



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:19 AM UTC

PDB ID : 7ESZ / pdb_00007esz
Title : Crystal structure of the complex formed by Wolbachia cytoplasmic incompatibility factors CinA and CinB with Mn²⁺ from wPip
Authors : Xiao, Y.J.; Wang, W.; Chen, X.; Ji, X.Y.; Yang, H.T.
Deposited on : 2021-05-12
Resolution : 2.48 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

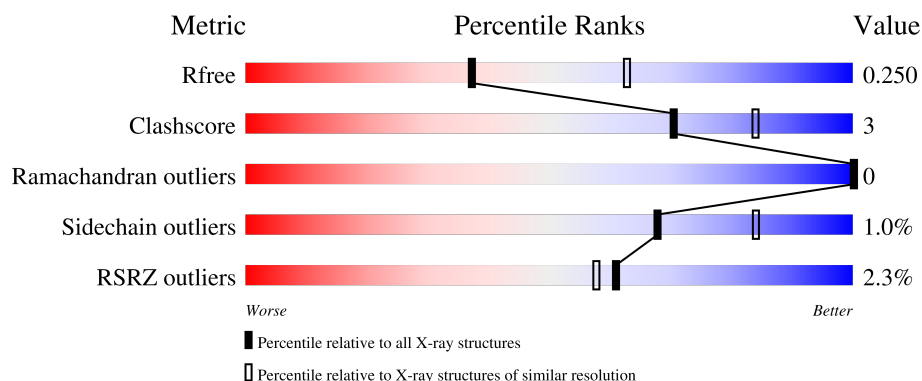
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

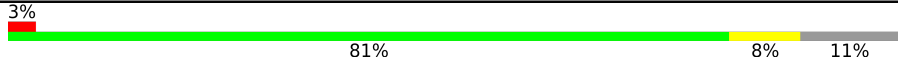
The reported resolution of this entry is 2.48 Å.

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	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (2.50-2.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	740	
1	C	740	
2	B	453	
2	D	453	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17282 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 BACTERIA FACTOR B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	659	Total	C	N	O	S	0	0	0
			5235	3366	873	980	16			
1	C	680	Total	C	N	O	S	0	0	0
			5390	3468	899	1007	16			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	733	LEU	-	expression tag	UNP B3CP74
A	734	GLU	-	expression tag	UNP B3CP74
A	735	HIS	-	expression tag	UNP B3CP74
A	736	HIS	-	expression tag	UNP B3CP74
A	737	HIS	-	expression tag	UNP B3CP74
A	738	HIS	-	expression tag	UNP B3CP74
A	739	HIS	-	expression tag	UNP B3CP74
A	740	HIS	-	expression tag	UNP B3CP74
C	733	LEU	-	expression tag	UNP B3CP74
C	734	GLU	-	expression tag	UNP B3CP74
C	735	HIS	-	expression tag	UNP B3CP74
C	736	HIS	-	expression tag	UNP B3CP74
C	737	HIS	-	expression tag	UNP B3CP74
C	738	HIS	-	expression tag	UNP B3CP74
C	739	HIS	-	expression tag	UNP B3CP74
C	740	HIS	-	expression tag	UNP B3CP74

- Molecule 2 is a protein called BACTERIA FACTOR A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	408	Total	C	N	O	S	0	0	0
			3316	2105	552	645	14			
2	D	401	Total	C	N	O	S	0	0	0
			3245	2066	536	629	14			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	446	LEU	-	expression tag	UNP B3CP73
B	447	GLU	-	expression tag	UNP B3CP73
B	448	HIS	-	expression tag	UNP B3CP73
B	449	HIS	-	expression tag	UNP B3CP73
B	450	HIS	-	expression tag	UNP B3CP73
B	451	HIS	-	expression tag	UNP B3CP73
B	452	HIS	-	expression tag	UNP B3CP73
B	453	HIS	-	expression tag	UNP B3CP73
D	446	LEU	-	expression tag	UNP B3CP73
D	447	GLU	-	expression tag	UNP B3CP73
D	448	HIS	-	expression tag	UNP B3CP73
D	449	HIS	-	expression tag	UNP B3CP73
D	450	HIS	-	expression tag	UNP B3CP73
D	451	HIS	-	expression tag	UNP B3CP73
D	452	HIS	-	expression tag	UNP B3CP73
D	453	HIS	-	expression tag	UNP B3CP73

