Full wwPDB X-ray Structure Validation Report (i)

Jun 7, 2023 – 04:35 pm BST

PDB ID	:	8C0J
Title	:	Structure of AmiB enzymatic domain bound to the EnvC LytM domain
Authors	:	Crow, A.
Deposited on	:	2022-12-17
Resolution	:	3.38 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 (i)) were used in the production of this report:

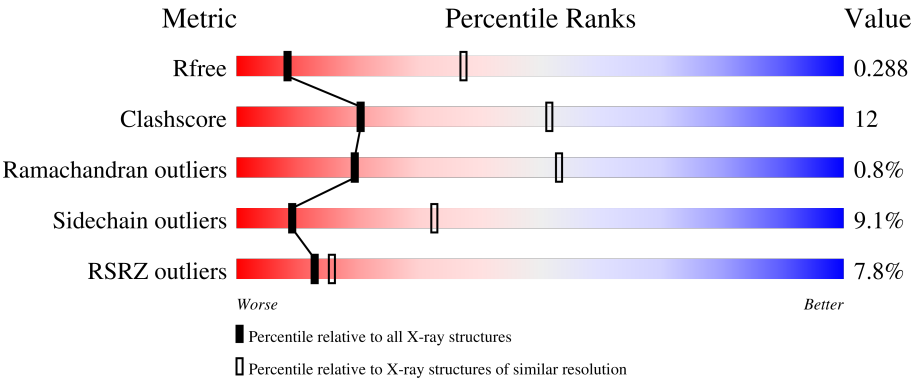
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.33
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

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 3.38 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	1691 (3.46-3.30)
Clashscore	141614	1762 (3.46-3.30)
Ramachandran outliers	138981	1732 (3.46-3.30)
Sidechain outliers	138945	1731 (3.46-3.30)
RSRZ outliers	127900	1635 (3.46-3.30)

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	234	3% 65% 17% • 15%
1	C	234	14% 66% 15% • 16%
2	B	149	% 54% 29% 5% 12%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4057 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 N-acetylmuramoyl-L-alanine amidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	200	Total	C	N	O	S	0	0	0
			1539	960	286	290	3			
1	C	197	Total	C	N	O	S	0	0	0
			1514	946	282	283	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	189	MET	-	initiating methionine	UNP A0A482PQR2
C	189	MET	-	initiating methionine	UNP A0A482PQR2

- Molecule 2 is a protein called Murein hydrolase activator EnvC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	131	Total	C	N	O	S	0	0	0
			992	625	185	180	2			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	279	MET	-	initiating methionine	UNP A0A482PID1
B	280	GLY	-	expression tag	UNP A0A482PID1
B	281	SER	-	expression tag	UNP A0A482PID1
B	282	SER	-	expression tag	UNP A0A482PID1
B	283	HIS	-	expression tag	UNP A0A482PID1
B	284	HIS	-	expression tag	UNP A0A482PID1
B	285	HIS	-	expression tag	UNP A0A482PID1
B	286	HIS	-	expression tag	UNP A0A482PID1
B	287	HIS	-	expression tag	UNP A0A482PID1
B	288	HIS	-	expression tag	UNP A0A482PID1
B	289	SER	-	expression tag	UNP A0A482PID1
B	290	GLN	-	expression tag	UNP A0A482PID1

