



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:37 AM UTC

PDB ID : 7WI7 / pdb_00007wi7
Title : Crystal structure of human MCM8/9 complex
Authors : Li, J.; Liu, Y.
Deposited on : 2022-01-03
Resolution : 6.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

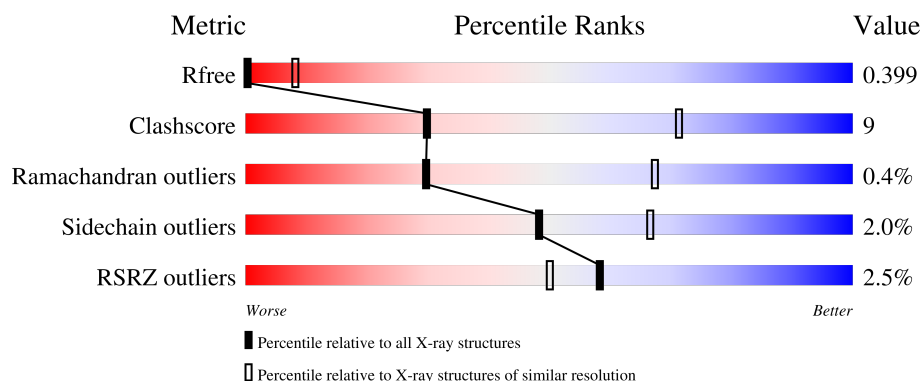
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

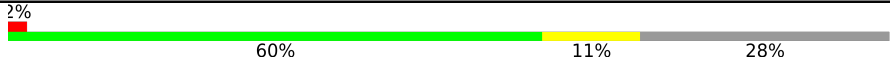
The reported resolution of this entry is 6.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1162 (9.00-4.00)
Clashscore	190562	1000 (9.00-4.04)
Ramachandran outliers	187476	1050 (9.00-4.00)
Sidechain outliers	187428	1014 (9.00-4.00)
RSRZ outliers	180081	1155 (9.00-4.00)

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	787	
2	B	684	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8839 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 helicase MCM8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	565	Total	C	N	O	S	0	1	0
			4406	2791	758	831	26			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	MET	-	initiating methionine	UNP Q9UJA3
A	841	HIS	-	expression tag	UNP Q9UJA3
A	842	HIS	-	expression tag	UNP Q9UJA3
A	843	HIS	-	expression tag	UNP Q9UJA3
A	844	HIS	-	expression tag	UNP Q9UJA3
A	845	HIS	-	expression tag	UNP Q9UJA3
A	846	HIS	-	expression tag	UNP Q9UJA3

- Molecule 2 is a protein called DNA helicase MCM9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	566	Total	C	N	O	S	0	0	0
			4431	2800	758	840	33			

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

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

- Molecule 1: DNA helicase MCM8





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	185.62Å 185.62Å 185.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.50 – 6.60 41.50 – 6.60	Depositor EDS
% Data completeness (in resolution range)	98.4 (41.50-6.60) 92.6 (41.50-6.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.28 (at 6.68Å)	Xtriage
Refinement program	PHENIX 1.17_3644	Depositor
R, R_{free}	0.321 , 0.398 0.323 , 0.399	Depositor DCC
R_{free} test set	415 reflections (9.89%)	wwPDB-VP
Wilson B-factor (Å ²)	404.8	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 999.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.055 for l,-k,h	Xtriage
F_o, F_c correlation	0.76	EDS
Total number of atoms	8839	wwPDB-VP
Average B, all atoms (Å ²)	627.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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

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	0.10	0/4479	0.33	2/6049 (0.0%)
2	B	0.11	0/4496	0.30	0/6069
All	All	0.11	0/8975	0.32	2/12118 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	345	ARG	CA-C-N	6.16	132.79	121.70
1	A	345	ARG	C-N-CA	6.16	132.79	121.70

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	4406	0	4472	56	0
2	B	4431	0	4494	99	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	8839	0	8966	152	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 9.

