Full wwPDB X-ray Structure Validation Report (i)

Nov 22, 2023 – 06:34 PM JST

PDB ID	:	7WI7
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 (i) 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 (1)) were used in the production of this report:

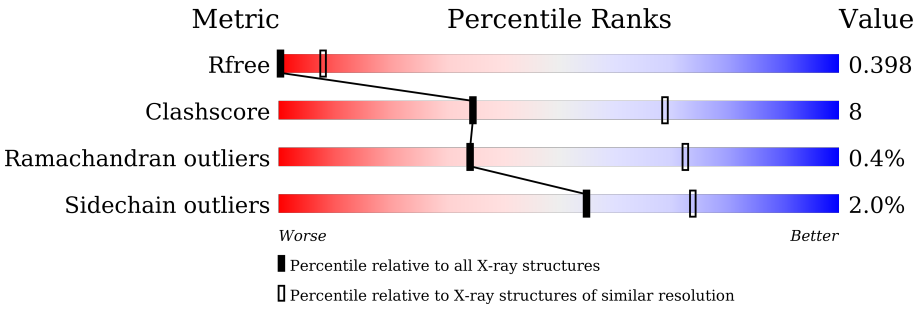
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	1000 (9.00-3.90)
Clashscore	141614	1064 (9.00-3.90)
Ramachandran outliers	138981	1012 (9.00-3.88)
Sidechain outliers	138945	1010 (9.00-3.84)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	787	60% 11% 28%
2	B	684	61% 20% • 17%

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	565	4406	2791	758	831	26	0	1	0

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
			Total	C	N	O	S			
2	B	566	4431	2800	758	840	33	0	0	0

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

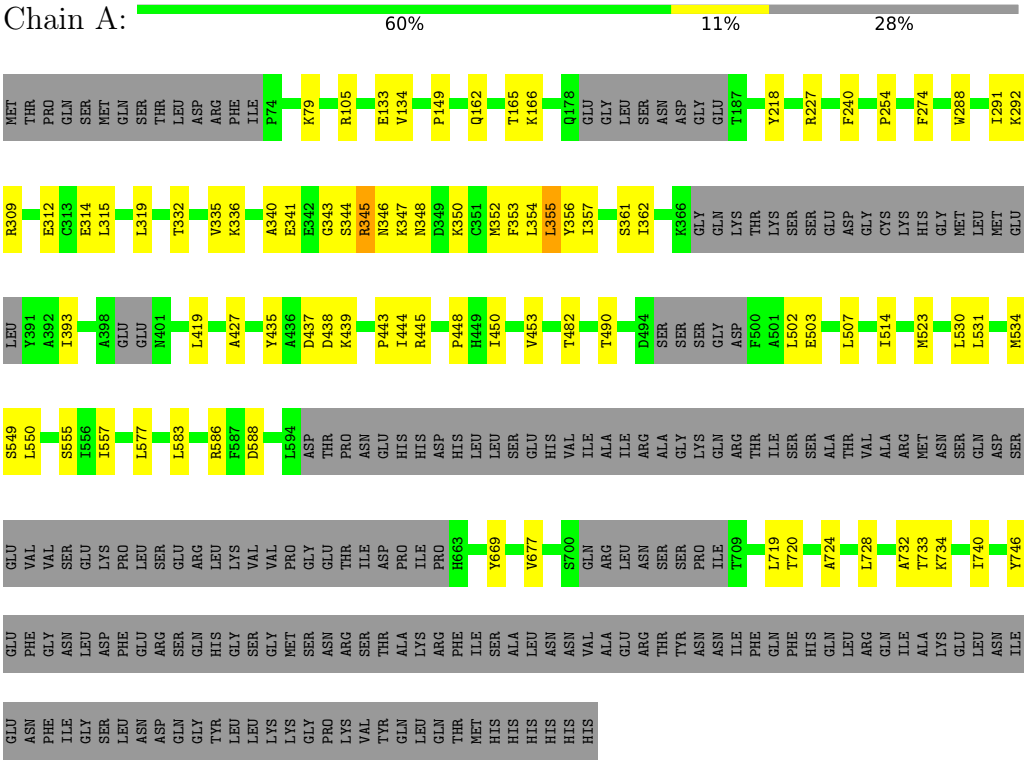
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	A	1	1	1	0	0
3	B	1	Total	Zn	0	0
			1	1		

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. 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. 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.