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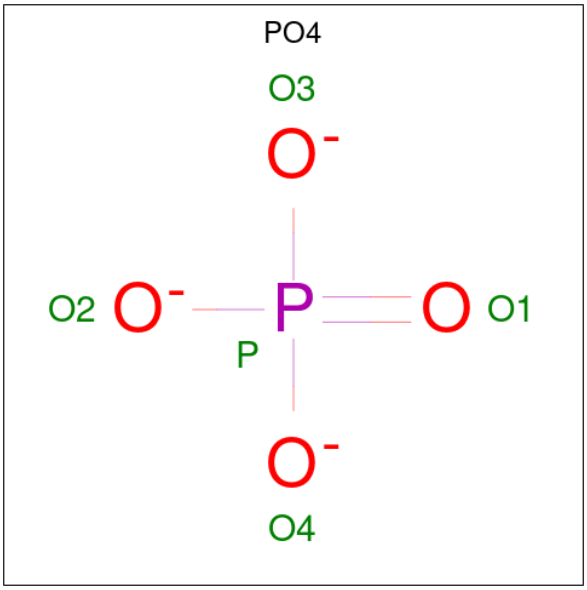
Chain	Residue	Modelled	Actual	Comment	Reference
B	291	ASP	-	expression tag	UNP A0A482PID1
B	292	PRO	-	expression tag	UNP A0A482PID1

- 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	A	1	Total Zn 1 1	0	0
3	C	1	Total Zn 1 1	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



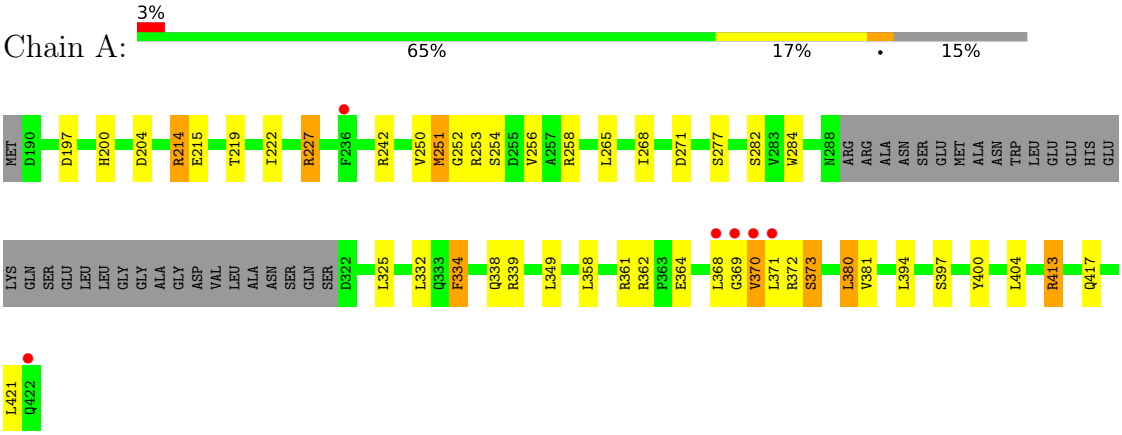
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O P 5 4 1	0	0
4	C	1	Total O P 5 4 1	0	0

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.

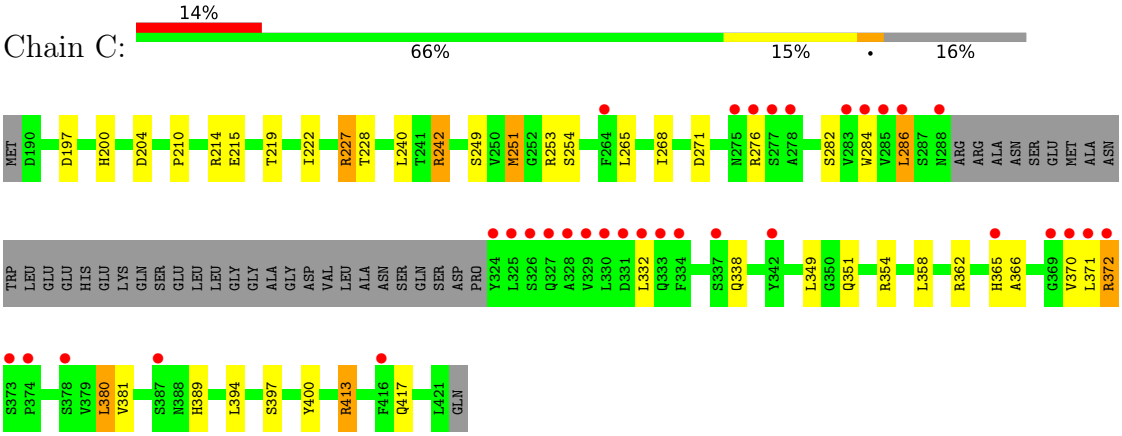
• Molecule 1: N-acetylmuramoyl-L-alanine amidase

