



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:24 PM UTC

PDB ID : 6SNV / pdb_00006snv
Title : DNA mismatch repair proteins MLH1 and MLH3
Authors : Dai, J.; Chervy, P.; Legrand, P.; Ropars, V.; Charbonnier, J.B.
Deposited on : 2019-08-27
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

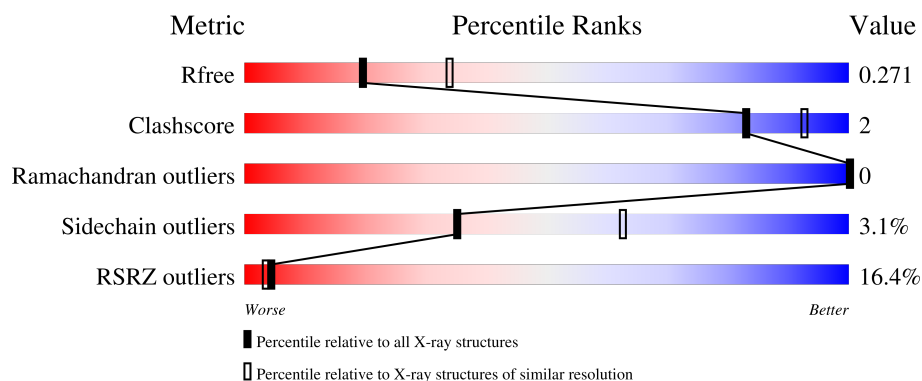
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	265	11% 89% 9% .
1	D	265	28% 85% 13% .
2	B	239	11% 85% 8% 7%
2	E	239	12% 82% 10% 7%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7871 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 DNA mismatch repair protein MLH1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	0	0
			2129	1372	345	405	7			
1	D	260	Total	C	N	O	S	0	0	0
			2129	1372	345	405	7			

- Molecule 2 is a protein called DNA mismatch repair protein MLH3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	222	Total	C	N	O	S	0	0	0
			1792	1153	299	326	14			
2	E	222	Total	C	N	O	S	0	0	0
			1792	1153	299	326	14			

- 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	2	Total	Zn	0	0
			2	2		
3	E	2	Total	Zn	0	0
			2	2		

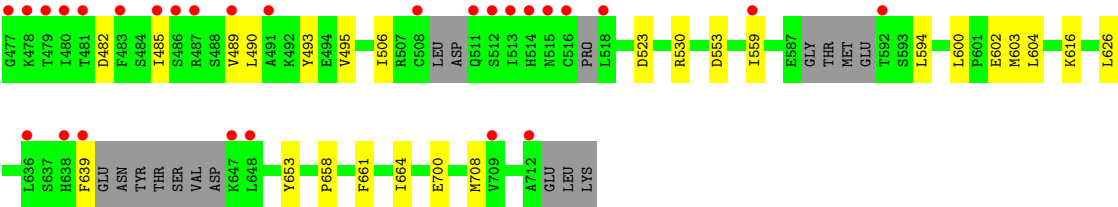
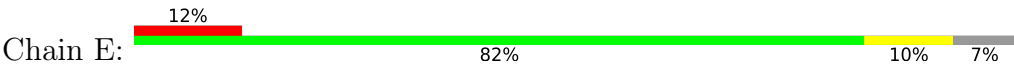
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	O	0	0
			3	3		
4	B	7	Total	O	0	0
			7	7		
4	D	1	Total	O	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	14	Total	O	0	0
			14	14		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	90.89Å 134.81Å 102.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.66 – 2.50 44.66 – 2.50	Depositor EDS
% Data completeness (in resolution range)	68.1 (44.66-2.50) 68.1 (44.66-2.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.51Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.229 , 0.271 (Not available) , 0.271	Depositor DCC
R_{free} test set	1496 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	59.5	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 74.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7871	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 63.05 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0259e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.76	0/2167	1.31	0/2926
1	D	0.76	0/2167	1.30	5/2926 (0.2%)
2	B	0.76	0/1826	1.34	2/2458 (0.1%)
2	E	0.76	0/1826	1.31	7/2458 (0.3%)
All	All	0.76	0/7986	1.32	14/10768 (0.1%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	523	ASP	CA-CB-CG	6.34	118.94	112.60
1	D	698	ILE	N-CA-CB	5.70	115.86	109.99
2	E	626	LEU	CA-C-N	5.55	127.72	120.28
2	E	626	LEU	C-N-CA	5.55	127.72	120.28
2	E	653	TYR	CA-C-N	5.37	127.48	120.28
2	E	653	TYR	C-N-CA	5.37	127.48	120.28
2	B	666	ASN	CA-CB-CG	5.30	117.90	112.60
1	D	687	ASP	CA-C-N	5.25	125.80	119.98
1	D	687	ASP	C-N-CA	5.25	125.80	119.98
1	D	563	GLY	CA-C-N	5.23	127.24	120.44
1	D	563	GLY	C-N-CA	5.23	127.24	120.44
2	B	523	ASP	CA-CB-CG	5.16	117.75	112.60
2	E	602	GLU	CA-C-N	5.06	127.02	120.44
2	E	602	GLU	C-N-CA	5.06	127.02	120.44