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

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

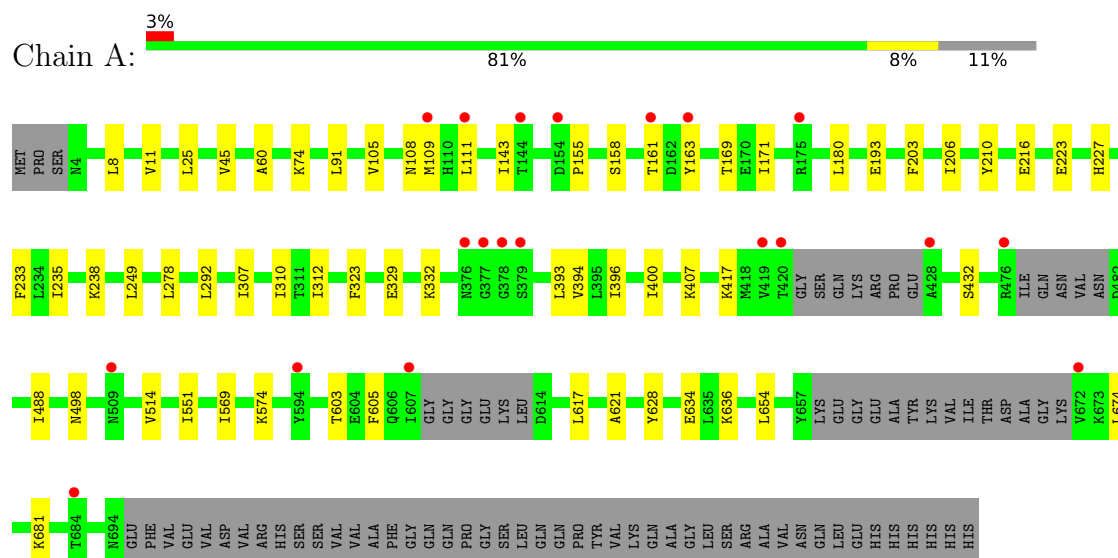
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	35	Total O 35 35	0	0
4	B	31	Total O 31 31	0	0
4	C	17	Total O 17 17	0	0
4	D	11	Total O 11 11	0	0

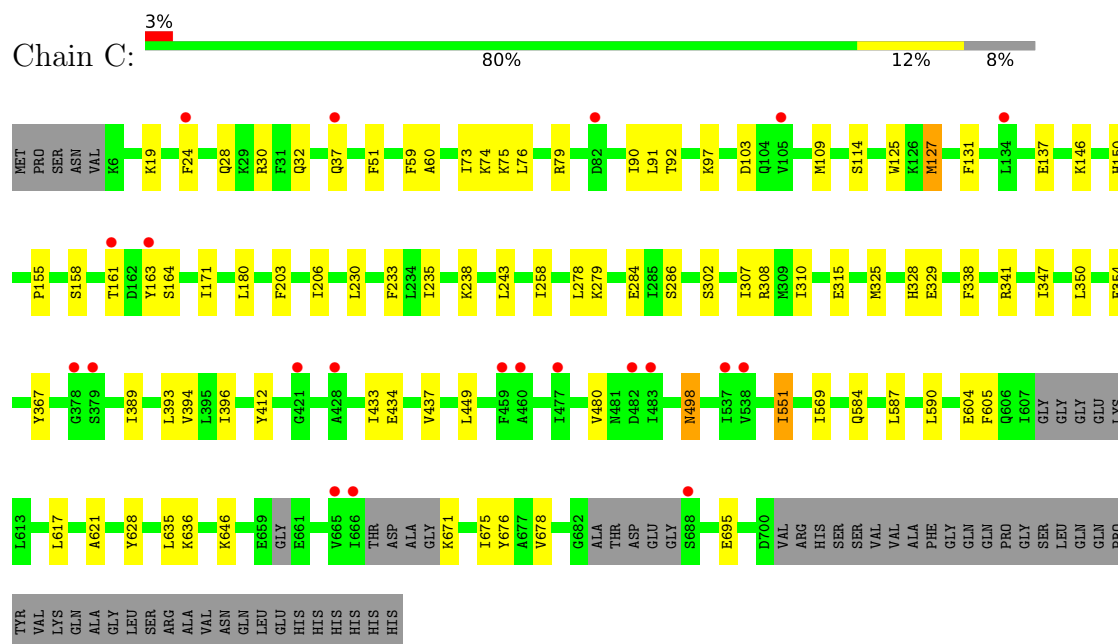
3 Residue-property plots

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.