All (152) 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:571:SER:HA	2:B:574:ARG:HD2	1.63	0.79
2:B:546:LEU:HD22	2:B:572:LEU:HD22	1.66	0.76
2:B:580:ALA:HB1	2:B:585:ARG:HB2	1.69	0.74
2:B:209:GLN:HB3	2:B:371:ARG:HG2	1.71	0.73
2:B:531:ILE:HG22	2:B:581:ARG:HG2	1.71	0.73
1:A:482:THR:HG21	1:A:523:MET:HG2	1.72	0.72
2:B:546:LEU:HD13	2:B:572:LEU:HB3	1.71	0.70
1:A:149:PRO:HB3	1:A:218:TYR:HB2	1.76	0.68
2:B:345:GLU:HB3	2:B:452:THR:HB	1.75	0.67
2:B:532:ARG:HA	2:B:581:ARG:HE	1.58	0.67
2:B:431:MET:HB3	2:B:567:ARG:HH12	1.61	0.65
2:B:577:GLU:O	2:B:581:ARG:N	2.17	0.65
2:B:398:LEU:HD21	2:B:447:LEU:HD22	1.78	0.64
1:A:548:CYS:SG	1:A:549:SER:N	2.71	0.63
2:B:566:ILE:HD12	2:B:570:GLU:HG3	1.81	0.63
2:B:387:VAL:HG11	2:B:438:VAL:HG22	1.81	0.63
2:B:582:LEU:HB3	2:B:583:MET:HE2	1.81	0.62
2:B:368:ILE:HG13	2:B:521:MET:HG3	1.81	0.61
2:B:55:GLY:O	2:B:59:ASN:ND2	2.31	0.61
2:B:549:TYR:OH	2:B:604:MET:SD	2.52	0.61
2:B:473:ILE:HG21	2:B:480:LEU:HD21	1.83	0.61
2:B:346:SER:O	2:B:347:HIS:ND1	2.33	0.60
1:A:453:VAL:HG13	1:A:577:LEU:HD13	1.84	0.60
2:B:370:PRO:HD3	2:B:525:LYS:HG3	1.83	0.59
1:A:535:GLU:OE1	1:A:586:ARG:NH1	2.36	0.59
2:B:568:LEU:O	2:B:572:LEU:HG	2.02	0.59
2:B:139:LEU:HD22	2:B:140:GLU:H	1.69	0.58
1:A:724:ALA:HB2	1:A:732:ALA:HB2	1.85	0.58
1:A:288:TRP:NE1	1:A:314:GLU:OE1	2.37	0.58
1:A:332:THR:HG1	1:A:361:SER:HG	1.50	0.58
2:B:329:ALA:HB1	2:B:581:ARG:HD3	1.85	0.57
2:B:317:MET:HE3	2:B:489:LEU:HD22	1.85	0.57
1:A:531:LEU:HG	1:A:583:LEU:HD13	1.86	0.56
2:B:445:CYS:SG	2:B:446:LYS:N	2.79	0.56
2:B:524:MET:HA	2:B:527:TYR:HD2	1.71	0.56
2:B:303:ARG:HH21	2:B:579:HIS:HB3	1.70	0.56
2:B:225:GLU:OE2	2:B:264:LYS:HE3	2.06	0.55
2:B:142:GLU:OE2	2:B:157:LYS:NZ	2.28	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:221:LYS:HD2	2:B:260:GLU:OE2	2.07	0.54
2:B:306:ILE:HG23	2:B:524:MET:HE1	1.90	0.54
1:A:340:ALA:HB3	1:A:341:GLU:HA	1.90	0.53
2:B:53:GLU:HB3	2:B:57:TYR:CE2	2.43	0.53
1:A:319:LEU:HD22	1:A:362:ILE:HG22	1.90	0.53
2:B:576:ALA:HB1	2:B:588:VAL:HG11	1.90	0.52
1:A:507:LEU:HD21	1:A:530:LEU:HD12	1.90	0.52
1:A:346:ASN:HB3	1:A:347:LYS:HB2	1.91	0.52
2:B:386:THR:HG21	2:B:426:SER:HB3	1.90	0.52
2:B:132:ARG:HB3	2:B:203:LYS:HB3	1.92	0.52
2:B:386:THR:HB	2:B:436:ILE:HG21	1.92	0.52
2:B:569:LEU:HA	2:B:572:LEU:HD12	1.90	0.52
