Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2024 – 02:36 PM EST

PDB ID	:	8SNK
Title	:	Crystal structure of metformin hydrolase (MfmAB) from Pseudomonas mendocina sp. MET-2 mutant (MfmA/D188N)
Authors	:	Tassoulas, L.J.; Rankin, J.A.; Elias, M.H.; Wackett, L.P.
Deposited on	:	2023-04-27
Resolution	:	1.85 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:

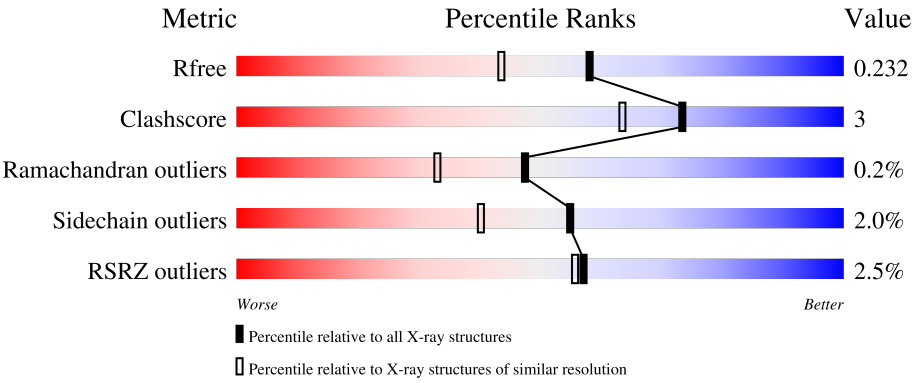
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson 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 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	364	86% 9% 5%
1	I	364	86% 8% • 5%
2	B	348	2% 87% 6% • 6%
2	C	348	3% 88% 5% • 6%
2	D	348	5% 82% 10% • 6%

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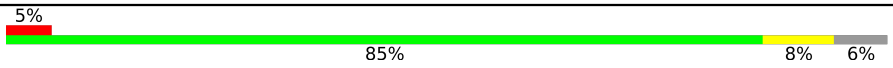
Mol	Chain	Length	Quality of chain
2	E	348	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 16893 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 metformin hydrolase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	345	Total	C	N	O	S	0	0	0
			2697	1700	473	501	23			
1	A	345	Total	C	N	O	S	0	0	0
			2697	1700	473	501	23			

- Molecule 2 is a protein called metformin hydrolase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	326	Total	C	N	O	S	0	0	0
			2511	1581	439	472	19			
2	B	326	Total	C	N	O	S	0	0	0
			2511	1581	439	472	19			
2	D	326	Total	C	N	O	S	0	0	0
			2511	1581	439	472	19			
2	E	326	Total	C	N	O	S	0	0	0
			2511	1581	439	472	19			

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

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	287	Total	O	0	0
			287	287		

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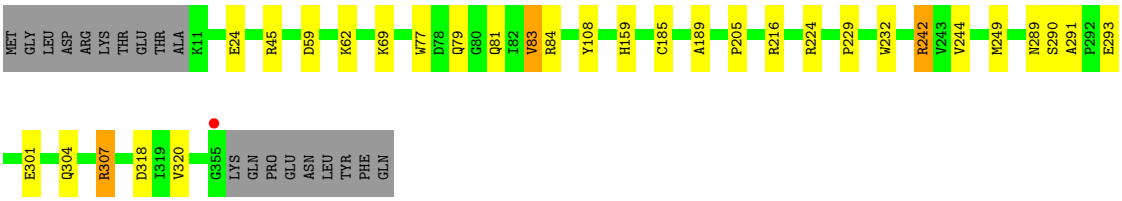
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	281	Total O 281 281	0	0
4	C	231	Total O 231 231	0	0
4	B	272	Total O 272 272	0	0
4	D	196	Total O 196 196	0	0
4	E	186	Total O 186 186	0	0

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.

