 (8%)	17,17,17	2.37	8 (47%)
3	GOL	B	507	-	5,5,5	1.26	1 (20%)	5,5,5	1.06	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
3	GOL	A	507	-	-	2/4/4/4	-
4	CIT	B	504	-	-	5/16/16/16	-
3	GOL	B	506	-	-	2/4/4/4	-
4	CIT	B	505	-	-	4/16/16/16	-
3	GOL	A	506	-	-	4/4/4/4	-
3	GOL	A	504	-	-	0/4/4/4	-
4	CIT	A	505	-	-	5/16/16/16	-
3	GOL	B	507	-	-	2/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	506	GOL	C3-C2	2.34	1.60	1.51
3	B	507	GOL	C1-C2	2.30	1.60	1.51
3	B	506	GOL	C1-C2	2.27	1.60	1.51
4	A	505	CIT	C3-C6	2.07	1.55	1.53

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	505	CIT	O6-C6-C3	5.24	123.19	113.14
4	B	505	CIT	O6-C6-C3	4.61	121.99	113.14
4	B	504	CIT	O6-C6-C3	4.36	121.51	113.14
4	B	504	CIT	O7-C3-C6	-3.37	104.18	108.96
4	A	505	CIT	O2-C1-O1	-3.24	114.99	123.33
4	A	505	CIT	O7-C3-C2	-3.01	102.50	109.38
4	A	505	CIT	C2-C3-C6	2.99	116.66	110.03
4	B	504	CIT	O2-C1-C2	2.82	123.28	114.35
4	A	505	CIT	O4-C5-C4	2.77	123.12	114.35
4	A	505	CIT	O4-C5-O3	-2.61	116.62	123.33
4	A	505	CIT	O7-C3-C6	-2.54	105.36	108.96
4	B	504	CIT	O4-C5-C4	2.39	121.91	114.35
3	A	506	GOL	C3-C2-C1	-2.35	103.18	111.80
4	B	504	CIT	O2-C1-O1	-2.24	117.56	123.33
4	B	505	CIT	O4-C5-C4	2.23	121.41	114.35
4	A	505	CIT	O6-C6-O5	-2.18	116.87	123.86
4	B	505	CIT	O7-C3-C6	2.11	111.96	108.96
3	A	507	GOL	C3-C2-C1	-2.03	104.34	111.80

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	506	GOL	O1-C1-C2-O2
3	A	506	GOL	O1-C1-C2-C3
3	A	506	GOL	C1-C2-C3-O3
3	A	507	GOL	O1-C1-C2-C3
3	B	507	GOL	C1-C2-C3-O3
4	A	505	CIT	C2-C3-C6-O5
4	A	505	CIT	C2-C3-C6-O6
4	A	505	CIT	O7-C3-C6-O5
4	A	505	CIT	O7-C3-C6-O6
4	B	504	CIT	C2-C3-C6-O5

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Mol	Chain	Res	Type	Atoms
4	B	504	CIT	C2-C3-C6-O6
4	B	504	CIT	O7-C3-C6-O5
4	B	504	CIT	O7-C3-C6-O6
4	B	505	CIT	O7-C3-C6-O5
4	B	505	CIT	O7-C3-C6-O6
4	B	505	CIT	C4-C3-C6-O5
4	B	505	CIT	C4-C3-C6-O6
3	B	507	GOL	O2-C2-C3-O3
3	A	507	GOL	O1-C1-C2-O2
3	A	506	GOL	O2-C2-C3-O3
4	B	504	CIT	O7-C3-C4-C5
3	B	506	GOL	O2-C2-C3-O3
3	B	506	GOL	O1-C1-C2-C3
4	A	505	CIT	O7-C3-C4-C5

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	506	GOL	2	0
4	B	505	CIT	1	0
3	A	506	GOL	1	0
3	A	504	GOL	1	0
4	A	505	CIT	1	0