Chain A:



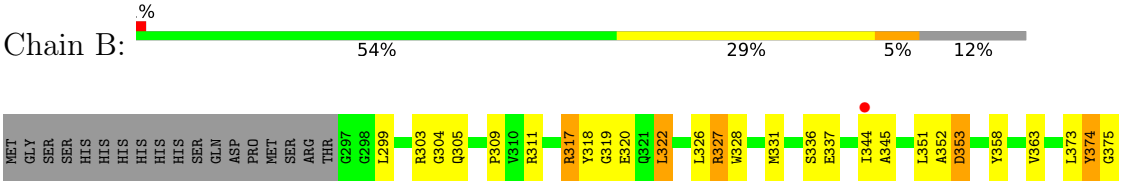
• Molecule 1: N-acetylmuramoyl-L-alanine amidase

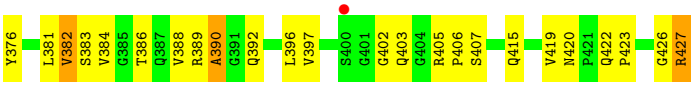
Chain C:



• Molecule 2: Murein hydrolase activator EnvC

Chain B:




Y376
L381
V382
S383
V384
G385
T386
Q387
V388
R389
A390
G391
Q392
L396
V397
S400
G401
G402
Q403
G404
R405
P406
S407
Q415
V419
N420
P421
Q422
P423
G426
R427

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41 3 2	Depositor
Cell constants a, b, c, α, β, γ	237.36Å 237.36Å 237.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.01 – 3.38 48.45 – 3.38	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.01-3.38) 99.6 (48.45-3.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.32 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.249 , 0.291 0.252 , 0.288	Depositor DCC
R_{free} test set	821 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	103.3	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 85.4	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	0.90	EDS
Total number of atoms	4057	wwPDB-VP
Average B, all atoms (Å^2)	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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, PO4

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	0.39	0/1567	0.79	0/2119
1	C	0.35	0/1541	0.71	0/2084
2	B	0.39	0/1015	0.79	0/1373
All	All	0.38	0/4123	0.76	0/5576

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	2
1	C	0	3
All	All	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	214	ARG	Sidechain
1	A	361	ARG	Sidechain
1	C	214	ARG	Sidechain
1	C	242	ARG	Sidechain
1	C	371	LEU	Peptide

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	1539	0	1524	39	0
1	C	1514	0	1505	26	0
2	B	992	0	982	42	1
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	5	0	0	0	0
4	C	5	0	0	0	0
All	All	4057	0	4011	100	1

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 12.