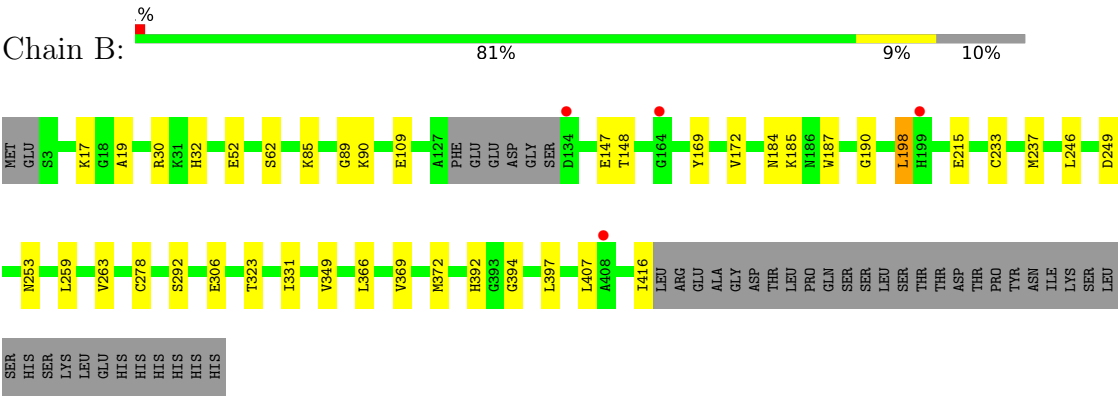
• Molecule 1: BACTERIA FACTOR B



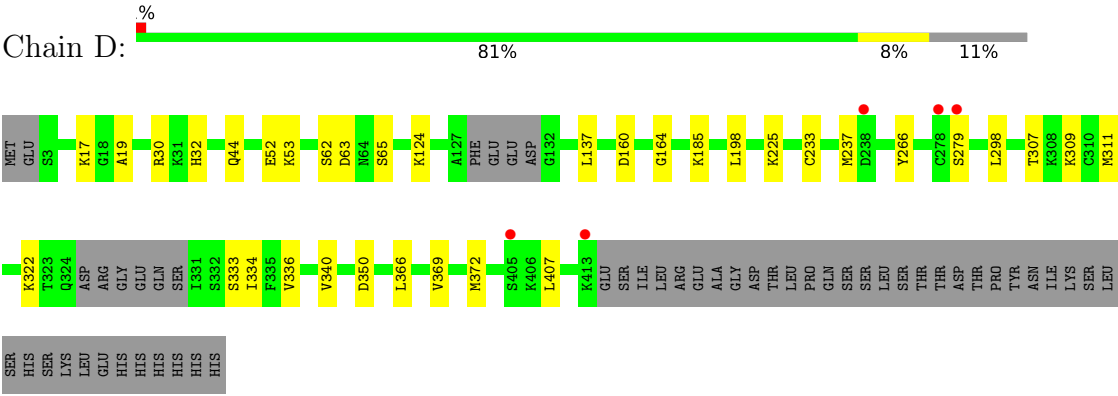
• Molecule 1: BACTERIA FACTOR B



● Molecule 2: BACTERIA FACTOR A



● Molecule 2: BACTERIA FACTOR A



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	85.47Å 86.38Å 93.02Å 110.06° 91.86° 115.38°	Depositor
Resolution (Å)	41.07 – 2.48 41.07 – 2.48	Depositor EDS
% Data completeness (in resolution range)	93.3 (41.07-2.48) 93.3 (41.07-2.48)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.198 , 0.250 0.198 , 0.250	Depositor DCC
R_{free} test set	3693 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å ²)	43.1	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 33.8	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	0.95	EDS
Total number of atoms	17282	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% 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: MN

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	0.11	0/5324	0.29	0/7152
1	C	0.11	0/5481	0.28	0/7363
2	B	0.12	0/3368	0.30	0/4518
2	D	0.11	0/3296	0.27	0/4421
All	All	0.11	0/17469	0.28	0/23454

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 [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	5235	0	5277	33	0
1	C	5390	0	5434	48	0
2	B	3316	0	3301	23	0
2	D	3245	0	3231	19	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	35	0	0	1	0
4	B	31	0	0	0	0
4	C	17	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	11	0	0	0	0
All	All	17282	0	17243	118	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 3.