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2129	0	2145	8	0
1	D	2129	0	2145	13	0
2	B	1792	0	1790	6	0
2	E	1792	0	1790	11	0
3	B	2	0	0	0	0
3	E	2	0	0	0	0
4	A	3	0	0	0	0
4	B	7	0	0	0	0
4	D	1	0	0	0	0
4	E	14	0	0	0	0
All	All	7871	0	7870	38	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 2.

All (38) 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)
2:B:530:ARG:HD3	2:B:700:GLU:O	1.94	0.67
2:E:603:MET:HG2	2:E:664:ILE:HG21	1.84	0.59
1:D:672:ARG:HG2	1:D:676:GLU:HG3	1.86	0.58
2:E:530:ARG:HD3	2:E:700:GLU:O	2.06	0.56
2:E:559:ILE:HG21	2:E:616:LYS:HB2	1.92	0.52
1:D:760:PRO:HA	1:D:763:TYR:CD2	2.46	0.51
1:D:634:GLU:HB3	1:D:650:LYS:HB3	1.93	0.51
2:E:600:LEU:HD22	2:E:604:LEU:HD23	1.93	0.50
2:E:490:LEU:HD11	2:E:708:MET:HE1	1.94	0.50
2:B:651:TRP:HA	2:B:654:SER:HB2	1.94	0.49
1:D:633:ILE:HD11	1:D:693:ILE:HD11	1.94	0.49
2:B:658:PRO:HD2	2:B:661:PHE:HD2	1.78	0.48
1:D:544:GLU:HB3	1:D:702:VAL:HB	1.96	0.47
2:E:658:PRO:HD2	2:E:661:PHE:HD2	1.80	0.47
1:A:633:ILE:HD11	1:A:693:ILE:HD11	1.96	0.47
2:B:603:MET:HG2	2:B:664:ILE:HG21	1.96	0.47
1:A:731:LEU:HA	1:A:735:LEU:HB2	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:485:ILE:O	2:E:489:VAL:HG23	2.15	0.46
2:E:530:ARG:HA	2:E:530:ARG:HD2	1.71	0.46
2:E:482:ASP:HA	2:E:485:ILE:HD12	1.98	0.46
1:D:538:TYR:HA	1:D:551:ILE:HG22	1.98	0.45
1:D:597:LEU:HA	1:D:600:LEU:HD12	1.98	0.45
1:A:669:PHE:O	1:A:673:LEU:HB2	2.16	0.45
1:D:731:LEU:HA	1:D:735:LEU:HB2	1.97	0.45
1:D:616:ILE:HG23	1:D:674:GLY:HA3	1.98	0.45
2:B:530:ARG:HA	2:B:530:ARG:HD2	1.79	0.44
2:B:600:LEU:HD22	2:B:604:LEU:HD23	1.98	0.44
1:D:596:VAL:HA	1:D:648:LYS:HG2	1.98	0.44
1:A:760:PRO:HA	1:A:763:TYR:CD2	2.54	0.43
1:D:688:GLY:HA2	1:D:691:ARG:HE	1.84	0.42
1:A:616:ILE:HG23	1:A:674:GLY:HA3	2.00	0.42
1:D:569:LEU:HD13	1:D:743:PHE:HB2	2.02	0.42
1:D:614:GLU:HA	1:D:617:ILE:HD12	2.01	0.41
2:E:495:VAL:HA	2:E:506:ILE:HG22	2.01	0.41
1:A:659:TYR:HB2	1:A:734:VAL:HG11	2.02	0.41
2:E:489:VAL:O	2:E:493:TYR:HD1	2.03	0.41
1:A:533:PHE:O	1:A:536:LEU:HD23	2.21	0.40
1:A:634:GLU:HB3	1:A:650:LYS:HB3	2.02	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	256/265 (97%)	251 (98%)	5 (2%)	0	100	100
1	D	256/265 (97%)	249 (97%)	7 (3%)	0	100	100
2	B	212/239 (89%)	201 (95%)	11 (5%)	0	100	100
2	E	212/239 (89%)	204 (96%)	8 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	936/1008 (93%)	905 (97%)	31 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	242/247 (98%)	233 (96%)	9 (4%)	30	57
1	D	242/247 (98%)	235 (97%)	7 (3%)	37	65
2	B	200/222 (90%)	192 (96%)	8 (4%)	28	54
2	E	200/222 (90%)	197 (98%)	3 (2%)	57	80
All	All	884/938 (94%)	857 (97%)	27 (3%)	35	62