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)
1:C:351:GLN:NE2	1:C:354:ARG:HH21	1.81	0.78
2:B:311:ARG:NH2	2:B:427:ARG:OXT	2.22	0.72
1:A:227:ARG:HB3	1:A:227:ARG:NH1	2.07	0.70
2:B:363:VAL:HG22	2:B:373:LEU:HG	1.74	0.70
1:C:286:LEU:HD22	1:C:370:VAL:HB	1.73	0.69
2:B:415:GLN:HE21	2:B:415:GLN:HA	1.59	0.65
1:C:351:GLN:HE21	1:C:354:ARG:HH21	1.42	0.64
2:B:374:TYR:CD1	2:B:374:TYR:N	2.67	0.63
2:B:422:GLN:HB3	2:B:423:PRO:HD3	1.81	0.63
2:B:382:VAL:HG12	2:B:386:THR:HG21	1.80	0.62
1:C:413:ARG:HG2	1:C:413:ARG:HH11	1.64	0.62
2:B:351:LEU:HD12	2:B:352:ALA:N	2.14	0.62
2:B:397:VAL:HG13	2:B:407:SER:O	2.01	0.60
1:A:250:VAL:HG13	1:A:251:MET:H	1.67	0.60
1:A:332:LEU:HB3	2:B:358:TYR:CE2	2.37	0.60
1:A:349:LEU:HD22	1:A:358:LEU:HD13	1.84	0.60
1:A:197:ASP:OD1	1:A:253:ARG:NH1	2.35	0.59
1:A:413:ARG:HH11	1:A:413:ARG:HG2	1.67	0.59
1:A:284:TRP:HB2	1:A:380:LEU:HB3	1.84	0.58
2:B:345:ALA:HA	2:B:390:ALA:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:LEU:HD11	2:B:351:LEU:CD2	2.33	0.58
1:C:365:HIS:O	1:C:366:ALA:HB2	2.03	0.58
1:A:215:GLU:O	1:A:219:THR:HG23	2.04	0.57
2:B:381:LEU:HD21	2:B:396:LEU:CD1	2.35	0.57
1:A:250:VAL:HG13	1:A:251:MET:N	2.20	0.56
2:B:304:GLY:O	2:B:426:GLY:HA3	2.05	0.56
1:C:215:GLU:O	1:C:219:THR:HG23	2.05	0.56
1:C:227:ARG:HG3	1:C:228:THR:N	2.19	0.56
1:C:210:PRO:HG3	1:C:276:ARG:HH22	1.70	0.56
2:B:351:LEU:HD11	2:B:353:ASP:HB2	1.88	0.55
1:C:413:ARG:HH11	1:C:413:ARG:CG	2.20	0.55
2:B:415:GLN:HA	2:B:415:GLN:NE2	2.22	0.55
1:A:413:ARG:O	1:A:417:GLN:HB2	2.07	0.55
1:A:369:GLY:O	1:A:370:VAL:HB	2.07	0.54
1:A:394:LEU:O	1:A:397:SER:HB3	2.07	0.54
1:C:284:TRP:HB2	1:C:380:LEU:HB3	1.88	0.54
2:B:351:LEU:HD12	2:B:352:ALA:H	1.71	0.54
2:B:373:LEU:C	2:B:374:TYR:CD1	2.81	0.54
1:C:413:ARG:O	1:C:417:GLN:HB2	2.09	0.53
1:A:413:ARG:HH11	1:A:413:ARG:CG	2.22	0.53
1:A:200:HIS:O	1:A:242:ARG:NE	2.42	0.53
1:C:413:ARG:CG	1:C:413:ARG:NH1	2.72	0.52
1:C:370:VAL:O	1:C:372:ARG:N	2.35	0.52
1:C:394:LEU:O	1:C:397:SER:HB3	2.08	0.52
1:C:200:HIS:O	1:C:242:ARG:NE	2.43	0.52
1:A:332:LEU:HB3	2:B:358:TYR:HE2	1.75	0.51
1:C:197:ASP:OD1	1:C:253:ARG:NH1	2.38	0.51
1:A:325:LEU:HD11	2:B:351:LEU:HD23	1.91	0.51
2:B:383:SER:O	2:B:384:VAL:C	2.47	0.51
1:A:284:TRP:CZ2	1:A:364:GLU:OE2	2.64	0.51
1:A:334:PHE:HE1	1:A:338:GLN:HE21	1.59	0.51