All (118) 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:A:45:VAL:HG11	1:A:143:ILE:HD13	1.69	0.75
1:A:109:MET:HB3	1:A:163:TYR:CD2	2.24	0.72
2:D:19:ALA:HB1	2:D:62:SER:HB3	1.73	0.71
2:D:366:LEU:HD13	2:D:407:LEU:HD11	1.77	0.66
1:C:37:GLN:NE2	1:C:604:GLU:OE2	2.31	0.63
1:A:109:MET:HB3	1:A:163:TYR:HD2	1.63	0.63
1:A:238:LYS:NZ	4:A:901:HOH:O	2.33	0.62
1:C:24:PHE:HA	1:C:30:ARG:HD3	1.83	0.61
2:D:322:LYS:HD2	2:D:334:ILE:HD13	1.83	0.60
1:C:127:MET:HB2	1:C:131:PHE:HB2	1.83	0.60
1:A:488:ILE:HG13	1:A:514:VAL:HG12	1.85	0.59
2:B:52:GLU:OE1	2:B:90:LYS:NZ	2.33	0.59
1:A:574:LYS:O	1:A:681:LYS:NZ	2.36	0.59
1:C:75:LYS:NZ	1:C:125:TRP:O	2.36	0.58
1:C:109:MET:HB3	1:C:163:TYR:CE2	2.38	0.58
1:C:347:ILE:HD11	1:C:389:ILE:HG23	1.87	0.57
2:B:249:ASP:OD1	2:B:253:ASN:ND2	2.35	0.57
2:B:172:VAL:HA	2:B:198:LEU:HD11	1.86	0.56
2:D:63:ASP:OD2	2:D:65:SER:OG	2.22	0.56
1:A:74:LYS:HB2	1:A:91:LEU:HD22	1.87	0.56
1:C:394:VAL:HG11	1:C:569:ILE:HG21	1.86	0.56
1:A:654:LEU:HD22	1:A:674:LEU:HB3	1.87	0.55
1:C:32:GLN:NE2	1:C:146:LYS:O	2.22	0.55
1:C:180:LEU:HD13	1:C:233:PHE:HE1	1.72	0.55
2:D:334:ILE:HG13	2:D:340:VAL:HG21	1.89	0.55
1:C:60:ALA:HA	1:C:171:ILE:HD13	1.89	0.54
1:A:108:ASN:HB3	1:A:111:LEU:HG	1.89	0.54
1:C:621:ALA:HB3	1:C:628:TYR:HB2	1.88	0.54
1:A:621:ALA:HB3	1:A:628:TYR:HB2	1.90	0.54
1:A:180:LEU:HD13	1:A:233:PHE:HE1	1.72	0.54
2:B:366:LEU:HD13	2:B:407:LEU:HD11	1.89	0.54
1:A:417:LYS:HA	1:A:432:SER:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:LEU:HD23	1:C:258:ILE:HD12	1.90	0.53
1:C:203:PHE:HA	1:C:206:ILE:HG22	1.90	0.53
1:A:249:LEU:O	1:A:498:ASN:ND2	2.41	0.53
2:B:85:LYS:HE3	2:B:89:GLY:HA2	1.90	0.52
1:A:155:PRO:HG2	1:A:158:SER:HB2	1.92	0.52
1:C:354:GLU:OE1	2:D:53:LYS:NZ	2.30	0.52
1:C:279:LYS:HD3	1:C:286:SER:HA	1.91	0.52
1:C:617:LEU:HB2	1:C:635:LEU:HD21	1.92	0.51
1:C:73:ILE:HD13	1:C:92:THR:HG22	1.93	0.51
2:B:246:LEU:HD13	2:B:278:CYS:SG	2.50	0.50
1:C:28:GLN:HB2	1:C:150:HIS:HB3	1.93	0.50
1:C:59:PHE:HD1	1:C:76:LEU:HD11	1.76	0.50
2:B:394:GLY:HA2	2:B:397:LEU:HG	1.92	0.50
1:A:605:PHE:CE1	1:A:617:LEU:HD13	2.47	0.49
2:B:30:ARG:NH1	2:B:306:GLU:OE1	2.45	0.49
1:C:238:LYS:HA	1:C:243:LEU:HB2	1.94	0.49
2:B:233:CYS:HB3	2:B:237:MET:HE3	1.94	0.49
1:C:302:SER:HB2	1:C:367:TYR:CZ	2.48	0.48
1:A:396:ILE:O	1:A:407:LYS:NZ	2.42	0.48
1:A:60:ALA:HA	1:A:171:ILE:HD13	1.95	0.47
2:B:323:THR:HG23	2:B:331:ILE:HD11	1.96	0.47
1:A:105:VAL:HA	1:A:111:LEU:HD11	1.97	0.47
1:C:315:GLU:OE1	2:D:225:LYS:NZ	2.37	0.47
2:D:369:VAL:HA	2:D:372:MET:HE2	1.95	0.47
1:A:8:LEU:HD12	1:A:25:LEU:HD22	1.97	0.47
2:B:349:VAL:HG21	2:B:392:HIS:CE1	2.49	0.47
1:A:169:THR:OG1	1:A:216:GLU:HG2	2.14	0.47
1:A:394:VAL:HG11	1:A:569:ILE:HG21	1.98	0.46
2:B:17:LYS:HE3	2:B:32:HIS:HB3	1.96	0.46
1:C:308:ARG:HD2	1:C:338:PHE:CD1	2.50	0.46
2:D:298:LEU:HD11	2:D:350:ASP:HA	1.98	0.46
1:A:292:LEU:HD22	1:A:332:LYS:HB3	1.97	0.46
1:C:498:ASN:OD1	1:C:498:ASN:N	2.48	0.45
1:A:329:GLU:OE2	1:A:329:GLU:N	2.40	0.45