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	649	LEU
1	A	652	LEU
1	A	697	TYR
1	A	700	ASP
1	A	730	LEU
1	A	749	ILE
1	A	750	LEU
1	A	754	VAL
1	A	762	LEU
2	B	494	GLU
2	B	553	ASP
2	B	594	LEU
2	B	608	TYR
2	B	618	VAL
2	B	632	LEU
2	B	636	LEU
2	B	639	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	560	ILE
1	D	617	ILE
1	D	649	LEU
1	D	673	LEU
1	D	749	ILE
1	D	750	LEU
1	D	755	GLU
2	E	553	ASP
2	E	594	LEU
2	E	639	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	628	ASN
2	B	666	ASN
2	B	683	GLN
2	B	696	HIS
2	B	697	ASN
1	D	553	HIS
1	D	628	ASN
2	E	696	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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 4 ligands modelled in this entry, 4 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

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	260/265 (98%)	0.92	29 (11%)	10 8	42, 92, 170, 193	0
1	D	260/265 (98%)	1.33	74 (28%)	1 1	41, 104, 200, 206	0
2	B	222/239 (92%)	0.69	27 (12%)	8 7	32, 64, 155, 184	0
2	E	222/239 (92%)	0.54	28 (12%)	8 6	28, 56, 149, 191	0
All	All	964/1008 (95%)	0.89	158 (16%)	4 3	28, 80, 178, 206	0