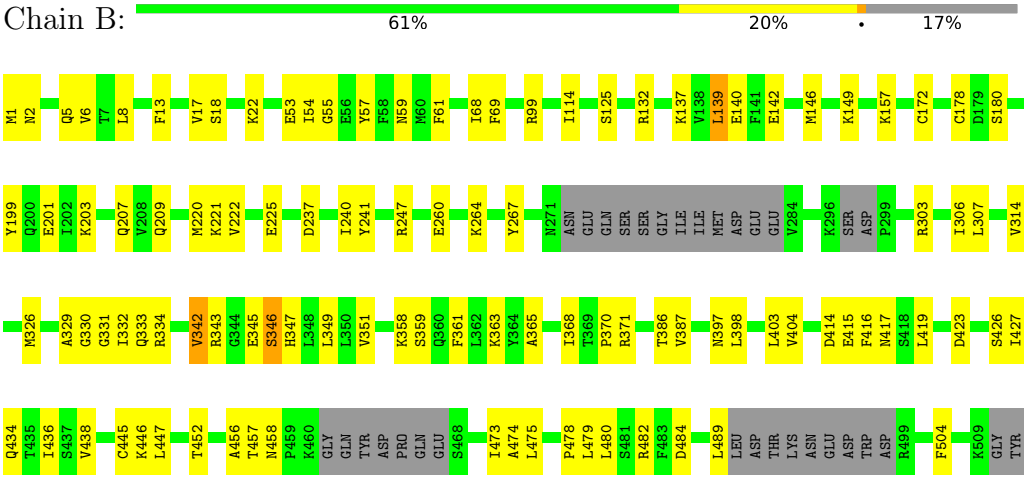
- Molecule 1: DNA helicase MCM8

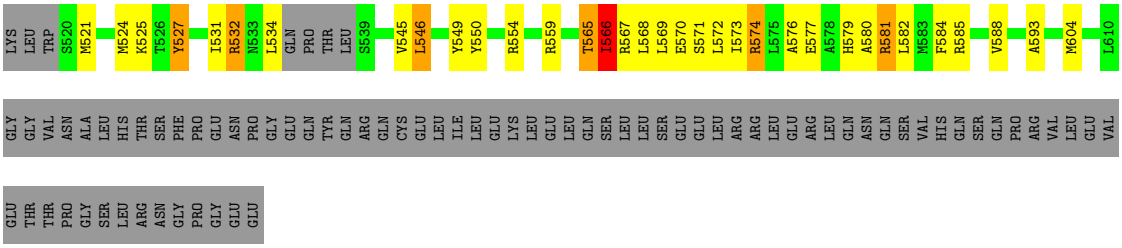
Chain A:



- Molecule 2: DNA helicase MCM9

Chain B:




LYS LEU TRP S520 M521 M524 K525 T526 Y527 I531 R532 N533 L534 GLN PRO THR LEU S539 V545 L546 Y549 Y550 R554 R559 T565 I566 R567 L568 L569 E570 S571 L572 I573 R574 L575 A576 E577 A578 H579 A580 R581 L582 M583 F584 R585 V588 A593 M604 L610
GLY GLY VAL ASN ALA LEU HIS THR SER PHE PRO GLU ASN PRO GLY GLU GLN TYR GLN ARG GLN CYS GLU LEU ILE LEU GLU LYS LEU GLU LEU GLN SER LEU LEU SER GLU GLU LEU ARG ARG LEU GLU ARG LEU GLN ASN GLN SER VAL HIS GLN SER GLN PRO ARG VAL LEU GLU VAL
GLU THR THR PRO GLY SER LEU ARG ASN GLY PRO GLY GLU GLU

4 Data and refinement statistics (i)

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 49.61 – 6.60	Depositor EDS
% Data completeness (in resolution range)	98.4 (41.50-6.60) 92.9 (49.61-6.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	5.28 (at 6.68Å)	Xtriage
Refinement program	PHENIX 1.17_3644	Depositor
R, R_{free}	0.321 , 0.398 0.322 , 0.398	Depositor DCC
R_{free} test set	415 reflections (9.96%)	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)	0.33 , 641.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.055 for l,-k,h	Xtriage
F_o,F_c correlation	0.75	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.24	0/4479	0.43	0/6049
2	B	0.24	0/4496	0.43	0/6069
All	All	0.24	0/8975	0.43	0/12118

There are no bond length outliers.