1:C:433:ILE:O	1:C:437:VAL:HG22	2.16	0.45
2:B:109:GLU:OE2	2:B:169:TYR:OH	2.23	0.45
2:B:369:VAL:HA	2:B:372:MET:HE2	1.98	0.45
1:C:675:ILE:HG13	1:C:676:TYR:H	1.82	0.45
2:D:160:ASP:HB3	2:D:164:GLY:H	1.81	0.45
1:A:393:LEU:O	1:A:396:ILE:HG22	2.17	0.45
1:C:76:LEU:HD22	1:C:171:ILE:HB	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:GLU:OE2	2:B:292:SER:OG	2.31	0.44
2:B:369:VAL:HG13	2:B:372:MET:HE2	1.98	0.44
1:A:603:THR:HG23	1:A:617:LEU:HD11	1.99	0.44
2:D:17:LYS:HE2	2:D:32:HIS:HB3	2.00	0.44
2:D:124:LYS:HG2	2:D:137:LEU:HD13	2.00	0.44
1:C:114:SER:OG	1:C:161:THR:O	2.32	0.44
1:C:636:LYS:HB2	1:C:678:VAL:HG22	1.99	0.44
2:D:30:ARG:NH2	2:D:266:TYR:O	2.31	0.44
2:B:184:ASN:OD1	2:B:185:LYS:HD2	2.19	0.43
1:A:396:ILE:HG13	1:A:400:ILE:HD11	2.00	0.43
1:C:341:ARG:HA	2:D:44:GLN:HB3	1.99	0.43
1:C:636:LYS:HD2	1:C:646:LYS:HD2	1.99	0.43
1:C:74:LYS:HB2	1:C:91:LEU:HD22	2.00	0.43
1:C:584:GLN:HG3	1:C:605:PHE:CE1	2.54	0.43
2:B:19:ALA:HB1	2:B:62:SER:HB3	2.00	0.43
2:B:215:GLU:OE1	1:C:19:LYS:HE3	2.18	0.43
1:C:551:ILE:HD12	1:C:551:ILE:HA	1.79	0.43
1:A:223:GLU:HG2	1:A:227:HIS:CE1	2.54	0.43
1:C:587:LEU:HD23	1:C:590:LEU:HD12	2.01	0.42
1:C:307:ILE:HD12	1:C:310:ILE:HD11	2.01	0.42
1:C:51:PHE:HB3	1:C:103:ASP:HB3	2.00	0.42
2:D:333:SER:O	2:D:336:VAL:HG22	2.19	0.42
2:D:185:LYS:HD2	2:D:185:LYS:HA	1.77	0.42
1:C:155:PRO:HG2	1:C:158:SER:HB2	2.02	0.42
1:C:393:LEU:O	1:C:396:ILE:HG22	2.20	0.42
1:C:412:TYR:N	1:C:434:GLU:OE2	2.53	0.42
2:B:259:LEU:O	2:B:263:VAL:HG22	2.20	0.42
1:A:307:ILE:HD12	1:A:310:ILE:HD11	2.01	0.42
2:B:147:GLU:HG3	2:B:148:THR:HG23	2.01	0.41
1:C:109:MET:HE3	1:C:163:TYR:HE2	1.85	0.41
1:C:325:MET:HG2	1:C:328:HIS:HB2	2.03	0.41
2:D:309:LYS:HE3	2:D:309:LYS:HB2	1.93	0.41
1:C:97:LYS:HE2	1:C:137:GLU:OE2	2.20	0.41
1:A:203:PHE:HA	1:A:206:ILE:HG22	2.03	0.41
2:D:233:CYS:HB3	2:D:237:MET:HE3	2.03	0.41
1:C:79:ARG:NH2	1:C:164:SER:HB3	2.36	0.40
1:A:210:TYR:CD1	1:A:323:PHE:HB3	2.55	0.40
2:B:416:ILE:HD12	2:B:416:ILE:HA	1.80	0.40
1:C:329:GLU:OE1	1:C:329:GLU:N	2.42	0.40
1:A:109:MET:CB	1:A:163:TYR:HD2	2.33	0.40
1:A:634:GLU:OE1	1:A:636:LYS:NZ	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:187:TRP:CD1	2:B:190:GLY:H	2.40	0.40
1:C:350:LEU:HD13	1:C:449:LEU:HD21	2.03	0.40
1:C:671:LYS:HE3	1:C:671:LYS:HB2	1.85	0.40
2:D:307:THR:O	2:D:311:MET:HG3	2.22	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	649/740 (88%)	634 (98%)	15 (2%)	0	100	100
1	C	670/740 (90%)	656 (98%)	14 (2%)	0	100	100
2	B	404/453 (89%)	399 (99%)	5 (1%)	0	100	100
2	D	395/453 (87%)	390 (99%)	5 (1%)	0	100	100
All	All	2118/2386 (89%)	2079 (98%)	39 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	570/655 (87%)	564 (99%)	6 (1%)	65	83
1	C	585/655 (89%)	576 (98%)	9 (2%)	57	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	369/416 (89%)	368 (100%)	1 (0%)	86	93
2	D	360/416 (86%)	357 (99%)	3 (1%)	73	87
All	All	1884/2142 (88%)	1865 (99%)	19 (1%)	68	84