2:B:199:TYR:OH	2:B:247:ARG:NH1	2.42	0.52
2:B:193:PRO:HB2	2:B:195:ARG:HG3	1.92	0.52
1:A:340:ALA:H	1:A:341:GLU:HG3	1.75	0.52
1:A:536:GLN:HE22	2:B:363:LYS:HD3	1.75	0.51
2:B:416:PHE:HB3	2:B:457:THR:HG22	1.92	0.51
1:A:343:GLY:HA3	1:A:344:SER:HB3	1.92	0.51
2:B:222:VAL:HG11	2:B:240:ILE:HD13	1.92	0.51
2:B:351:VAL:HG11	2:B:473:ILE:HG12	1.93	0.51
2:B:414:ASP:OD1	2:B:415:GLU:N	2.41	0.51
2:B:132:ARG:HE	2:B:203:LYS:HB2	1.76	0.51
2:B:349:LEU:HD11	2:B:457:THR:HG23	1.93	0.51
1:A:490:THR:HB	1:A:503:GLU:HB2	1.93	0.50
2:B:404:VAL:HG11	2:B:447:LEU:HD21	1.92	0.50
2:B:322:LEU:O	2:B:326:MET:HG2	2.10	0.50
1:A:502:LEU:HD13	1:A:550:LEU:HD21	1.93	0.50
2:B:329:ALA:HA	2:B:581:ARG:CZ	2.42	0.50
2:B:306:ILE:HG21	2:B:582:LEU:HD21	1.94	0.50
2:B:545:VAL:HG11	2:B:593:ALA:HB1	1.94	0.50
2:B:428:HIS:CD2	2:B:479:LEU:HD13	2.47	0.49
2:B:370:PRO:HD3	2:B:525:LYS:HE2	1.94	0.49
1:A:355:LEU:HD22	1:A:356:TYR:H	1.77	0.49
1:A:438:ASP:OD2	1:A:439:LYS:NZ	2.46	0.49
2:B:54:ILE:HD11	2:B:69:PHE:HZ	1.78	0.49
1:A:295:GLU:HG3	1:A:297:MET:HG2	1.95	0.48
1:A:345:ARG:HB3	1:A:346:ASN:CG	2.38	0.48
1:A:720:THR:HA	1:A:740:ILE:HG13	1.95	0.48
1:A:450:ILE:HB	1:A:557:ILE:HG13	1.96	0.48
2:B:343:ARG:N	2:B:570:GLU:OE1	2.47	0.48
2:B:114:ILE:HD12	2:B:220:MET:HB2	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:307:LEU:HD21	2:B:322:LEU:HB2	1.96	0.48
1:A:291:ILE:HD13	1:A:315:LEU:HD11	1.96	0.48
2:B:207:GLN:NE2	2:B:237:ASP:OD1	2.41	0.48
2:B:550:TYR:OH	2:B:554:ARG:NH1	2.47	0.47
2:B:8:LEU:HD22	2:B:53:GLU:HB2	1.96	0.47
1:A:332:THR:OG1	1:A:361:SER:OG	2.26	0.47
2:B:334:ARG:C	2:B:342:VAL:HG23	2.40	0.47
2:B:330:GLY:HA2	2:B:331:GLY:HA2	1.70	0.46
2:B:527:TYR:O	2:B:531:ILE:HG13	2.15	0.46
2:B:475:LEU:HD22	2:B:479:LEU:HD23	1.98	0.46
1:A:162:GLN:HE21	1:A:166:LYS:HE3	1.81	0.46
2:B:332:ILE:HD12	2:B:577:GLU:OE2	2.15	0.46
2:B:334:ARG:HE	2:B:573:ILE:HD13	1.79	0.46
2:B:315:PHE:HE2	2:B:504:PHE:HB3	1.81	0.46
2:B:1:MET:HG3	2:B:61:PHE:CD2	2.50	0.46
2:B:358:LYS:HD2	2:B:456:ALA:HB1	1.98	0.46
2:B:365:ALA:HA	2:B:368:ILE:HG22	1.98	0.46
2:B:534:LEU:HD21	2:B:584:PHE:CE1	2.50	0.45
2:B:199:TYR:HE1	2:B:201:GLU:HG3	1.81	0.45
1:A:427:ALA:HA	1:A:448:PRO:HG2	1.99	0.45
2:B:430:ALA:HB2	2:B:436:ILE:HD11	1.98	0.45
2:B:314:VAL:HG21	2:B:361:PHE:CE1	2.52	0.45