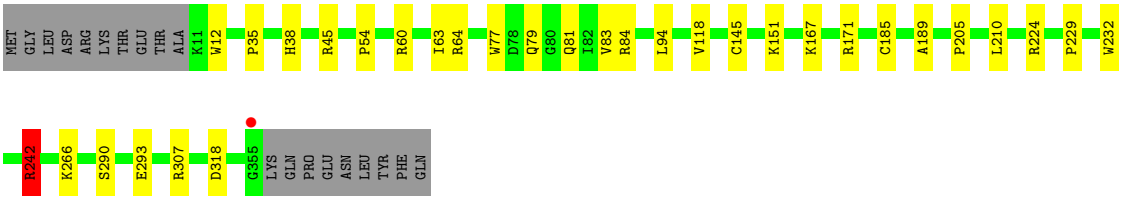
• Molecule 1: metformin hydrolase subunit A

Chain I:



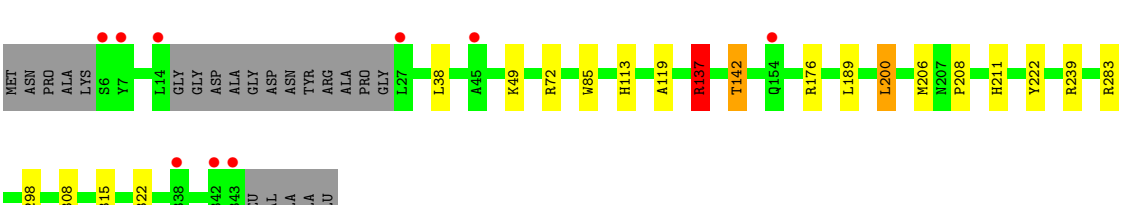
• Molecule 1: metformin hydrolase subunit A

Chain A:



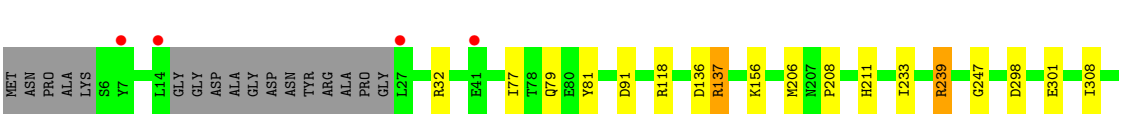
• Molecule 2: metformin hydrolase subunit B

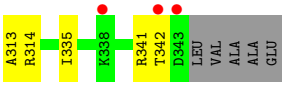
Chain C:



• Molecule 2: metformin hydrolase subunit B

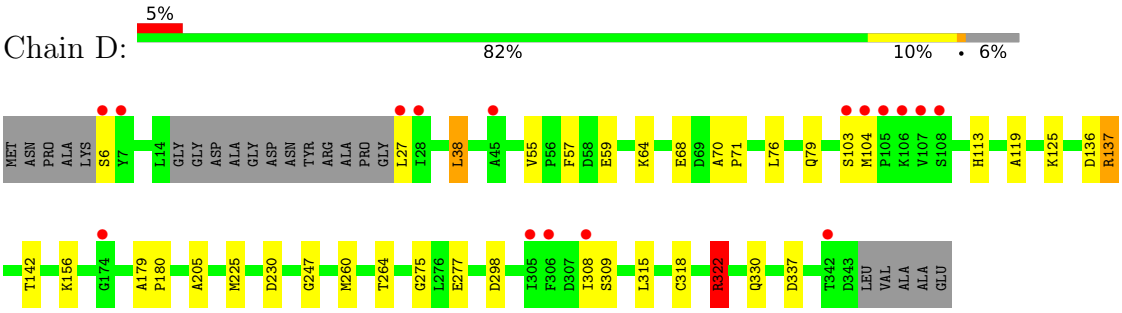
Chain B:





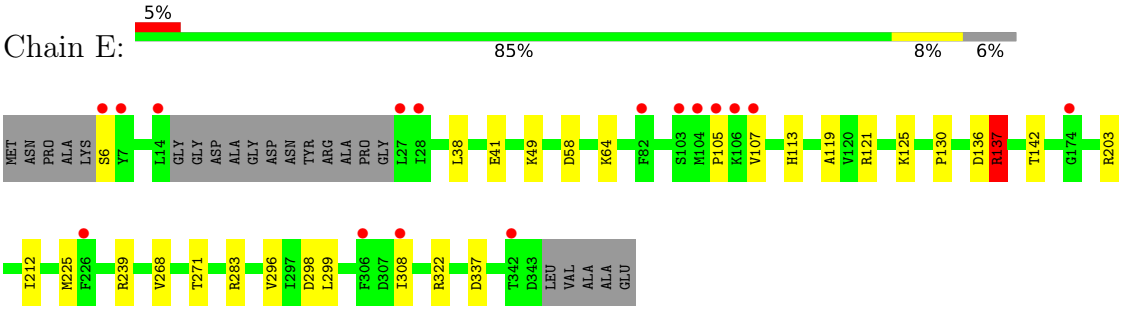
• Molecule 2: metformin hydrolase subunit B