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	VAL
1	A	161	THR
1	A	235	ILE
1	A	278	LEU
1	A	312	ILE
1	A	551	ILE
2	B	198	LEU
1	C	90	ILE
1	C	127	MET
1	C	235	ILE
1	C	278	LEU
1	C	284	GLU
1	C	480	VAL
1	C	498	ASN
1	C	551	ILE
1	C	695	GLU
2	D	52	GLU
2	D	198	LEU
2	D	279	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	296	GLN
1	A	330	ASN
1	A	344	ASN
1	A	364	GLN
1	A	398	ASN
1	A	454	ASN
1	A	598	ASN
1	A	653	GLN
2	B	199	HIS
2	B	207	GLN

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Mol	Chain	Res	Type
1	C	104	GLN
1	C	110	HIS
1	C	198	ASN
1	C	314	ASN
1	C	364	GLN
1	C	398	ASN
1	C	454	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 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	659/740 (89%)	0.23	20 (3%)	52 49	26, 48, 93, 119	0
1	C	680/740 (91%)	0.41	21 (3%)	51 48	29, 57, 107, 134	0
2	B	408/453 (90%)	0.00	4 (0%)	79 77	28, 41, 80, 120	0
2	D	401/453 (88%)	0.14	5 (1%)	76 74	31, 48, 81, 108	0
All	All	2148/2386 (90%)	0.23	50 (2%)	61 58	26, 49, 95, 134	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	594	TYR	4.1
1	A	161	THR	4.1
2	B	134	ASP	3.8
1	C	134	LEU	3.4
1	C	459	PHE	3.3
1	C	24	PHE	3.2
1	C	421	GLY	3.2
1	C	163	TYR	3.1
1	A	378	GLY	3.1
1	C	666	ILE	3.0
1	A	109	MET	3.0
1	C	161	THR	2.9
2	B	199	HIS	2.8
2	D	278	CYS	2.8
2	D	405	SER	2.6
1	A	144	THR	2.6
1	A	509	ASN	2.5
1	C	460	ALA	2.5
1	C	482	ASP	2.5
1	A	175	ARG	2.5
2	B	164	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	377	GLY	2.4
1	A	163	TYR	2.4
1	A	672	VAL	2.4
2	B	408	ALA	2.4
1	C	378	GLY	2.4
1	A	376	ASN	2.4
1	A	607	ILE	2.3
1	C	82	ASP	2.3
1	C	483	ILE	2.3
1	C	379	SER	2.2
1	C	477	ILE	2.2
2	D	279	SER	2.2
1	A	154	ASP	2.2
1	A	428	ALA	2.2
2	D	413	LYS	2.2
1	A	684	THR	2.2
1	C	688	SER	2.2
1	A	476	ARG	2.2
1	C	37	GLN	2.1
1	C	105	VAL	2.1
1	C	665	VAL	2.1
2	D	238	ASP	2.1
1	A	419	VAL	2.1
1	C	428	ALA	2.1
1	A	379	SER	2.1
1	C	538	VAL	2.0
1	C	537	ILE	2.0
1	A	111	LEU	2.0
1	A	420	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