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	441/499 (88%)	0.69	63 (14%) 6 3	6, 24, 82, 113	0
1	B	441/499 (88%)	0.97	92 (20%) 2 2	5, 28, 88, 115	0
All	All	882/998 (88%)	0.83	155 (17%) 4 3	5, 26, 86, 115	0

All (155) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	108	ILE	8.6
1	B	40	TRP	6.5
1	A	109	ARG	6.1
1	A	97	THR	5.9
1	A	115	LEU	5.7
1	A	92	PRO	5.5
1	B	101	LEU	5.5
1	B	113	VAL	5.4
1	A	82	HIS	5.2
1	B	56	PRO	5.1
1	B	39	ILE	4.8
1	B	80	ILE	4.8
1	B	85	GLN	4.8
1	A	90	LEU	4.7
1	A	104	VAL	4.7
1	B	86	GLY	4.7
1	B	90	LEU	4.7
1	B	108	ILE	4.7
1	B	57	LEU	4.6
1	B	111	ASN	4.5
1	A	105	ARG	4.4
1	B	100	GLY	4.4
1	B	25	CYS	4.4
1	B	121	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	143	ARG	4.2
1	A	93	GLY	4.2
1	A	118	GLY	4.1
1	B	51	SER	4.1
1	A	98	ARG	4.1
1	B	115	LEU	4.1
1	B	33	GLN	4.0
1	A	91	ASP	4.0
1	A	107	GLY	3.9
1	B	95	TYR	3.9
1	B	98	ARG	3.9
1	A	79	VAL	3.9
1	A	85	GLN	3.9
1	B	10	CYS	3.8
1	A	89	PRO	3.8
1	B	119	ASP	3.8
1	A	196	THR	3.8
1	A	112	GLU	3.8
1	B	122	SER	3.8
1	B	82	HIS	3.8
1	A	119	ASP	3.7
1	B	99	ARG	3.7
1	B	120	TYR	3.7
1	B	104	VAL	3.7
1	A	114	ASP	3.6
1	B	52	GLU	3.6
1	B	97	THR	3.6
1	A	87	LEU	3.6
1	A	77	ARG	3.6
1	B	43	HIS	3.6
1	B	96	GLN	3.6
1	A	86	GLY	3.6
1	B	102	VAL	3.5
1	B	205	THR	3.5
1	B	47	SER	3.5
1	A	84	GLU	3.4
1	A	103	SER	3.4
1	B	107	GLY	3.4
1	B	55	PRO	3.4
1	B	16	TYR	3.4
1	A	184	LEU	3.4
1	B	109	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	117	ASP	3.4
1	A	122	SER	3.4
1	A	203	SER	3.4
1	B	123	THR	3.4
1	B	116	PRO	3.3
1	B	45	ALA	3.3
1	B	78	THR	3.3
1	B	42	GLY	3.3
1	B	444	HIS	3.3
1	B	87	LEU	3.3
1	A	11	GLY	3.3
1	A	3	LYS	3.2
1	B	48	GLY	3.2
1	B	106	ARG	3.2
1	B	118	GLY	3.1
1	B	112	GLU	3.1
1	B	15	PRO	3.1
1	B	89	PRO	3.1
1	B	30	HIS	3.1
1	B	79	VAL	3.1
1	A	205	THR	3.0
1	A	106	ARG	3.0
1	B	58	GLY	3.0
1	B	103	SER	3.0
1	B	114	ASP	3.0
1	B	36	PRO	3.0
1	B	203	SER	3.0
1	B	92	PRO	3.0
1	A	183	ALA	3.0
1	B	37	VAL	2.9
1	B	46	GLY	2.9
1	B	44	PRO	2.9
1	A	88	THR	2.9
1	B	94	ARG	2.9
1	A	110	GLY	2.9
1	B	206	GLY	2.9
1	B	84	GLU	2.9
1	A	185	GLY	2.8
1	A	116	PRO	2.8
1	B	105	ARG	2.8
1	A	198	GLN	2.8
1	A	120	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	26	VAL	2.8
1	B	83	VAL	2.8
1	A	194	GLY	2.8
1	A	443	GLU	2.8
1	B	443	GLU	2.8
1	A	80	ILE	2.8
1	A	51	SER	2.8
1	A	193	ALA	2.7
1	B	54	GLU	2.7
1	B	143	ARG	2.7
1	B	198	GLN	2.7
1	B	88	THR	2.6
1	B	75	PRO	2.6
1	B	49	SER	2.6
1	A	111	ASN	2.6
1	A	161	GLN	2.6
1	A	52	GLU	2.5
1	A	6	MET	2.5
1	B	59	LYS	2.5
1	B	38	ILE	2.5
1	B	77	ARG	2.5
1	A	95	TYR	2.4
1	B	91	ASP	2.4
1	B	117	ASP	2.4
1	A	94	ARG	2.4
1	B	124	ALA	2.4
1	B	73	TYR	2.3
1	A	199	PHE	2.3
1	A	121	ALA	2.3
1	A	186	THR	2.3
1	A	99	ARG	2.3
1	A	83	VAL	2.3
1	B	441	GLU	2.2
1	B	41	CYS	2.2
1	A	81	MET	2.2
1	B	125	LEU	2.2
1	B	24	VAL	2.1
1	A	76	PRO	2.1
1	B	189	PHE	2.1
1	B	187	CYS	2.1
1	B	13	PRO	2.1
1	A	78	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	200	PRO	2.0
1	A	160	LEU	2.0
1	B	408	ARG	2.0
1	B	128	THR	2.0
1	B	438	ALA	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](#)