Chain D:



• Molecule 2: metformin hydrolase subunit B

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	102.70Å 162.30Å 152.70Å 90.00° 101.10° 90.00°	Depositor
Resolution (Å)	19.75 – 1.85 19.75 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.2 (19.75-1.85) 99.3 (19.75-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.55 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.8.0411	Depositor
R, R_{free}	0.188 , 0.223 0.199 , 0.232	Depositor DCC
R_{free} test set	10338 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	26.3	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 53.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	16893	wwPDB-VP
Average B, all atoms (Å^2)	32.0	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 43.82 % 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 1.6677e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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	0.53	0/2769	0.85	1/3754 (0.0%)
1	I	0.54	2/2769 (0.1%)	0.85	1/3754 (0.0%)
2	B	0.55	1/2562 (0.0%)	0.83	2/3465 (0.1%)
2	C	0.53	0/2562	0.85	3/3465 (0.1%)
2	D	0.46	0/2562	0.77	2/3465 (0.1%)
2	E	0.48	0/2562	0.79	0/3465
All	All	0.52	3/15786 (0.0%)	0.82	9/21368 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	I	0	3
2	B	0	3
2	C	0	2
2	D	0	1
2	E	0	2
All	All	0	14

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	GLU	CD-OE1	6.43	1.32	1.25
1	I	24	GLU	CD-OE1	-5.38	1.19	1.25
1	I	301	GLU	CD-OE2	-5.08	1.20	1.25

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	72	ARG	NE-CZ-NH1	6.17	123.38	120.30
2	B	239	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	I	242	ARG	NE-CZ-NH2	-5.87	117.36	120.30
2	C	176	ARG	NE-CZ-NH1	5.76	123.18	120.30
2	D	322	ARG	CG-CD-NE	5.42	123.17	111.80
2	B	239	ARG	NE-CZ-NH2	-5.42	117.59	120.30
2	C	200	LEU	CA-CB-CG	5.18	127.21	115.30
1	A	242	ARG	CG-CD-NE	-5.11	101.08	111.80
2	D	337	ASP	CB-CA-C	-5.05	100.31	110.40

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	242	ARG	Sidechain
1	A	307	ARG	Sidechain
1	A	45	ARG	Sidechain
2	B	118	ARG	Sidechain
2	B	137	ARG	Sidechain
2	B	314	ARG	Sidechain
2	C	137	ARG	Sidechain
2	C	322	ARG	Sidechain
2	D	137	ARG	Sidechain
2	E	137	ARG	Sidechain
2	E	322	ARG	Sidechain
1	I	216	ARG	Sidechain
1	I	307	ARG	Sidechain
1	I	45	ARG	Sidechain