1:A:344:SER:HB3	1:A:350:LYS:HD2	1.99	0.45
2:B:478:PRO:O	2:B:482:ARG:HG3	2.16	0.45
1:A:445:ARG:HG3	1:A:537:GLN:HE21	1.82	0.45
1:A:435:TYR:HD1	1:A:443:PRO:HD3	1.81	0.45
1:A:449:HIS:CG	1:A:534:MET:HE3	2.52	0.45
2:B:149:LYS:HD2	2:B:180:SER:HB2	1.98	0.45
1:A:514:ILE:HG12	1:A:555:SER:HB3	1.99	0.44
1:A:535:GLU:OE2	2:B:363:LYS:NZ	2.49	0.44
1:A:437:ASP:OD1	1:A:437:ASP:N	2.51	0.44
1:A:309:ARG:HD3	1:A:309:ARG:HA	1.84	0.44
2:B:566:ILE:HA	2:B:566:ILE:HD13	1.66	0.44
1:A:105:ARG:NH1	1:A:133:GLU:OE2	2.50	0.44
2:B:333:GLN:NE2	2:B:434:GLN:OE1	2.46	0.43
2:B:576:ALA:HB1	2:B:588:VAL:HG21	2.00	0.43
2:B:307:LEU:HD11	2:B:322:LEU:HA	2.01	0.43
1:A:335:VAL:HA	1:A:357:ILE:HD13	2.01	0.43
1:A:435:TYR:CD1	1:A:443:PRO:HD3	2.53	0.43
1:A:536:GLN:NE2	2:B:363:LYS:HD3	2.34	0.43
2:B:565:THR:HG23	2:B:566:ILE:H	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ARG:HB2	1:A:134:VAL:HG13	2.02	0.42
1:A:448:PRO:HA	1:A:588:ASP:OD2	2.19	0.42
2:B:2:ASN:OD1	2:B:5:GLN:HG3	2.19	0.42
2:B:419:LEU:HB3	2:B:423:ASP:HB2	2.00	0.42
2:B:18:SER:O	2:B:22:LYS:NZ	2.51	0.42
1:A:419:LEU:HG	1:A:746:TYR:CG	2.55	0.42
2:B:125:SER:HB3	2:B:241:TYR:CD2	2.55	0.42
2:B:570:GLU:HA	2:B:573:ILE:HD12	2.01	0.42
2:B:172:CYS:HB3	2:B:178:CYS:HB2	2.00	0.42
2:B:342:VAL:HG12	2:B:570:GLU:CD	2.45	0.42
2:B:403:LEU:HD11	2:B:427:ILE:HG12	2.01	0.42
2:B:13:PHE:O	2:B:17:VAL:HG23	2.19	0.42
1:A:336:LYS:HE2	1:A:336:LYS:HB3	1.91	0.41
1:A:227:ARG:NH1	1:A:292:LYS:HD2	2.34	0.41
2:B:417:ASN:HB2	2:B:474:ALA:HB3	2.02	0.41
1:A:393:ILE:HG23	1:A:669:TYR:CD1	2.55	0.41
1:A:297:MET:HE3	1:A:297:MET:HB3	1.99	0.41
2:B:314:VAL:HG11	2:B:361:PHE:CZ	2.54	0.41
1:A:719:LEU:HB3	1:A:740:ILE:HD12	2.02	0.41
2:B:6:VAL:HG13	2:B:68:ILE:HD13	2.02	0.41
1:A:79:LYS:HE2	1:A:79:LYS:HB3	1.91	0.41
1:A:240:PHE:HB3	1:A:274:PHE:HB3	2.03	0.41
2:B:99:ARG:HB3	2:B:267:TYR:HB2	2.03	0.41
2:B:484:ASP:OD2	2:B:574:ARG:NH1	2.53	0.41
1:A:162:GLN:HA	1:A:165:THR:HG22	2.03	0.41
1:A:227:ARG:NH2	1:A:312:GLU:OE2	2.53	0.41
2:B:397:ASN:OD1	2:B:398:LEU:N	2.46	0.40
1:A:340:ALA:N	1:A:341:GLU:HG3	2.35	0.40
1:A:677:VAL:HG21	1:A:728:LEU:HA	2.03	0.40
1:A:345:ARG:HH11	1:A:348:ASN:ND2	2.20	0.40
1:A:733:THR:OG1	1:A:734:LYS:N	2.55	0.40
2:B:207:GLN:HE22	2:B:237:ASP:CG	2.28	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries

of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	552/787 (70%)	524 (95%)	26 (5%)	2 (0%)	30	67
2	B	552/684 (81%)	505 (92%)	45 (8%)	2 (0%)	30	67
All	All	1104/1471 (75%)	1029 (93%)	71 (6%)	4 (0%)	30	67

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	254	PRO
1	A	444	ILE
2	B	566	ILE
2	B	527	TYR

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	483/681 (71%)	476 (99%)	7 (1%)	59	72
2	B	502/610 (82%)	489 (97%)	13 (3%)	40	62
All	All	985/1291 (76%)	965 (98%)	20 (2%)	48	66

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	268	VAL
1	A	335	VAL
1	A	345	ARG
1	A	352	MET
1	A	354	LEU
1	A	355	LEU
1	A	751	THR
2	B	137	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	139	LEU
2	B	198	ASP
2	B	326	MET
2	B	342	VAL
2	B	346	SER
2	B	458	ASN
2	B	545	VAL
2	B	546	LEU
2	B	565	THR
2	B	566	ILE
2	B	574	ARG
2	B	581	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	162	GLN
1	A	206	GLN
1	A	348	ASN
1	A	536	GLN
1	A	537	GLN
1	A	663	HIS
1	A	712	GLN
2	B	162	GLN
2	B	246	GLN
2	B	271	ASN
2	B	458	ASN

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

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	565/787 (71%)	0.06	13 (2%)	61 53	367, 571, 750, 889	1 (0%)
2	B	566/684 (82%)	0.07	15 (2%)	56 48	388, 662, 895, 1054	0
All	All	1131/1471 (76%)	0.06	28 (2%)	58 50	367, 617, 826, 1054	1 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	310	LEU	5.1
2	B	324	VAL	4.5
2	B	306	ILE	4.1
2	B	232	CYS	3.7
1	A	681	LEU	3.6
1	A	422	ALA	3.5
1	A	530	LEU	3.1
1	A	507	LEU	3.1
1	A	403	PHE	3.0
1	A	198	VAL	3.0
2	B	261	ILE	2.9
2	B	400	ALA	2.8
2	B	320	VAL	2.8
1	A	506	ALA	2.7
2	B	399	GLU	2.6
1	A	137	LEU	2.4
2	B	582	LEU	2.4
1	A	97	GLN	2.4
1	A	226[A]	VAL	2.3
1	A	674	ARG	2.3
2	B	224	LEU	2.3
2	B	387	VAL	2.2
2	B	569	LEU	2.2
2	B	425	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	325	ALA	2.1
1	A	547	VAL	2.1
2	B	598	SER	2.1
1	A	509	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

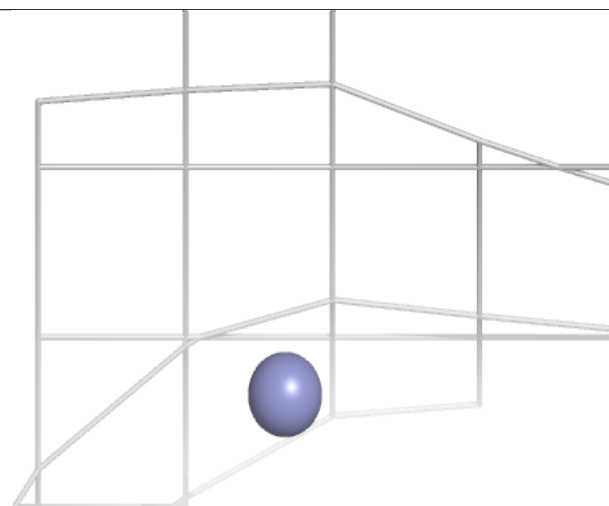
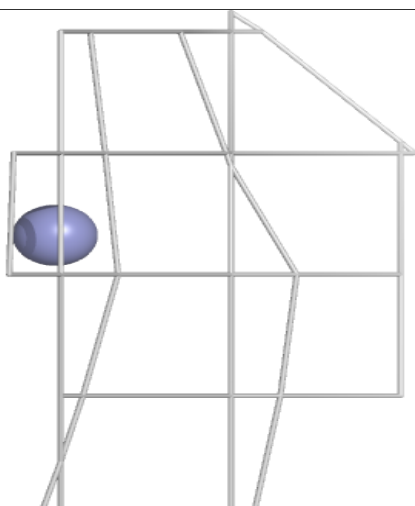
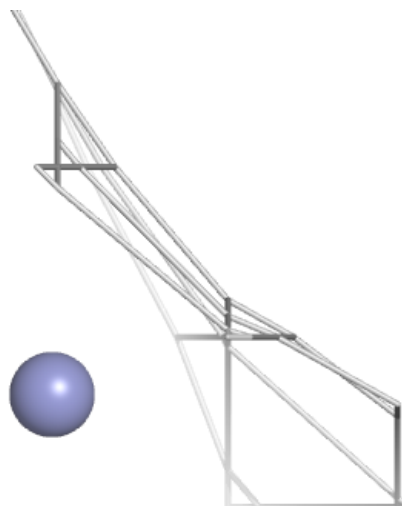
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