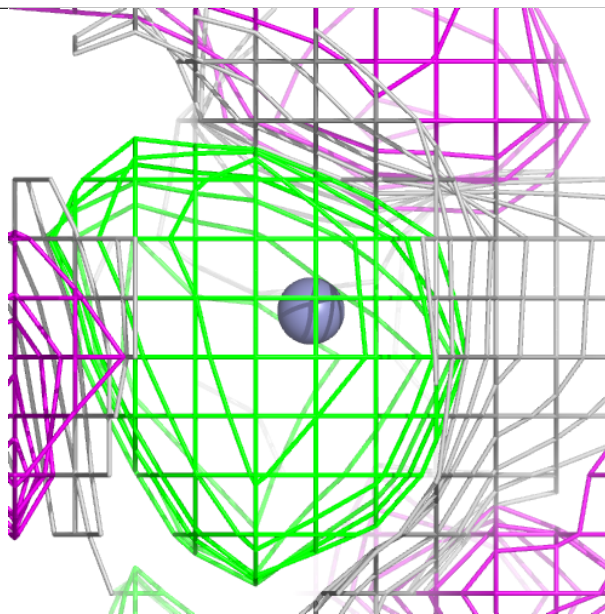
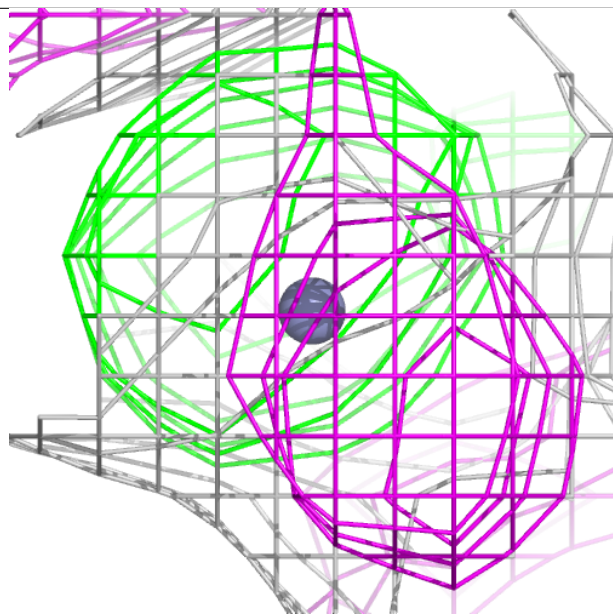
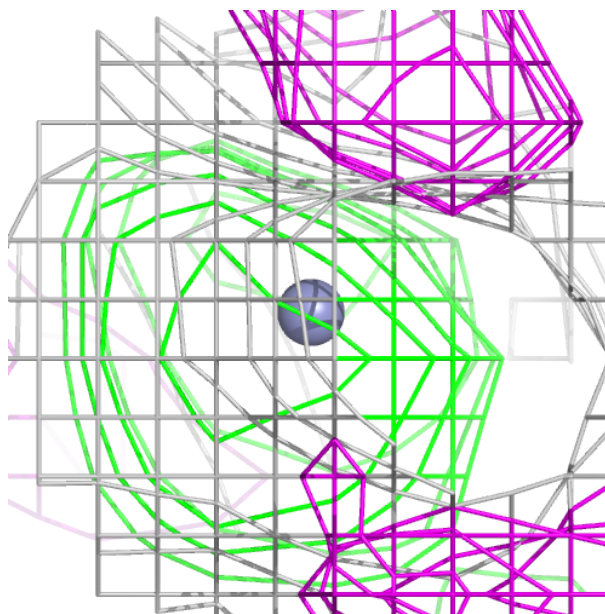
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CIT	A	505	13/13	0.78	0.20	23,45,56,57	0
4	CIT	B	504	13/13	0.80	0.19	29,39,50,57	0
4	CIT	B	505	13/13	0.80	0.17	43,54,68,68	0
3	GOL	A	507	6/6	0.83	0.18	41,42,53,55	0
2	ZN	B	501	1/1	0.83	0.29	213,213,213,213	0
3	GOL	A	504	6/6	0.89	0.15	35,38,42,44	0
3	GOL	B	507	6/6	0.90	0.10	27,34,40,43	0
3	GOL	A	506	6/6	0.91	0.13	18,19,25,27	0
3	GOL	B	506	6/6	0.91	0.15	20,31,35,36	0
2	ZN	B	502	1/1	0.97	0.05	97,97,97,97	0
2	ZN	B	503	1/1	0.99	0.02	51,51,51,51	0
2	ZN	A	502	1/1	0.99	0.03	71,71,71,71	0
2	ZN	A	503	1/1	0.99	0.02	20,20,20,20	0
2	ZN	A	501	1/1	1.00	0.02	24,24,24,24	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.