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	2697	0	2581	16	0
1	I	2697	0	2581	17	0
2	B	2511	0	2476	13	0
2	C	2511	0	2476	15	0
2	D	2511	0	2476	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	2511	0	2476	20	0
3	A	1	0	0	0	0
3	I	1	0	0	0	0
4	A	281	0	0	5	0
4	B	272	0	0	1	0
4	C	231	0	0	5	0
4	D	196	0	0	5	0
4	E	186	0	0	5	0
4	I	287	0	0	2	0
All	All	16893	0	15066	100	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 (100) 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:91:ASP:HB2	2:B:335:ILE:HD11	1.47	0.95
2:E:239:ARG:HD3	4:E:437:HOH:O	1.81	0.81
2:D:318:CYS:O	2:D:322:ARG:HG3	1.82	0.79
2:D:113:HIS:ND1	2:D:142:THR:HG21	1.98	0.78
2:E:105:PRO:HB2	4:E:435:HOH:O	1.85	0.75
2:C:38:LEU:HD21	2:C:119:ALA:HB1	1.68	0.74
2:B:239:ARG:HD2	4:B:843:HOH:O	1.88	0.72
2:B:308:ILE:HG23	2:E:308:ILE:HG13	1.72	0.72
2:C:189:LEU:O	4:C:401:HOH:O	2.08	0.72
2:C:308:ILE:HG23	2:D:308:ILE:HG13	1.71	0.71
2:C:38:LEU:HD21	2:C:119:ALA:CB	2.20	0.70
2:C:113:HIS:ND1	2:C:142:THR:HG21	2.08	0.68
1:A:266:LYS:HE3	4:A:727:HOH:O	1.95	0.66
2:D:277:GLU:OE1	4:D:401:HOH:O	2.15	0.64
2:D:6:SER:N	4:D:405:HOH:O	2.32	0.63
2:D:225:MET:HE3	2:D:275:GLY:HA2	1.81	0.62
2:E:203:ARG:NH1	2:E:225:MET:HE2	2.14	0.62
1:A:151:LYS:NZ	4:A:502:HOH:O	2.27	0.61
2:C:283:ARG:NH1	4:C:402:HOH:O	2.18	0.61
2:E:113:HIS:ND1	2:E:142:THR:HG21	2.16	0.61
2:C:239:ARG:HD2	4:C:502:HOH:O	2.01	0.60
1:A:60:ARG:O	1:A:64:ARG:HG3	2.03	0.59
2:C:113:HIS:ND1	2:C:142:THR:CG2	2.66	0.59
2:C:308:ILE:CG2	2:D:308:ILE:HG13	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:68:GLU:HG2	4:D:497:HOH:O	2.04	0.57
2:B:77:ILE:HD12	2:B:313:ALA:HB1	1.85	0.57
2:B:308:ILE:CG2	2:E:308:ILE:HG13	2.35	0.56
2:D:318:CYS:O	2:D:322:ARG:CG	2.51	0.56
1:I:81:GLN:HE22	1:I:83:VAL:HG23	1.70	0.56
2:E:41:GLU:HG2	4:E:552:HOH:O	2.05	0.56
2:D:125:LYS:HE2	4:D:568:HOH:O	2.05	0.55
1:A:167:LYS:HE2	1:A:171:ARG:NH2	2.22	0.54
1:I:185:CYS:SG	1:I:293:GLU:HG3	2.48	0.54
1:A:77:TRP:CH2	1:A:79:GLN:HB2	2.43	0.53
1:A:167:LYS:HG2	1:A:210:LEU:HD21	1.91	0.53
1:I:81:GLN:HE22	1:I:84:ARG:N	2.07	0.52
2:C:137:ARG:HG3	2:C:137:ARG:O	2.09	0.52
2:B:156:LYS:HE3	2:B:247:GLY:O	2.09	0.52
2:E:49:LYS:HG3	4:E:443:HOH:O	2.11	0.51
1:A:242:ARG:HD2	4:A:516:HOH:O	2.10	0.51
2:B:91:ASP:CB	2:B:335:ILE:HD11	2.30	0.51
2:E:268:VAL:HG22	2:E:271:THR:HG22	1.93	0.51
2:D:64:LYS:HD3	4:D:493:HOH:O	2.11	0.50
1:I:69:LYS:NZ	4:I:502:HOH:O	2.28	0.50
2:B:341:ARG:HG2	2:B:342:THR:N	2.26	0.50
1:I:244:VAL:HG12	1:I:249:MET:HG3	1.94	0.49
1:I:81:GLN:HE22	1:I:84:ARG:H	1.61	0.49
1:I:242:ARG:HG3	1:I:242:ARG:HH11	1.78	0.49