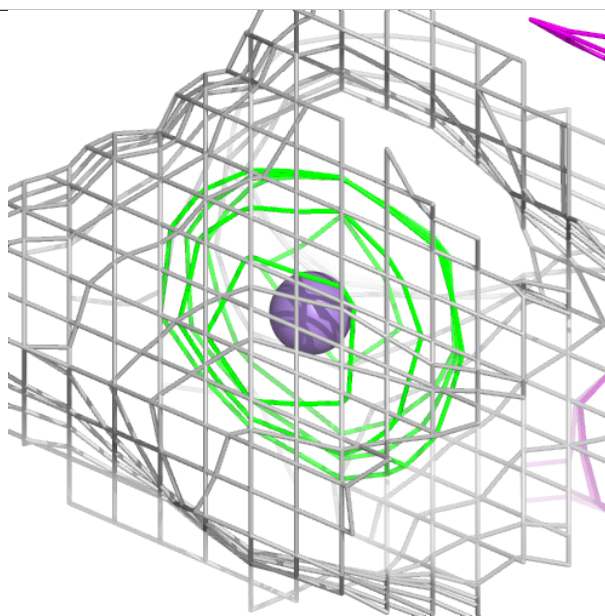
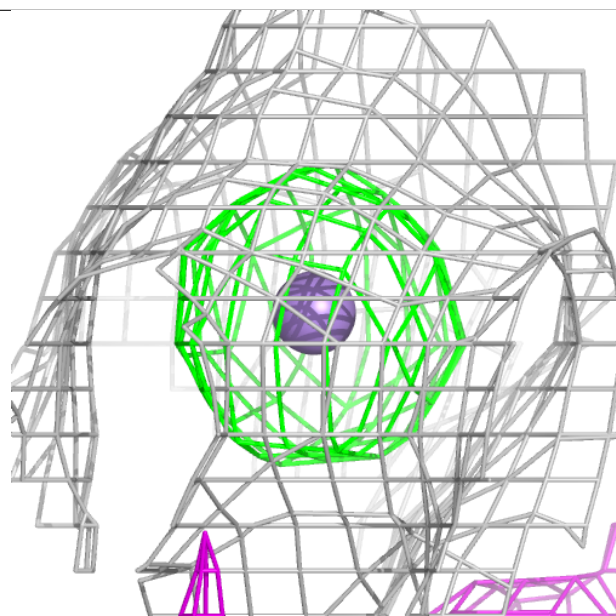
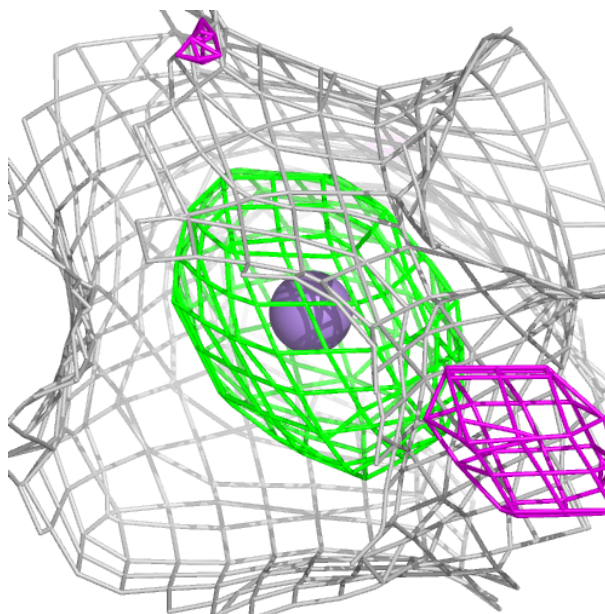
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	MN	A	801	1/1	0.99	0.12	67,67,67,67	0
3	MN	C	801	1/1	0.99	0.03	34,34,34,34	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.