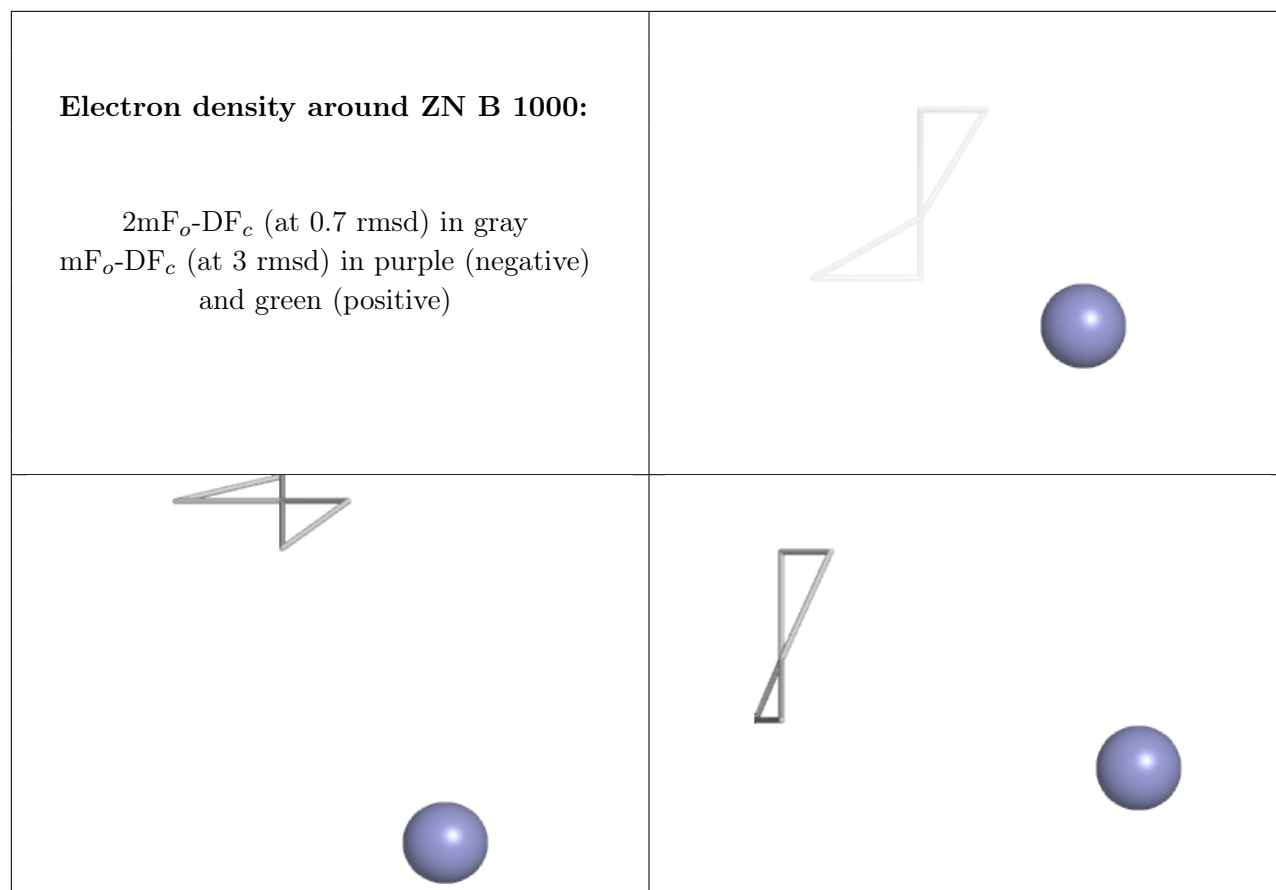
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ZN	A	1000	1/1	0.85	0.09	843,843,843,843	0
3	ZN	B	1000	1/1	0.87	0.07	940,940,940,940	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ZN A 1000:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.