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	516	CYS	7.7
2	E	516	CYS	6.3
2	E	485	ILE	5.7
2	B	515	ASN	5.6
2	E	515	ASN	5.5
2	E	639	PHE	5.2
2	B	639	PHE	5.0
1	D	640	LEU	4.9
1	D	600	LEU	4.8
1	A	620	ILE	4.6
1	D	508	ASN	4.5
1	D	507	VAL	4.3
1	A	640	LEU	4.2
2	B	514	HIS	4.2
1	A	508	ASN	4.2
1	D	597	LEU	4.1
2	B	592	THR	4.1
1	D	648	LYS	4.1
1	D	620	ILE	4.1
1	D	595	ILE	4.0
2	B	712	ALA	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	652	LEU	3.9
1	D	636	VAL	3.9
2	E	514	HIS	3.9
1	A	649	LEU	3.9
1	D	638	ASP	3.8
1	D	649	LEU	3.8
2	E	486	SER	3.8
1	D	509	VAL	3.8
2	B	485	ILE	3.8
1	D	598	TYR	3.7
2	E	513	ILE	3.7
2	B	486	SER	3.7
1	D	631	TYR	3.7
1	D	644	LEU	3.6
1	A	595	ILE	3.6
2	B	513	ILE	3.6
1	D	604	PHE	3.4
2	E	511	GLN	3.3
1	D	647	VAL	3.3
1	D	630	TYR	3.3
1	D	635	LEU	3.3
1	D	617	ILE	3.2
2	E	487	ARG	3.1
1	D	616	ILE	3.1
2	E	712	ALA	3.1
1	D	749	ILE	3.1
1	D	601	LEU	3.0
1	D	673	LEU	3.0
1	D	651	SER	3.0
2	B	479	THR	2.9
2	E	478	LYS	2.9
1	D	584	ILE	2.9
1	D	596	VAL	2.9
1	A	712	LEU	2.9
2	B	511	GLN	2.9
2	E	709	VAL	2.9
1	D	607	LEU	2.9
1	D	599	ASN	2.9
2	E	512	SER	2.9
1	D	670	ILE	2.9
1	D	663	LEU	2.9
1	A	507	VAL	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	648	LYS	2.8
1	D	633	ILE	2.8
1	A	586	LEU	2.8
1	D	578	PHE	2.8
2	E	489	VAL	2.8
1	A	645	LYS	2.8
2	B	512	SER	2.7
1	A	607	LEU	2.7
2	B	478	LYS	2.7
1	D	737	PRO	2.7
1	D	712	LEU	2.7
2	E	592	THR	2.7
2	B	648	LEU	2.7
2	E	483	PHE	2.6
1	D	575	LEU	2.6
2	B	634	MET	2.6
1	D	710	ALA	2.6
2	B	480	ILE	2.6
1	D	666	LEU	2.6
2	E	636	LEU	2.6
1	D	619	LYS	2.6
1	D	623	MET	2.5
1	A	635	LEU	2.5
1	A	611	ALA	2.5
2	B	518	LEU	2.5
1	A	749	ILE	2.5
1	D	693	ILE	2.5
1	D	627	LEU	2.5
1	A	644	LEU	2.5
1	A	598	TYR	2.4
2	E	480	ILE	2.4
2	E	638	HIS	2.4
1	A	675	LYS	2.4
2	E	479	THR	2.4
1	A	584	ILE	2.4
2	E	559	ILE	2.4
1	A	630	TYR	2.4
1	D	579	ALA	2.4
1	D	705	VAL	2.3
1	D	751	LYS	2.3
1	A	592	SER	2.3
1	D	689	ILE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	508	CYS	2.3
1	D	611	ALA	2.3
1	D	674	GLY	2.3
1	A	601	LEU	2.3
2	B	555	LYS	2.3
1	D	668	PHE	2.3
1	D	506	ARG	2.3
2	E	481	THR	2.3
1	D	618	SER	2.3
1	D	594	ASP	2.3
1	D	570	PHE	2.3
1	D	725	GLU	2.3
1	D	769	CYS	2.3
1	D	614	GLU	2.2
1	A	647	VAL	2.2
2	B	487	ARG	2.2
1	D	645	LYS	2.2
1	A	708	SER	2.2
2	E	647	LYS	2.2
2	B	548	THR	2.2
2	E	518	LEU	2.2
2	B	559	ILE	2.2
1	D	653	PRO	2.2
1	A	509	VAL	2.2
2	B	481	THR	2.2
1	A	638	ASP	2.2
2	B	483	PHE	2.2
2	E	491	ALA	2.1
1	A	597	LEU	2.1
1	D	566	CYS	2.1
1	D	632	SER	2.1
2	B	484	SER	2.1
1	D	586	LEU	2.1
1	D	621	TRP	2.1
1	A	600	LEU	2.1
2	B	636	LEU	2.1
1	D	650	LYS	2.1
1	A	596	VAL	2.1
1	D	581	PHE	2.1
1	D	510	ASN	2.1
2	B	647	LYS	2.1
1	D	661	PRO	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	648	LEU	2.0
1	D	603	GLU	2.0
2	E	477	GLY	2.0
1	D	641	ASP	2.0
2	B	653	TYR	2.0
1	A	623	MET	2.0
1	D	646	SER	2.0
1	D	511	LEU	2.0
1	D	613	LYS	2.0
1	D	615	LYS	2.0
1	D	512	THR	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](#)