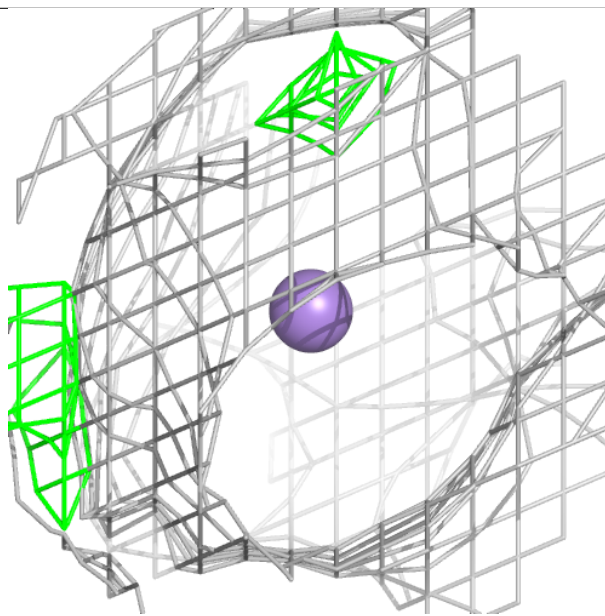
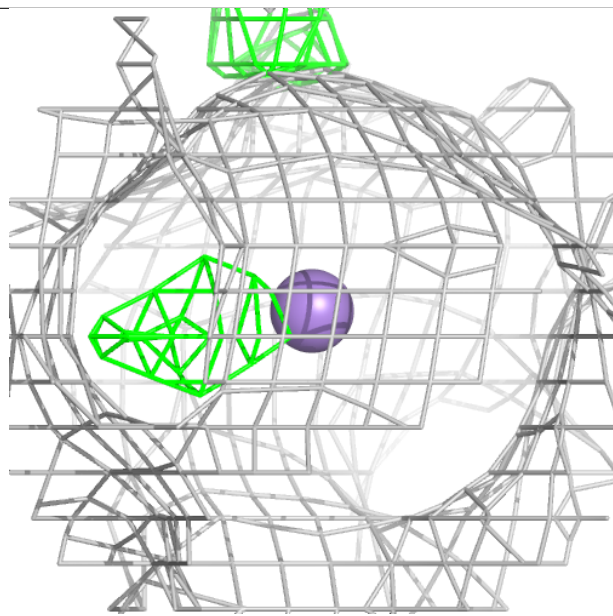
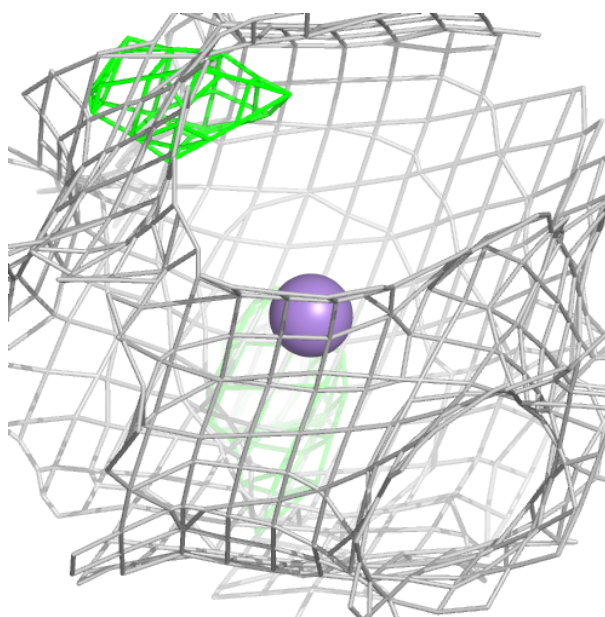
Electron density around MN A 801:

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



Electron density around MN C 801:

$2mF_o - DF_c$ (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.