

Full wwPDB X-ray Structure Validation Report (i)

Nov 4, 2021 – 12:09 PM JST

PDB ID : 7ESZ

Title : Crystal structure of the complex formed by Wolbachia cytoplasmic incompat-

ibility factors CinA and CinB with Mn2+ from wPip

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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 (i) symbol.

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 : 2.23.2buster-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) roteins) : Engh & Huber (2001)

Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

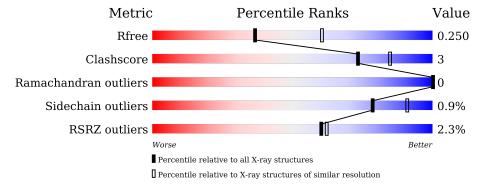
Validation Pipeline (wwPDB-VP) : 2.23.2

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 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	Similar resolution
Wietric	$(\# {\rm Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (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 <=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	81%	8%	11%
1	С	740	80%	11%	8%
2	В	453	82%	8%	10%
2	D	453	81%	8%	11%



2 Entry composition (i)

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 5235	C 3366	N 873	O 980	S 16	0	0	0
1	С	680	Total 5390	C 3468	N 899	O 1007	S 16	0	0	0

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
С	733	LEU	-	expression tag	UNP B3CP74
С	734	GLU	-	expression tag	UNP B3CP74
С	735	HIS	-	expression tag	UNP B3CP74
С	736	HIS	-	expression tag	UNP B3CP74
С	737	HIS	-	expression tag	UNP B3CP74
С	738	HIS	-	expression tag	UNP B3CP74
С	739	HIS	-	expression tag	UNP B3CP74
С	740	HIS	-	expression tag	UNP B3CP74

• Molecule 2 is a protein called BACTERIA FACTOR A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	В	408	Total 3316	C 2105		O 645	S 14	0	0	0
2	D	401	Total 3245	C 2066	- '	O 629	S 14	0	0	0



There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	446	LEU	-	expression tag	UNP B3CP73
В	447	GLU	-	expression tag	UNP B3CP73
В	448	HIS	-	expression tag	UNP B3CP73
В	449	HIS	-	expression tag	UNP B3CP73
В	450	HIS	-	expression tag	UNP B3CP73
В	451	HIS	-	expression tag	UNP B3CP73
В	452	HIS	-	expression tag	UNP B3CP73
В	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 (three-letter code: 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	С	1	Total Mn 1 1	0	0

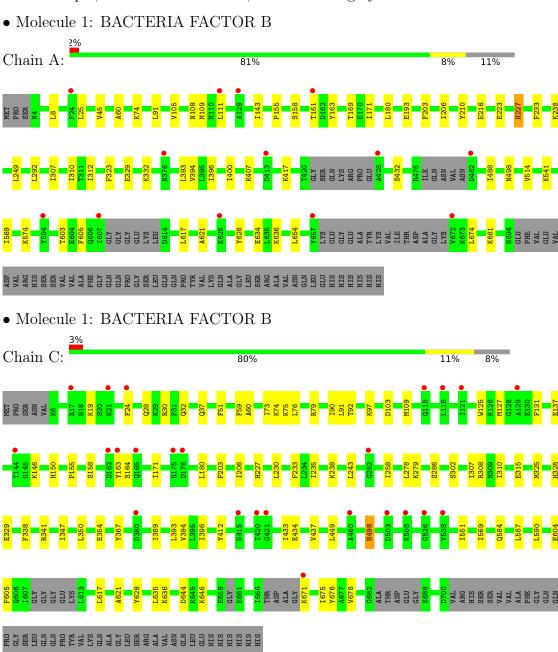
• Molecule 4 is water.

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



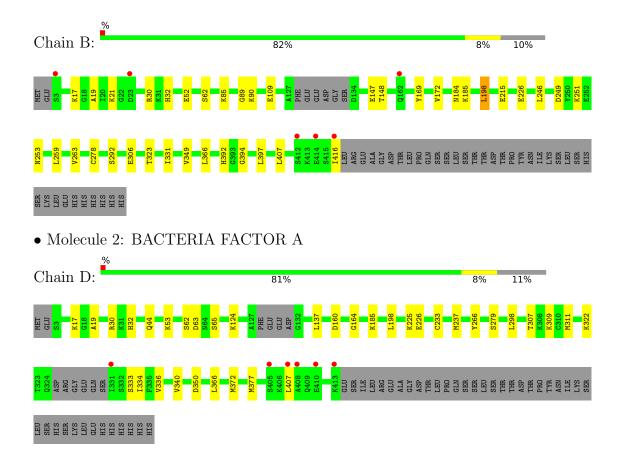
3 Residue-property plots (i)

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 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 2: BACTERIA FACTOR A