1:A:339:ARG:NH1	2:B:322:LEU:HD13	2.26	0.50
1:C:349:LEU:HD22	1:C:358:LEU:HD13	1.92	0.50
1:A:413:ARG:CG	1:A:413:ARG:NH1	2.73	0.50
1:A:380:LEU:HD23	1:A:381:VAL:N	2.26	0.50
1:A:265:LEU:C	1:A:265:LEU:HD23	2.33	0.49
2:B:336:SER:O	2:B:337:GLU:C	2.51	0.49
2:B:327:ARG:HH11	2:B:327:ARG:CB	2.25	0.49
1:C:222:ILE:HG22	1:C:268:ILE:HD13	1.95	0.48
1:C:227:ARG:HH21	1:C:240:LEU:HD12	1.78	0.48
1:A:339:ARG:HH12	2:B:322:LEU:HD13	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:VAL:CG1	1:A:373:SER:HB2	2.42	0.48
1:C:380:LEU:HD23	1:C:381:VAL:N	2.28	0.48
2:B:382:VAL:CG1	2:B:386:THR:HG21	2.43	0.47
1:A:370:VAL:O	1:A:372:ARG:N	2.47	0.47
1:A:227:ARG:HB3	1:A:227:ARG:HH11	1.79	0.47
1:A:369:GLY:O	1:A:370:VAL:CB	2.63	0.47
2:B:419:VAL:HG22	2:B:420:ASN:N	2.30	0.47
2:B:322:LEU:HG	2:B:328:TRP:NE1	2.29	0.47
1:A:222:ILE:HG22	1:A:268:ILE:HD13	1.96	0.46
2:B:309:PRO:HD3	2:B:344:ILE:HG22	1.97	0.46
2:B:375:GLY:O	2:B:376:TYR:HB2	2.15	0.46
1:A:325:LEU:HD11	2:B:351:LEU:HD22	1.97	0.46
1:C:265:LEU:C	1:C:265:LEU:HD23	2.35	0.46
1:C:394:LEU:O	1:C:400:TYR:HB3	2.15	0.46
1:A:394:LEU:O	1:A:400:TYR:HB3	2.16	0.45
1:A:258:ARG:HH22	1:A:373:SER:HB3	1.82	0.45
1:A:370:VAL:HG13	1:A:373:SER:HB2	1.99	0.45
2:B:381:LEU:HD21	2:B:396:LEU:HD13	1.99	0.45
2:B:388:VAL:HG12	2:B:392:GLN:NE2	2.32	0.45
2:B:381:LEU:HD11	2:B:396:LEU:HD11	2.00	0.44
2:B:402:GLY:O	2:B:403:GLN:HB2	2.18	0.43
1:C:286:LEU:HA	1:C:366:ALA:O	2.18	0.43
2:B:374:TYR:N	2:B:374:TYR:HD1	2.13	0.43
1:C:210:PRO:CG	1:C:276:ARG:HH22	2.31	0.43
2:B:381:LEU:HD11	2:B:396:LEU:CD1	2.49	0.43
1:C:210:PRO:HD3	1:C:276:ARG:HH12	1.82	0.43
2:B:319:GLY:O	2:B:320:GLU:C	2.56	0.43
1:A:400:TYR:CE2	1:A:404:LEU:HD11	2.54	0.43
2:B:299:LEU:O	2:B:305:GLN:NE2	2.52	0.42
1:A:250:VAL:CG1	1:A:251:MET:H	2.32	0.42
1:A:334:PHE:CE1	1:A:338:GLN:HG3	2.55	0.42
2:B:317:ARG:O	2:B:318:TYR:C	2.56	0.41
2:B:327:ARG:HH11	2:B:327:ARG:HB3	1.84	0.41
2:B:358:TYR:N	2:B:358:TYR:CD1	2.88	0.41
1:C:249:SER:HB2	1:C:251:MET:CE	2.51	0.41
1:A:421:LEU:HD23	1:A:421:LEU:HA	1.89	0.41
2:B:326:LEU:HD23	2:B:326:LEU:HA	1.89	0.40
1:A:252:GLY:O	1:A:256:VAL:HG23	2.22	0.40
1:A:214:ARG:O	1:A:215:GLU:C	2.59	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:353:ASP:OD2	2:B:353:ASP:OD2[48_555]	2.10	0.10