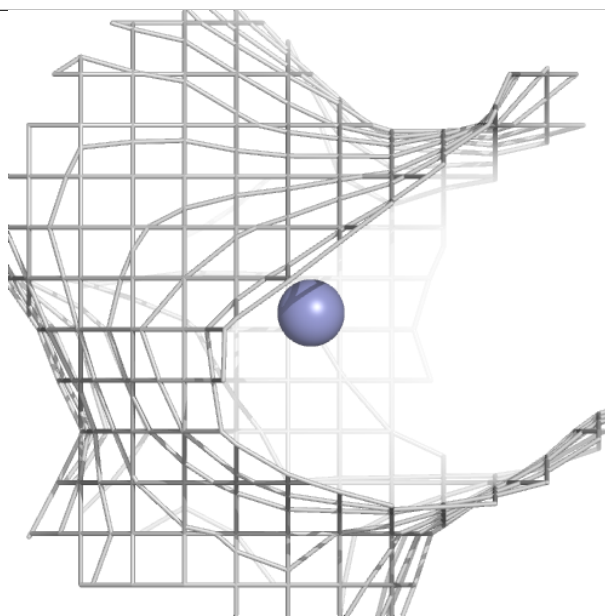
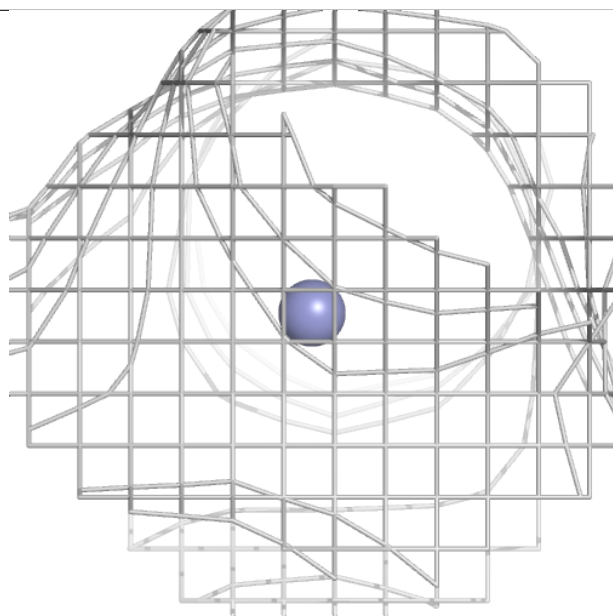
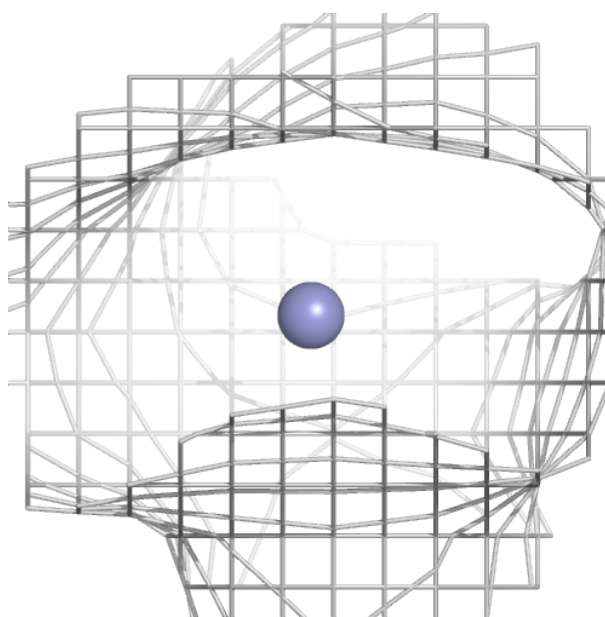
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ZN	B	901	1/1	0.99	0.02	55,55,55,55	0
3	ZN	B	902	1/1	0.99	0.03	84,84,84,84	0
3	ZN	E	902	1/1	0.99	0.03	76,76,76,76	0
3	ZN	E	901	1/1	1.00	0.03	54,54,54,54	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.