There are no bond angle outliers.

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	4406	0	4472	54	0
2	B	4431	0	4494	96	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	8839	0	8966	147	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 8.

All (147) 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: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:332:THR:HG1	1:A:361:SER:HG	1.47	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
2:B:329:ALA:HB1	2:B:581:ARG:HD3	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:317:MET:HE3	2:B:489:LEU:HD22	1.86	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
2:B:221:LYS:HD2	2:B:260:GLU:OE2	2.07	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:345:ARG:HB3	1:A:346:ASN:CG	2.38	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
2:B:359:SER:HB2	2:B:363:LYS:HZ2	1.82	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
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:534:MET:HB3	1:A:534:MET:HE2	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:334:ARG:C	2:B:342:VAL:HG23	2.40	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
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

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	552/787 (70%)	524 (95%)	26 (5%)	2 (0%)	34	72
2	B	552/684 (81%)	505 (92%)	45 (8%)	2 (0%)	34	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1104/1471 (75%)	1029 (93%)	71 (6%)	4 (0%)	34 72

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 (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	483/681 (71%)	477 (99%)	6 (1%)	71 83
2	B	502/610 (82%)	488 (97%)	14 (3%)	43 65
All	All	985/1291 (76%)	965 (98%)	20 (2%)	55 74

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

Mol	Chain	Res	Type
1	A	345	ARG
1	A	352	MET
1	A	353	PHE
1	A	354	LEU
1	A	355	LEU
1	A	751	THR
2	B	137	LYS
2	B	139	LEU
2	B	146	MET
2	B	198	ASP
2	B	342	VAL
2	B	346	SER
2	B	458	ASN
2	B	532	ARG

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Mol	Chain	Res	Type
2	B	546	LEU
2	B	559	ARG
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 (6) such sidechains are listed below:

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

There are no monosaccharides 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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

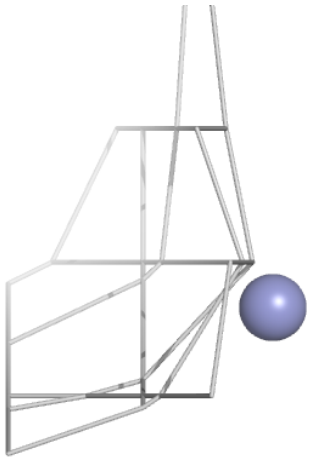
6.4 Ligands

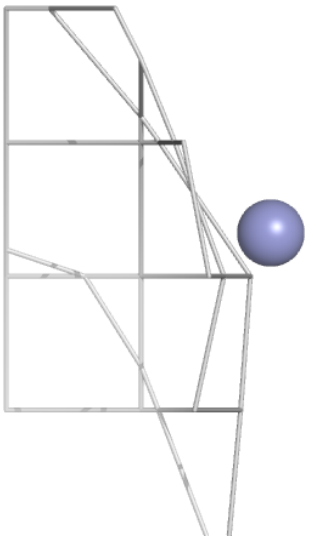
Unable to reproduce the depositors R factor - this section is therefore empty.

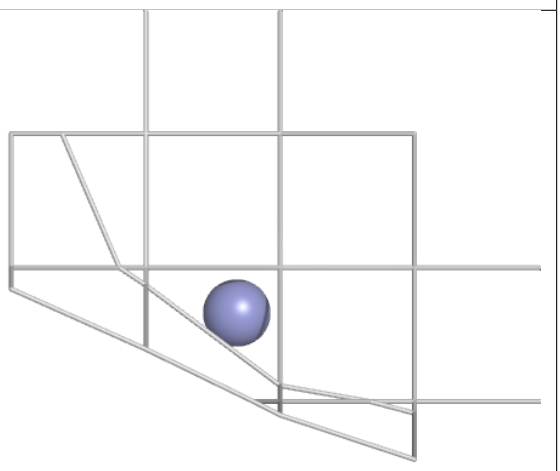
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