2:D:113:HIS:ND1	2:D:142:THR:CG2	2.72	0.49
1:I:189:ALA:HA	1:I:205:PRO:CD	2.43	0.49
2:E:113:HIS:HD1	2:E:142:THR:HG21	1.77	0.49
1:A:171:ARG:NH1	4:A:504:HOH:O	2.30	0.48
1:A:185:CYS:SG	1:A:293:GLU:HG3	2.53	0.48
2:E:38:LEU:HD21	2:E:119:ALA:HB1	1.94	0.48
1:I:77:TRP:CH2	1:I:79:GLN:HB2	2.48	0.48
1:A:189:ALA:HA	1:A:205:PRO:CD	2.45	0.47
2:B:32:ARG:NH1	2:B:79:GLN:O	2.47	0.47
2:B:81:TYR:HE2	4:E:478:HOH:O	1.97	0.47
2:D:76:LEU:O	2:D:79:GLN:HB2	2.15	0.47
2:D:260:MET:HG3	2:D:315:LEU:HD21	1.97	0.47
2:C:49:LYS:HG2	4:C:516:HOH:O	2.15	0.46
1:I:289:ASN:ND2	1:I:291:ALA:H	2.13	0.46
2:E:107:VAL:HG12	2:E:107:VAL:O	2.15	0.46
1:A:229:PRO:HD2	1:A:232:TRP:CD2	2.50	0.45
2:E:58:ASP:HA	2:E:136:ASP:OD1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ILE:HD13	1:A:145:CYS:HA	1.98	0.45
2:D:156:LYS:HE2	2:D:247:GLY:O	2.16	0.45
1:I:304:GLN:NE2	4:I:515:HOH:O	2.50	0.45
2:D:38:LEU:HD21	2:D:119:ALA:HA	1.98	0.45
1:I:81:GLN:NE2	1:I:84:ARG:N	2.65	0.45
2:E:299:LEU:HD23	2:E:299:LEU:N	2.32	0.45
1:A:94:LEU:C	1:A:94:LEU:HD13	2.38	0.44
2:D:57:PHE:CZ	2:D:59:GLU:HB2	2.53	0.44
1:I:289:ASN:HD22	1:I:291:ALA:H	1.65	0.44
1:I:59:ASP:OD1	1:I:62:LYS:HG2	2.17	0.44
2:C:222:TYR:OH	4:C:403:HOH:O	2.20	0.44
1:A:35:PRO:HB2	1:A:38:HIS:O	2.18	0.44
2:C:208:PRO:HG2	2:C:211:HIS:CD2	2.53	0.44
1:I:108:TYR:HE1	1:I:307:ARG:HE	1.66	0.43
1:I:229:PRO:HD2	1:I:232:TRP:CD2	2.53	0.43
2:E:121:ARG:O	2:E:125:LYS:HG3	2.18	0.43
2:D:70:ALA:HB3	2:D:71:PRO:HD3	2.01	0.43
2:C:85:TRP:CE2	2:D:205:ALA:HB2	2.54	0.43
2:D:55:VAL:O	2:D:55:VAL:HG12	2.19	0.43
2:E:299:LEU:HD23	2:E:299:LEU:H	1.84	0.43
1:I:159:HIS:CD2	1:I:320:VAL:HG21	2.54	0.43
4:A:543:HOH:O	2:D:264:THR:HG23	2.19	0.43
1:A:81:GLN:NE2	1:A:84:ARG:N	2.67	0.42
2:D:179:ALA:HB3	2:D:180:PRO:HD3	2.00	0.42
2:D:330:GLN:NE2	2:D:330:GLN:HA	2.35	0.42
2:B:77:ILE:CD1	2:B:313:ALA:CB	2.97	0.41
1:A:12:TRP:CD1	1:A:54:PRO:HG2	2.56	0.41
2:B:341:ARG:HG2	2:B:342:THR:H	1.86	0.41
2:D:57:PHE:HB2	2:D:104:MET:SD	2.60	0.41
2:E:137:ARG:O	2:E:137:ARG:HG3	2.21	0.40
2:C:315:LEU:O	2:C:315:LEU:HG	2.17	0.40
2:E:38:LEU:HD12	2:E:38:LEU:HA	1.87	0.40
2:E:130:PRO:HG2	2:E:296:VAL:HG22	2.02	0.40
2:B:208:PRO:HG2	2:B:211:HIS:CD2	2.56	0.40
2:E:212:ILE:N	2:E:212:ILE:HD13	2.36	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	343/364 (94%)	325 (95%)	17 (5%)	1 (0%)	41	26
1	I	343/364 (94%)	328 (96%)	14 (4%)	1 (0%)	41	26
2	B	322/348 (92%)	313 (97%)	8 (2%)	1 (0%)	41	26
2	C	322/348 (92%)	314 (98%)	8 (2%)	0	100	100
2	D	322/348 (92%)	311 (97%)	11 (3%)	0	100	100
2	E	322/348 (92%)	314 (98%)	8 (2%)	0	100	100
All	All	1974/2120 (93%)	1905 (96%)	66 (3%)	3 (0%)	47	33