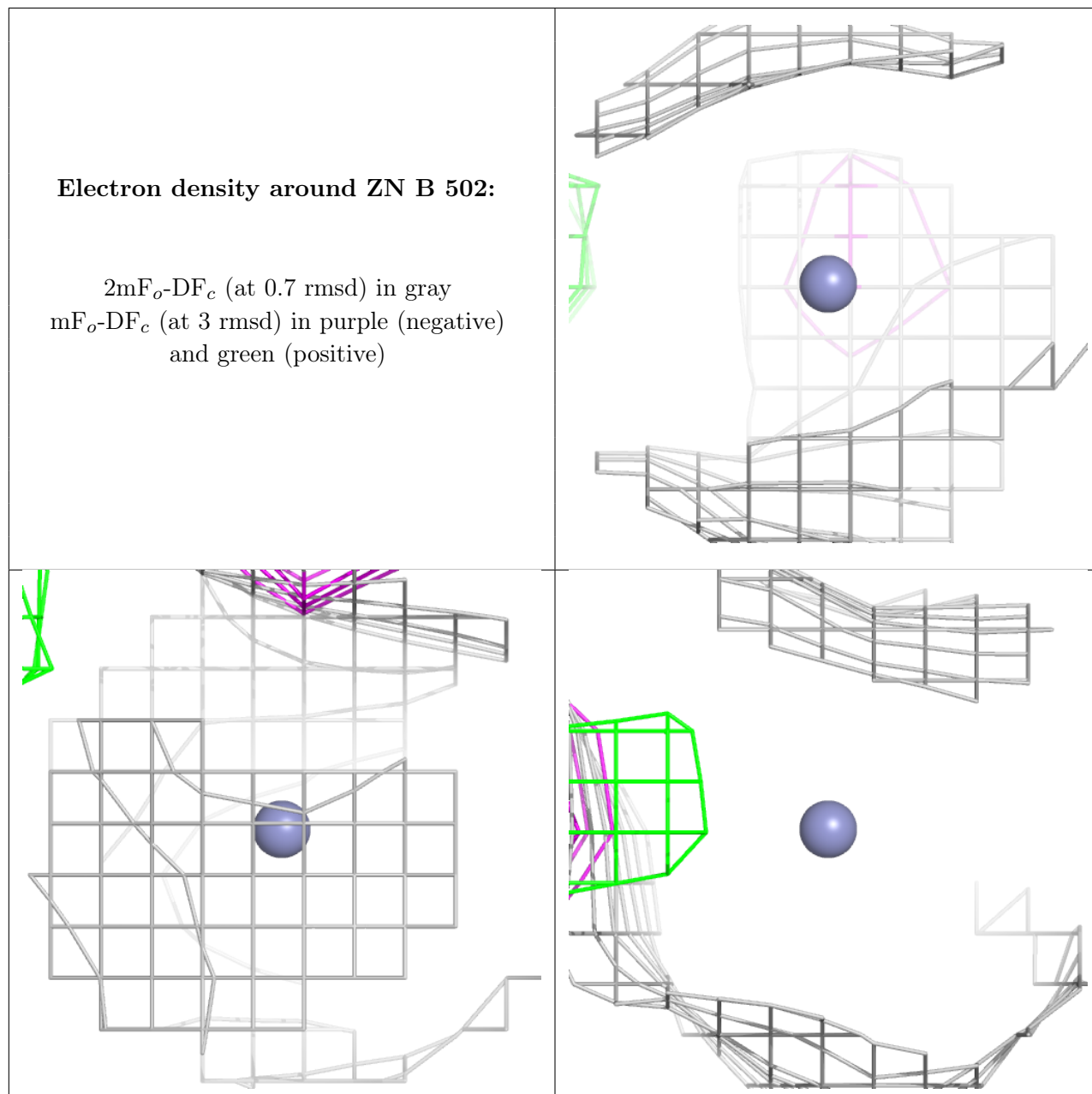
Electron density around ZN B 501:

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



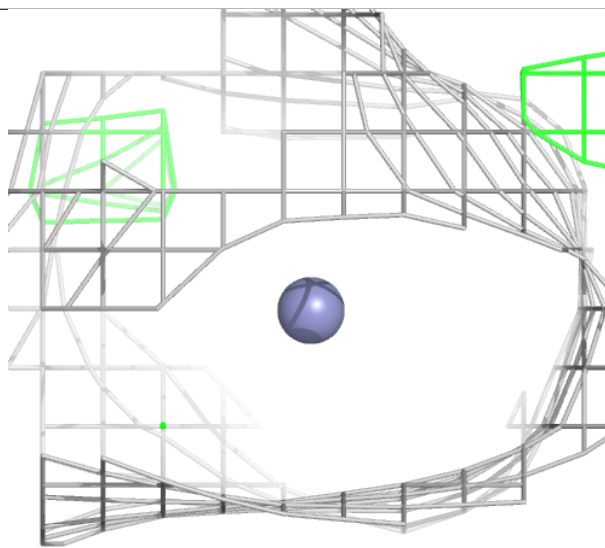
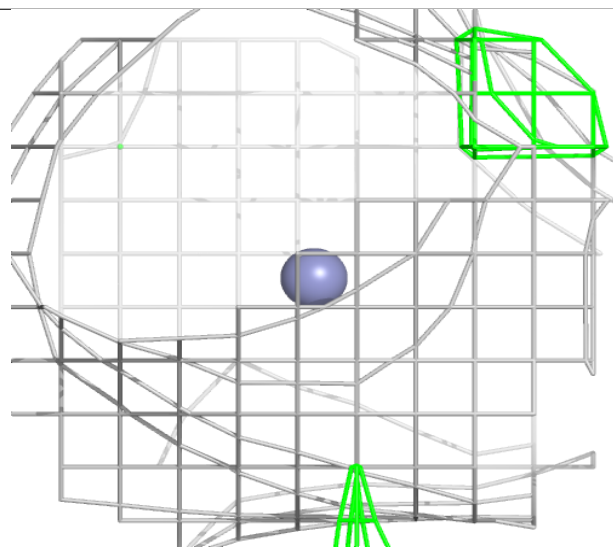
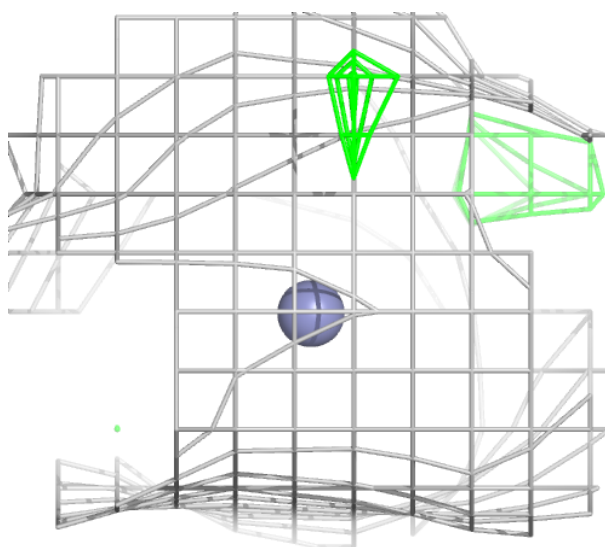
Electron density around ZN B 502:

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



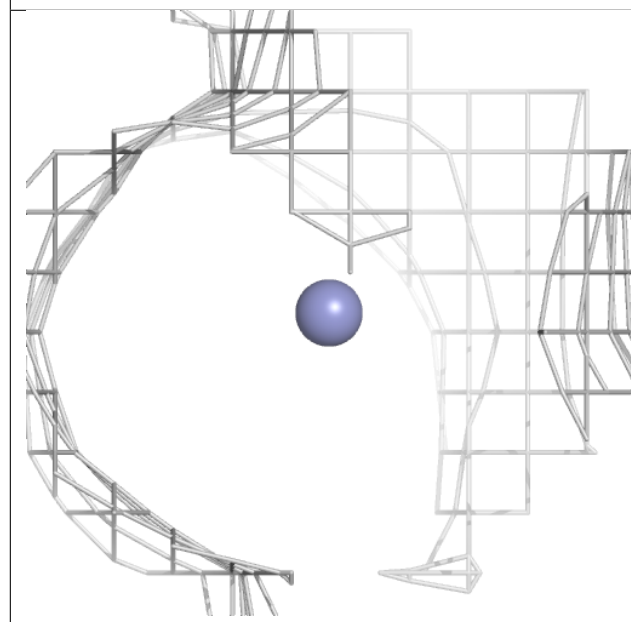
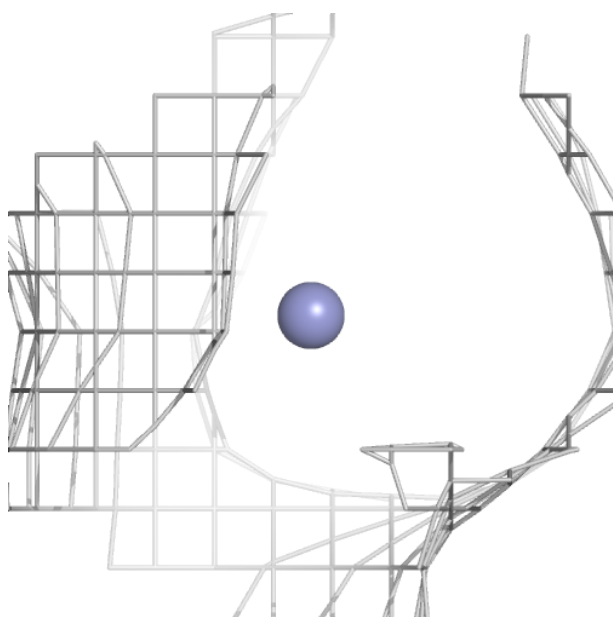
Electron density around ZN B 503:

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



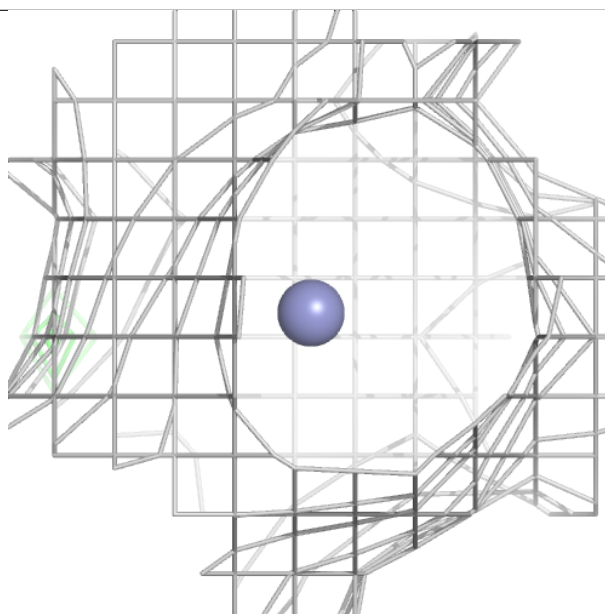
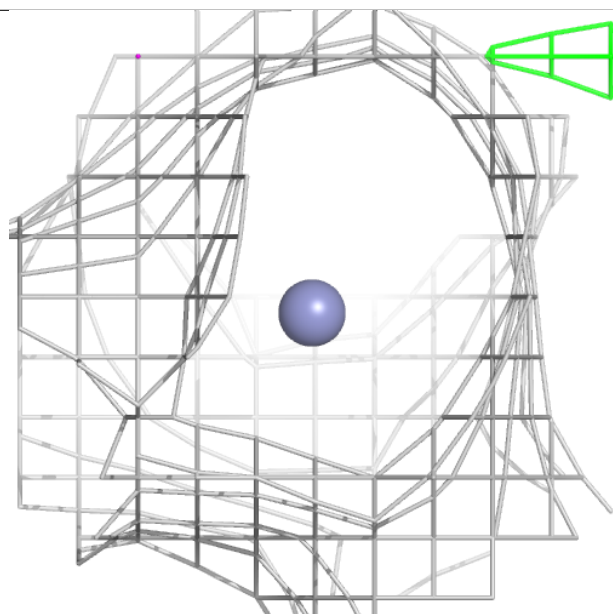
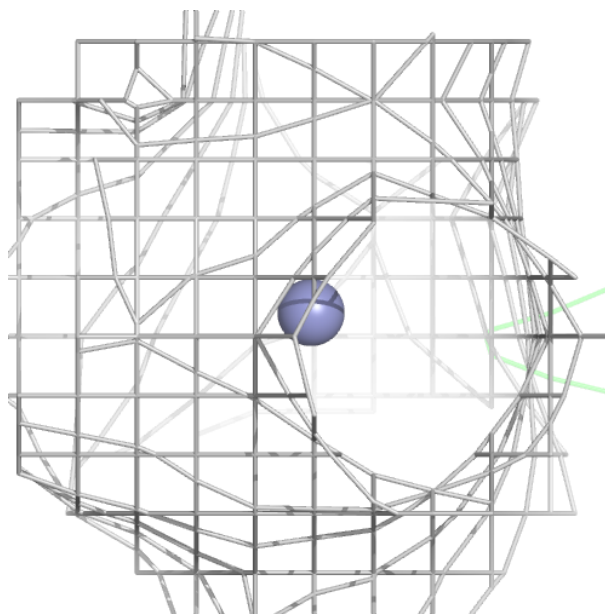
Electron density around ZN A 502:

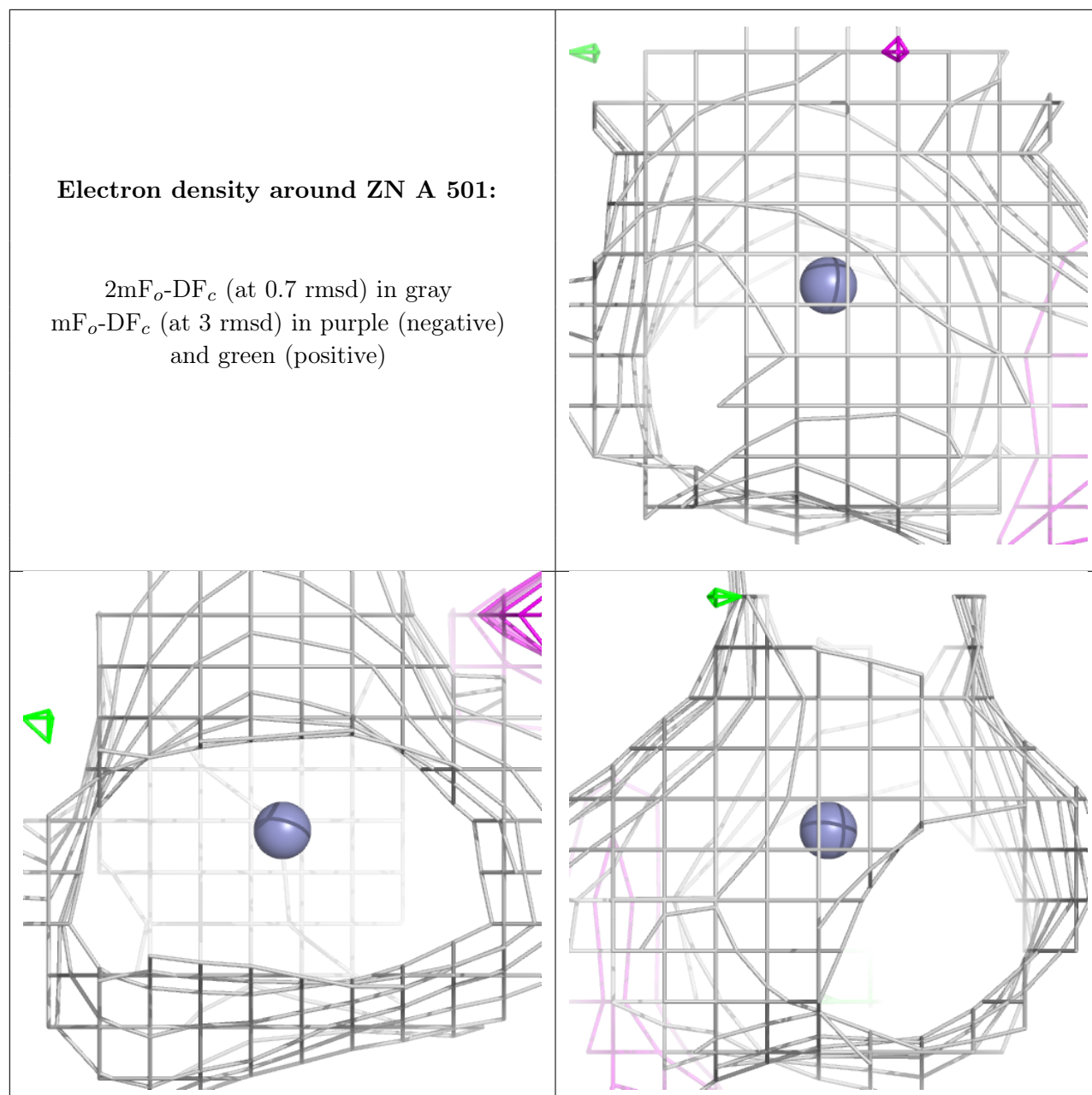
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN A 503:

$2mF_o-DF_c$ (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.