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	85.47Å 86.38Å 93.02Å	Donositor
a, b, c, α , β , γ	110.06° 91.86° 115.38°	Depositor
Resolution (Å)	41.07 - 2.48	Depositor
Resolution (A)	41.07 - 2.48	EDS
% Data completeness	93.3 (41.07-2.48)	Depositor
(in resolution range)	93.4 (41.07-2.48)	EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.87 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
D D.	0.198 , 0.250	Depositor
R, R_{free}	0.198 , 0.250	DCC
R_{free} test set	3672 reflections (5.00%)	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 , 32.4	EDS
L-test for twinning ²	$ < L > = 0.49, < L^2> = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	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.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.26	0/5324	0.43	0/7152	
1	С	0.25	0/5481	0.42	0/7363	
2	В	0.25	0/3368	0.40	0/4518	
2	D	0.24	0/3296	0.38	0/4421	
All	All	0.25	0/17469	0.41	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	С	5390	0	5434	46	0
2	В	3316	0	3301	19	0
2	D	3245	0	3231	19	0
3	A	1	0	0	0	0
3	С	1	0	0	0	0
4	A	35	0	0	1	0
4	В	31	0	0	0	0
4	С	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	112	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 (112) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash	
Atom-1	Atom-2	${\rm distance}(\mathring{\rm A})$	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:354:GLU:OE1	2:D:53:LYS:NZ	2.30	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	



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Continued from prev		Interatomic	Clash
Atom-1	Atom-2	${\rm distance} \; ({\rm \AA})$	overlap(A)
1:A:417:LYS:HA	1:A:432:SER:HA	1.90	0.54
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: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
1:C:302:SER:HB2	1:C:367:TYR:CZ	2.48	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
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
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
1:A:193:GLU:OE2	2:B:292:SER:OG	2.31	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



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Atom-1	Atom-2	Interatomic	Clash	
Atom-1	Atom-2	${\rm distance}({\rm \AA})$	overlap (Å)	
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	
2:D:233:CYS:HB3	2:D:237:MET:HE3	2.01	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	
2:D:372:MET:HE3	2:D:377:MET:HA	1.99	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	
1:A:396:ILE:O	1:A:407:LYS:NZ	2.42	0.42	
2:B:147:GLU:HG3	2:B:148:THR:HG23	2.01	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	
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	
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	В	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	hain Analysed Rotameric Outliers		Percentiles		
1	A	570/655 (87%)	566 (99%)	4 (1%)	84	93
1	C	585/655 (89%)	579 (99%)	6 (1%)	76	89
2	В	369/416 (89%)	365 (99%)	4 (1%)	73	88
2	D	360/416 (86%)	357 (99%)	3 (1%)	81	92
All	All	1884/2142 (88%)	1867 (99%)	17 (1%)	78	91

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	161	THR
1	A	227	HIS



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Mol	Chain	Res	Type
1	A	312	ILE
1	A	541	LYS
2	В	21	LYS
2	В	198	LEU
2	В	226	GLU
2	В	251	LYS
1	С	90	ILE
1	С	227	HIS
1	C C	235	ILE
1		278	LEU
1	С	498	ASN
1	С	644	ASP
2	D	198	LEU
2	D	226	GLU
2	D	279	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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 (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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95^{th} 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>	$\# \mathrm{RSRZ} {>} 2$	$OWAB(Å^2)$	Q<0.9
1	A	659/740 (89%)	-0.14	13 (1%) 65 67	26, 48, 93, 119	0
1	С	680/740 (91%)	0.08	24 (3%) 44 46	29, 57, 107, 134	0
2	В	408/453 (90%)	-0.32	6 (1%) 73 75	28, 41, 80, 120	0
2	D	401/453 (88%)	-0.27	6 (1%) 73 75	31, 48, 81, 108	0
All	All	2148/2386 (90%)	-0.13	49 (2%) 60 62	26, 49, 95, 134	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	671	LYS	4.6
1	С	129	ALA	4.2
1	С	24	PHE	4.0
1	С	538	VAL	3.9
1	С	526	GLY	3.7
1	A	482	ASP	3.7
1	С	21	LYS	3.6
2	В	23	ASP	3.6
1	С	144	THR	3.6
2	В	412	SER	3.4
1	С	460	ALA	3.3
1	A	672	VAL	3.3
1	С	163	TYR	3.2
1	С	421	GLY	3.2
2	В	3	SER	3.2
1	С	17	ARG	3.1
1	С	121	ILE	3.1
2	D	331	ILE	3.1
1	С	115	GLN	3.0
2	D	410	GLU	3.0
2	В	416	ILE	2.9