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	83	VAL
1	A	83	VAL
2	B	233	ILE

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	285/302 (94%)	280 (98%)	5 (2%)	59	45
1	I	285/302 (94%)	282 (99%)	3 (1%)	73	65
2	B	266/279 (95%)	262 (98%)	4 (2%)	65	53
2	C	266/279 (95%)	261 (98%)	5 (2%)	57	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	D	266/279 (95%)	257 (97%)	9 (3%)	37 19
2	E	266/279 (95%)	260 (98%)	6 (2%)	50 34
All	All	1634/1720 (95%)	1602 (98%)	32 (2%)	55 40

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	224	ARG
1	I	290	SER
1	I	318	ASP
1	A	118	VAL
1	A	224	ARG
1	A	242	ARG
1	A	290	SER
1	A	318	ASP
2	C	137	ARG
2	C	142	THR
2	C	200	LEU
2	C	206	MET
2	C	298	ASP
2	B	136	ASP
2	B	137	ARG
2	B	206	MET
2	B	298	ASP
2	D	27	LEU
2	D	38	LEU
2	D	103	SER
2	D	136	ASP
2	D	137	ARG
2	D	230	ASP
2	D	298	ASP
2	D	309	SER
2	D	322	ARG
2	E	6	SER
2	E	64	LYS
2	E	137	ARG
2	E	283	ARG
2	E	298	ASP
2	E	337	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	81	GLN
1	I	214	ASN
1	I	289	ASN
1	I	353	GLN
1	A	81	GLN
2	D	330	GLN

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

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>2			OWAB(Å^2)	Q<0.9
1	A	345/364 (94%)	-0.38	1 (0%)	94	93	16, 25, 37, 61	0
1	I	345/364 (94%)	-0.40	1 (0%)	94	93	16, 24, 38, 60	0
2	B	326/348 (93%)	-0.25	7 (2%)	63	63	15, 26, 47, 97	0
2	C	326/348 (93%)	-0.07	9 (2%)	53	52	16, 30, 53, 94	0
2	D	326/348 (93%)	0.09	16 (4%)	29	28	21, 34, 58, 107	0
2	E	326/348 (93%)	0.14	16 (4%)	29	28	21, 33, 56, 112	0
All	All	1994/2120 (94%)	-0.15	50 (2%)	57	56	15, 28, 52, 112	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	107	VAL	9.0
2	E	105	PRO	7.4
2	B	342	THR	6.7
2	B	343	ASP	6.0
2	D	107	VAL	6.0
2	C	342	THR	5.1
2	D	105	PRO	4.9
2	D	27	LEU	4.5
2	C	6	SER	4.2
2	C	343	ASP	4.1
1	A	355	GLY	4.0
2	E	7	TYR	3.9
1	I	355	GLY	3.9
2	D	104	MET	3.7
2	D	106	LYS	3.7
2	C	7	TYR	3.4
2	C	14	LEU	3.4
2	E	226	PHE	3.4
2	E	174	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
2	C	154	GLN	3.3
2	C	27	LEU	3.3
2	B	7	TYR	3.3
2	E	306	PHE	3.3
2	D	7	TYR	3.3
2	D	103	SER	3.2
2	B	41	GLU	3.1
2	D	174	GLY	3.1
2	D	6	SER	3.0
2	D	308	ILE	2.9
2	E	308	ILE	2.9
2	D	306	PHE	2.9
2	E	28	ILE	2.9
2	E	104	MET	2.8
2	C	338	LYS	2.7
2	B	14	LEU	2.7
2	C	45	ALA	2.7
2	B	338	LYS	2.7
2	E	103	SER	2.7
2	B	27	LEU	2.7
2	D	342	THR	2.7
2	E	6	SER	2.7
2	D	45	ALA	2.5
2	D	28	ILE	2.5
2	E	27	LEU	2.2
2	E	82	PHE	2.2
2	E	106	LYS	2.1
2	E	14	LEU	2.0
2	E	342	THR	2.0
2	D	305	ILE	2.0
2	D	108	SER	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)