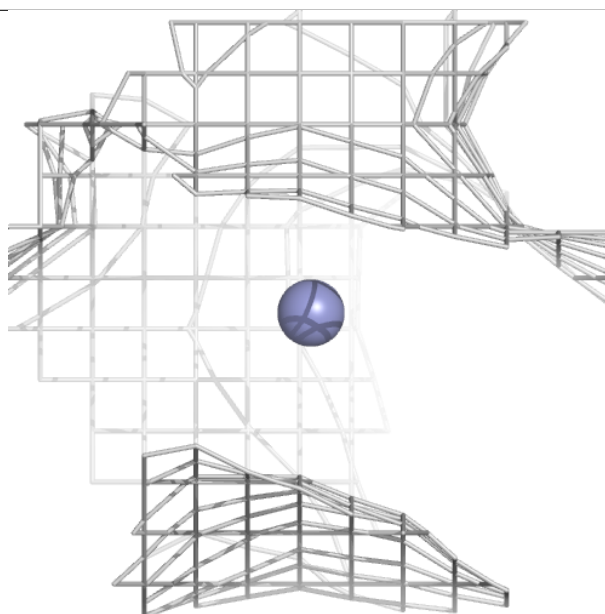
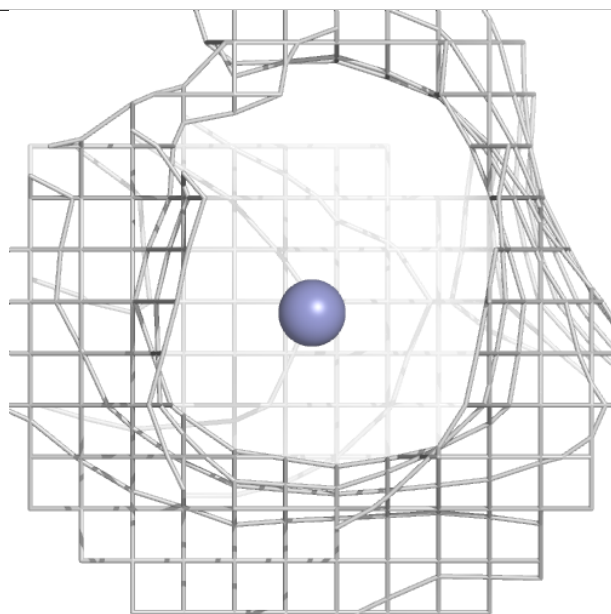
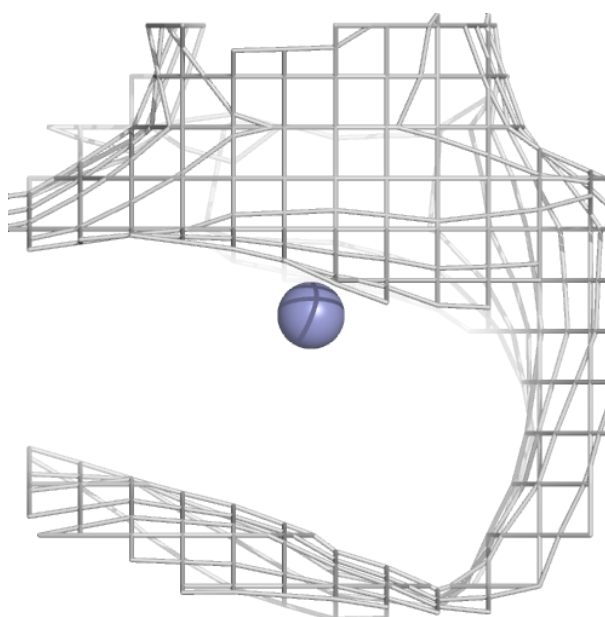
Electron density around ZN B 901:

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



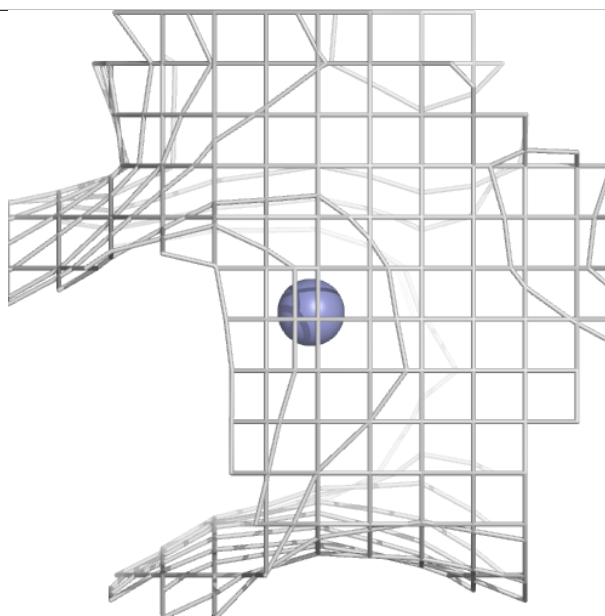
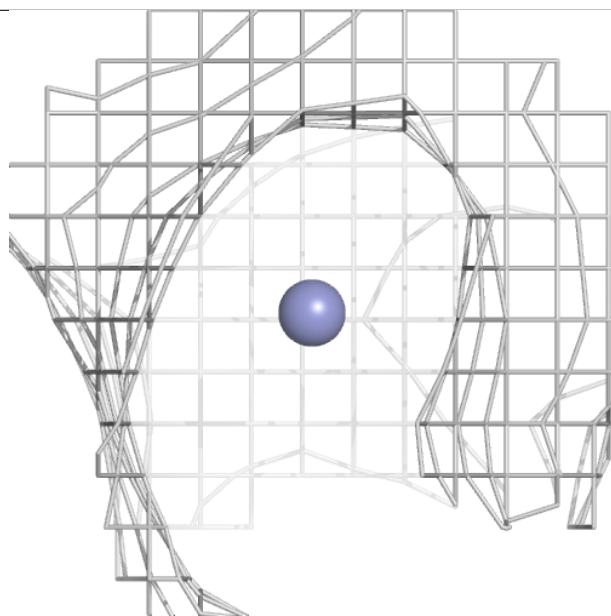
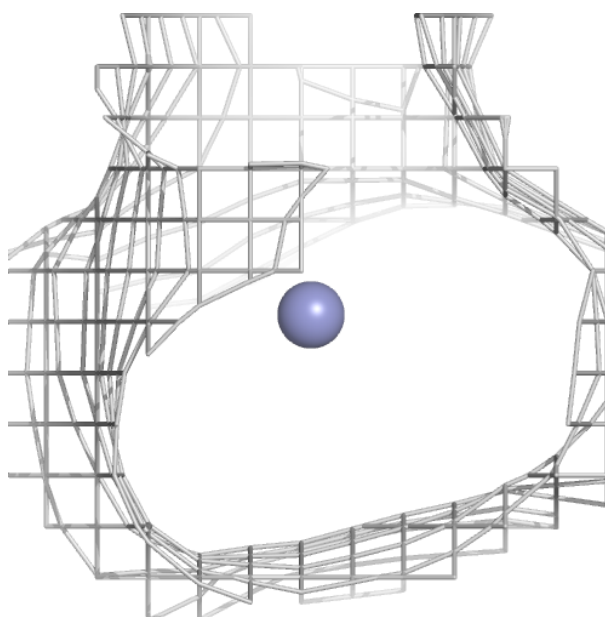
Electron density around ZN B 902:

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



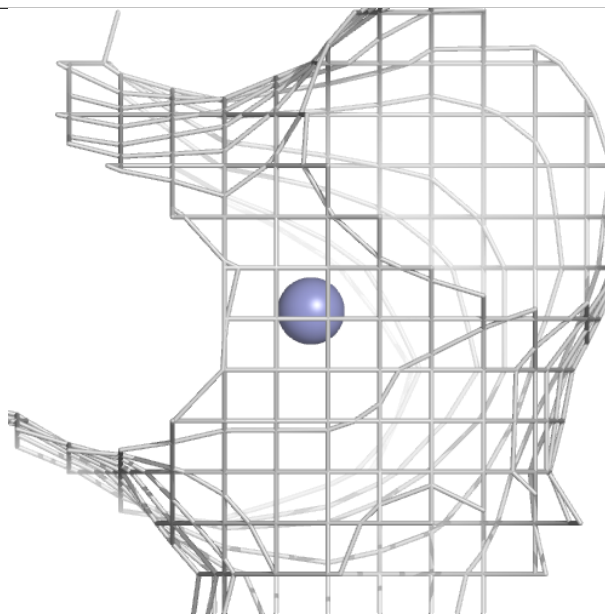
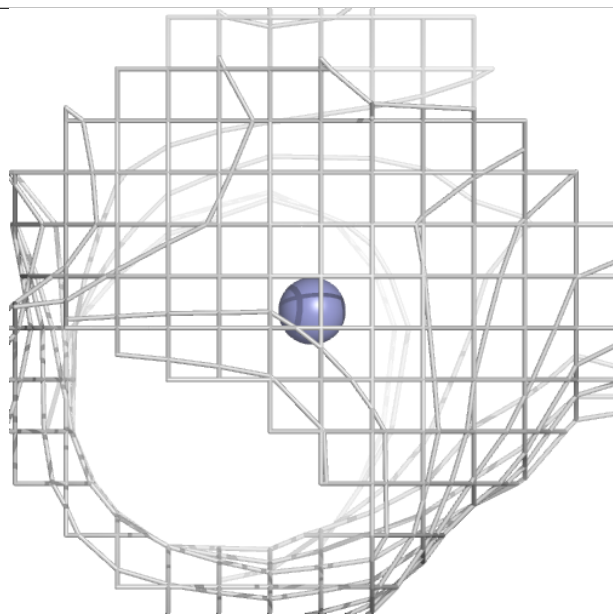
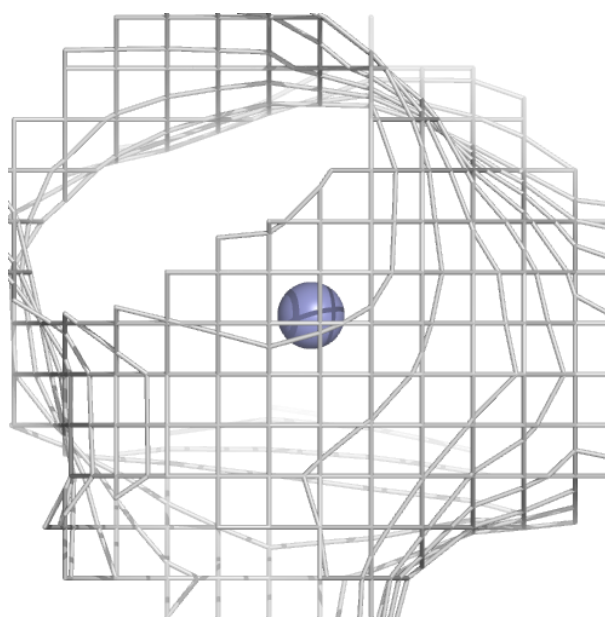
Electron density around ZN E 902:

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



Electron density around ZN E 901:

$2mF_o-DF_c$ (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.