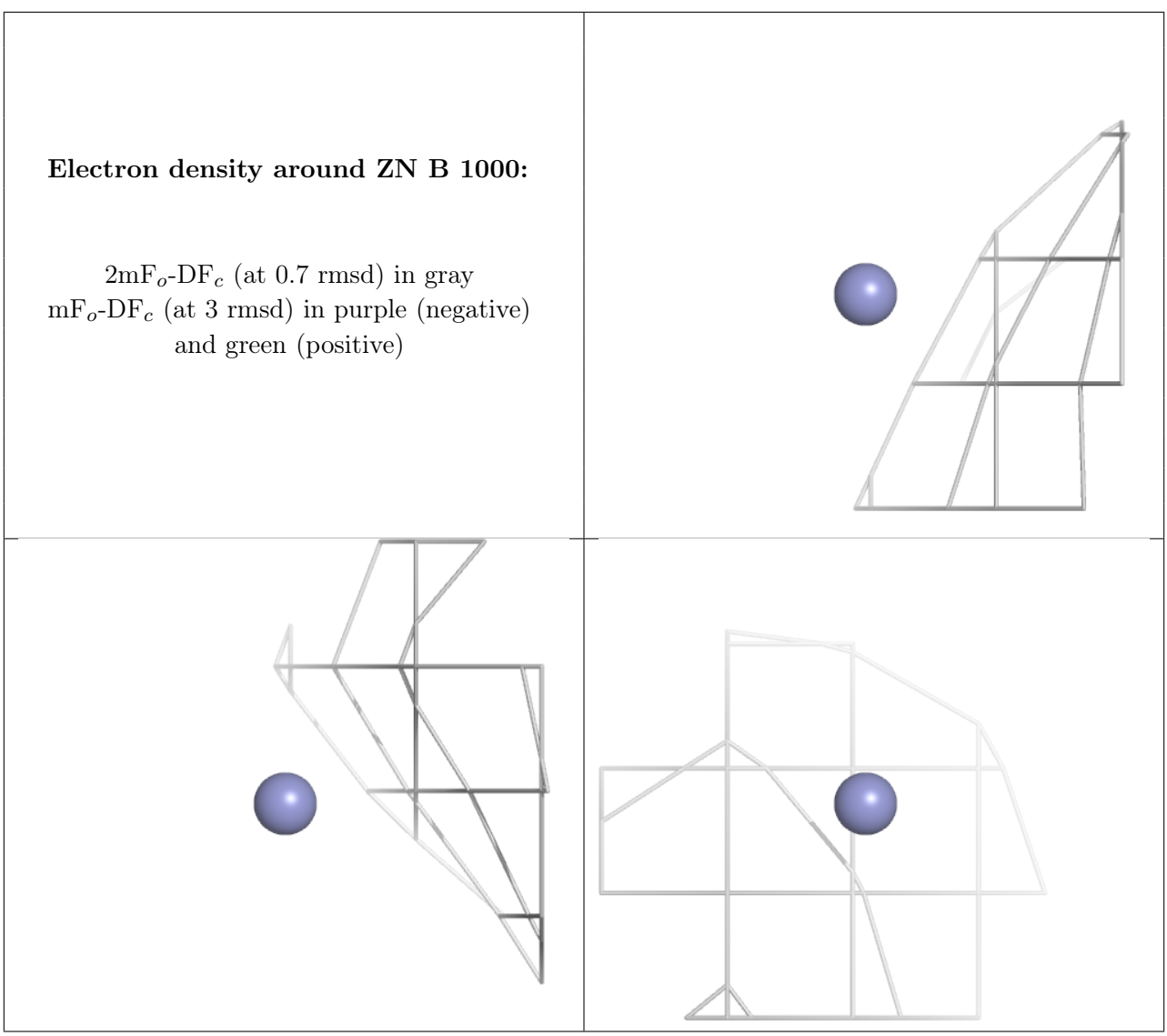






Electron density around ZN B 1000:

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.