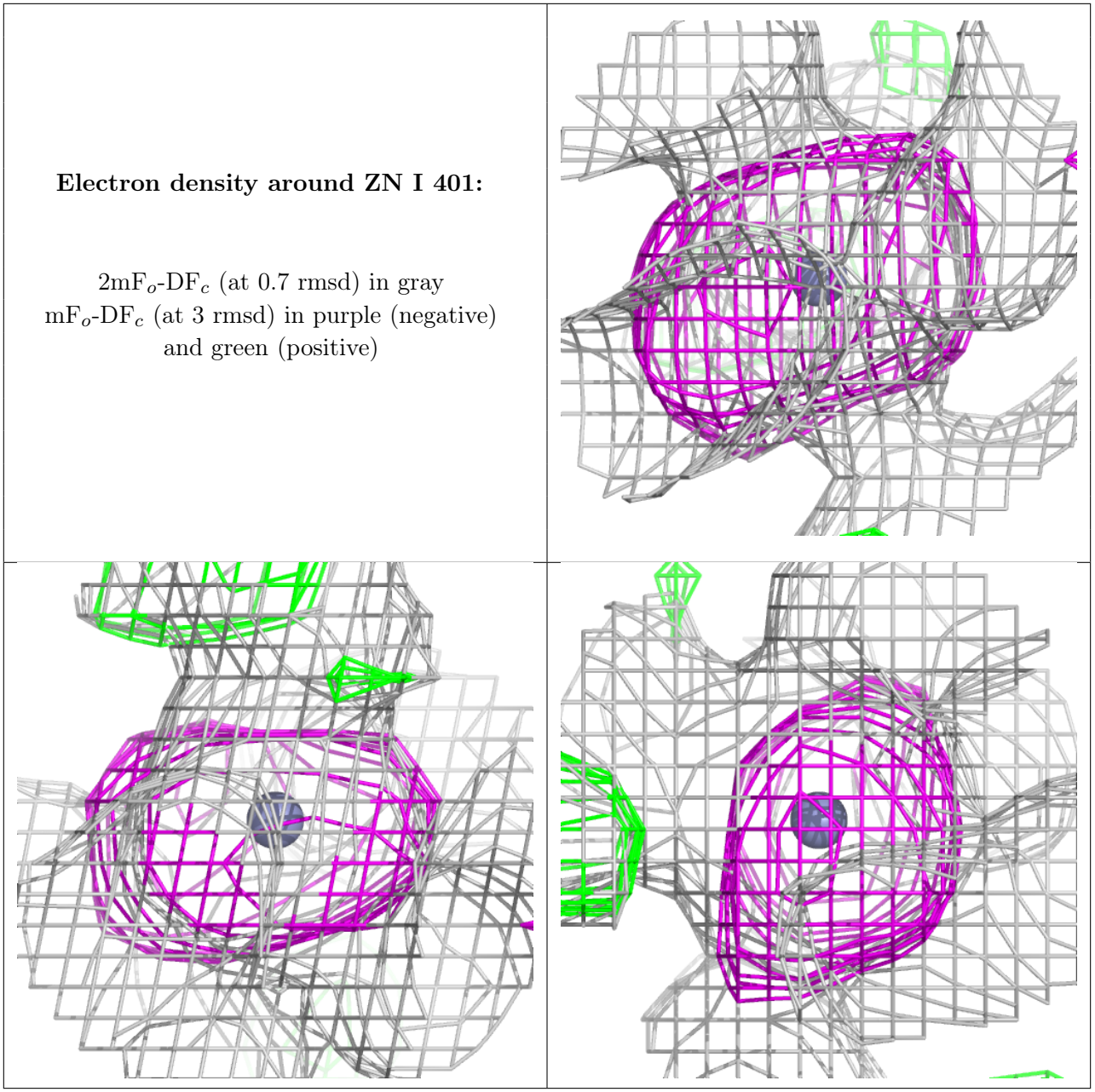
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ZN	I	401	1/1	0.99	0.05	30,30,30,30	0
3	ZN	A	401	1/1	1.00	0.03	29,29,29,29	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.