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Mol	Chain	Res	Type	RSRZ
2	D	407	LEU	2.8
1	A	161	THR	2.8
1	С	420	THR	2.8
1	С	165	GLN	2.7
1	С	252	GLY	2.7
1	A	594	TYR	2.7
2	D	408	ALA	2.7
	С	175	ARG	2.6
1	С	508	LYS	2.6
2	D	405	SER	2.6
1	A	376	ASN	2.6
1	A	607	ILE	2.5
2	В	414	GLU	2.5
1	С	162	ASP	2.5
1	С	118	LEU	2.5
1	С	380	ASP	2.4
1	С	415	ASN	2.4
1	A	129	ALA	2.2
1	A	24	PHE	2.2
2	В	162	GLN	2.1
1	A	657	TYR	2.1
1	A	625	LYS	2.1
2	D	413	LYS	2.1
1	A	413	ASP	2.0
1	С	176	ASP	2.0
1	A	428	ALA	2.0
1	A	111	LEU	2.0
1	С	503	ASP	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 monosaccharides in this entry.

6.4 Ligands (i)

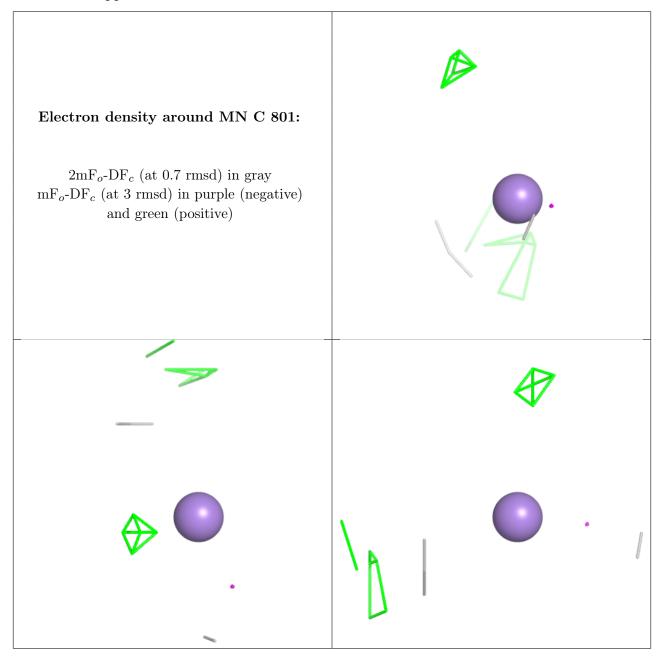
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,



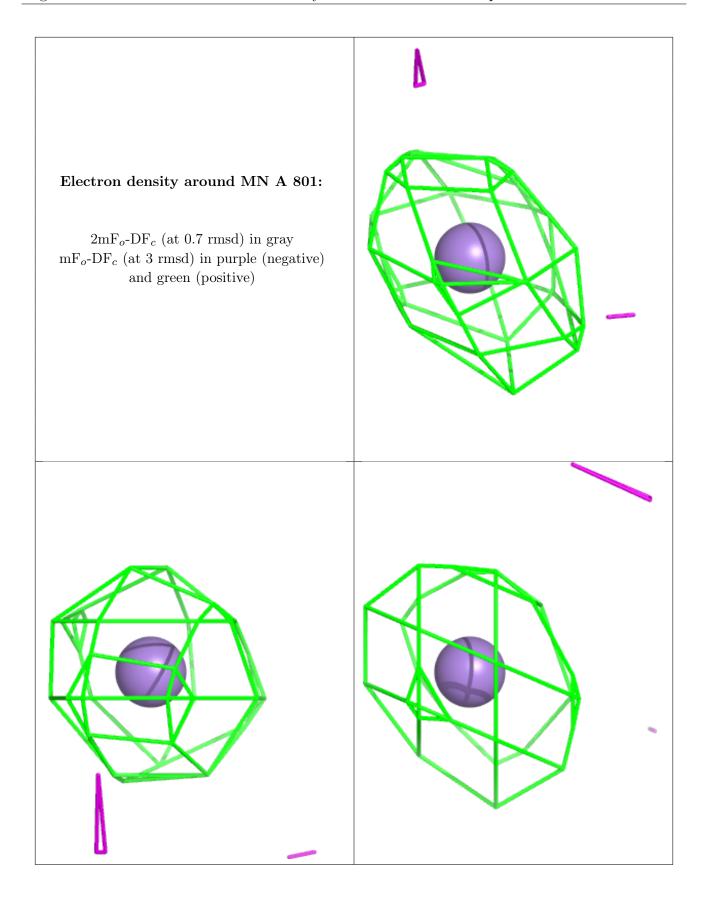
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mo	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
3	MN	С	801	1/1	0.97	0.09	34,34,34,34	0
3	MN	A	801	1/1	0.98	0.23	67,67,67,67	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.









6.5 Other polymers (i)

There are no such residues in this entry.