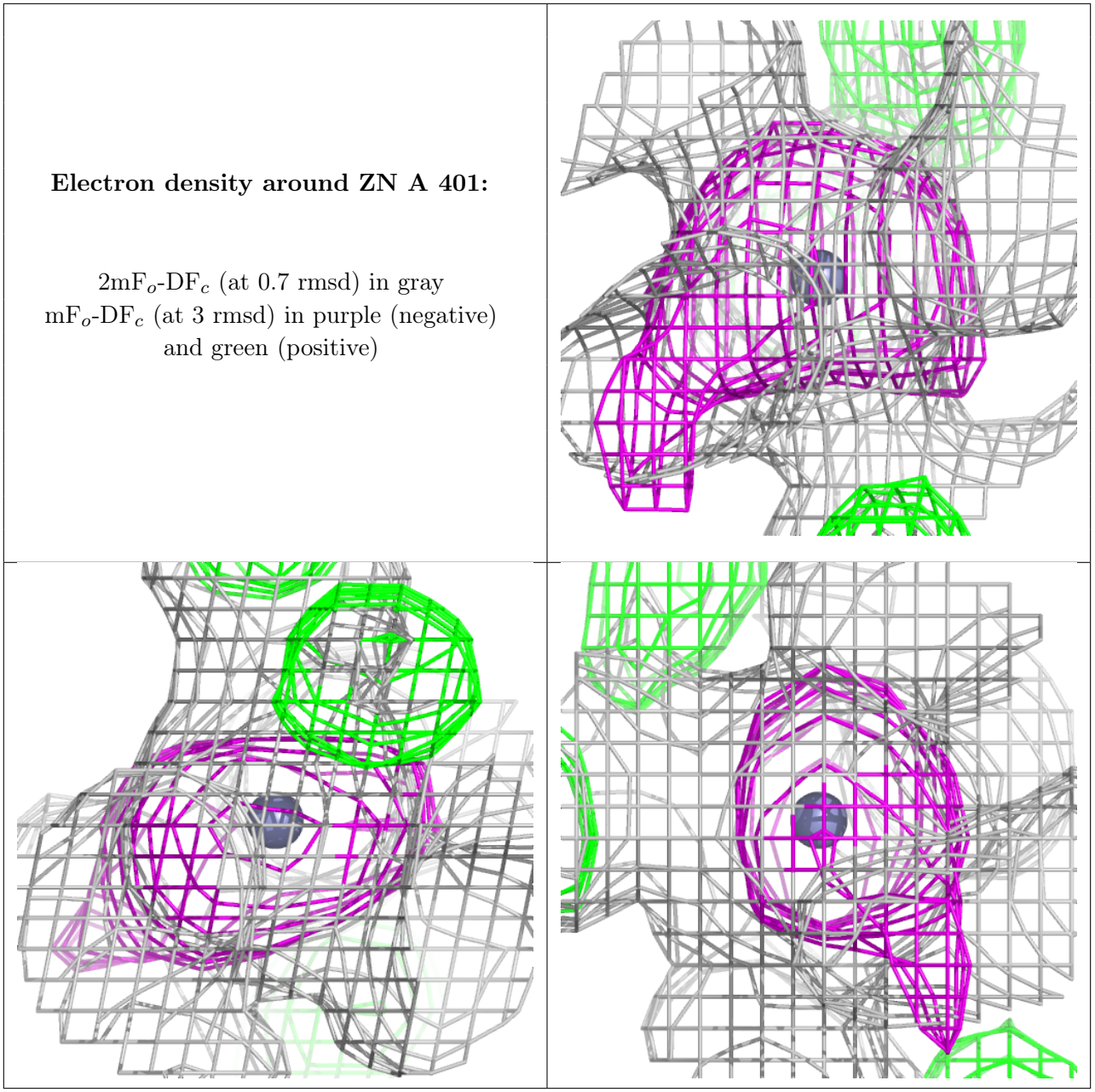
Electron density around ZN I 401:

$2mF_o$-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 A 401:

$2mF_o$-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.