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	196/234 (84%)	181 (92%)	13 (7%)	2 (1%)	15	48
1	C	193/234 (82%)	174 (90%)	18 (9%)	1 (0%)	29	63
2	B	129/149 (87%)	109 (84%)	19 (15%)	1 (1%)	19	53
All	All	518/617 (84%)	464 (90%)	50 (10%)	4 (1%)	19	53

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	370	VAL
1	C	372	ARG
1	A	371	LEU
2	B	390	ALA

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	161/188 (86%)	148 (92%)	13 (8%)	11	38
1	C	158/188 (84%)	145 (92%)	13 (8%)	11	38
2	B	98/115 (85%)	86 (88%)	12 (12%)	5	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	417/491 (85%)	379 (91%)	38 (9%)	9 32

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	204	ASP
1	A	227	ARG
1	A	251	MET
1	A	254	SER
1	A	271	ASP
1	A	277	SER
1	A	282	SER
1	A	334	PHE
1	A	362	ARG
1	A	368	LEU
1	A	373	SER
1	A	380	LEU
1	A	413	ARG
2	B	303	ARG
2	B	317	ARG
2	B	322	LEU
2	B	327	ARG
2	B	331	MET
2	B	353	ASP
2	B	374	TYR
2	B	382	VAL
2	B	389	ARG
2	B	405	ARG
2	B	406	PRO
2	B	427	ARG
1	C	204	ASP
1	C	227	ARG
1	C	251	MET
1	C	254	SER
1	C	271	ASP
1	C	282	SER
1	C	286	LEU
1	C	332	LEU
1	C	338	GLN
1	C	362	ARG
1	C	380	LEU
1	C	389	HIS

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Mol	Chain	Res	Type
1	C	413	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	351	GLN
2	B	415	GLN
2	B	417	GLN
1	C	338	GLN
1	C	351	GLN

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	PO4	C	502	-	4,4,4	0.82	0	6,6,6	0.40	0
4	PO4	A	502	-	4,4,4	0.78	0	6,6,6	0.51	0

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

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	200/234 (85%)	0.30	6 (3%) 50 54	63, 103, 163, 232	0
1	C	197/234 (84%)	0.80	33 (16%) 1 2	99, 134, 201, 252	0
2	B	131/149 (87%)	0.34	2 (1%) 73 77	75, 119, 174, 207	0
All	All	528/617 (85%)	0.50	41 (7%) 13 16	63, 119, 184, 252	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	422	GLN	7.8
1	C	369	GLY	6.1
1	C	325	LEU	6.0
1	C	374	PRO	5.6
1	C	326	SER	5.5
1	C	288	ASN	4.9
1	A	371	LEU	4.6
1	C	370	VAL	4.4
1	C	329	VAL	3.6
1	A	369	GLY	3.4
1	C	328	ALA	3.4
1	A	368	LEU	3.4
1	C	324	TYR	3.3
1	C	365	HIS	3.0
2	B	400	SER	3.0
1	C	371	LEU	2.9
1	C	334	PHE	2.9
1	C	331	ASP	2.8
1	C	330	LEU	2.8
1	C	285	VAL	2.7
1	C	372	ARG	2.7
1	C	387	SER	2.6
1	C	286	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	327	GLN	2.6
1	C	283	VAL	2.5
1	C	342	TYR	2.5
1	C	278	ALA	2.4
1	C	264	PHE	2.4
1	C	373	SER	2.4
1	C	378	SER	2.3
1	C	275	ASN	2.3
1	C	333	GLN	2.3
2	B	344	ILE	2.2
1	C	416	PHE	2.2
1	C	337	SER	2.2
1	A	370	VAL	2.2
1	C	284	TRP	2.2
1	C	332	LEU	2.1
1	C	276	ARG	2.1
1	C	277	SER	2.0
1	A	236	PHE	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)

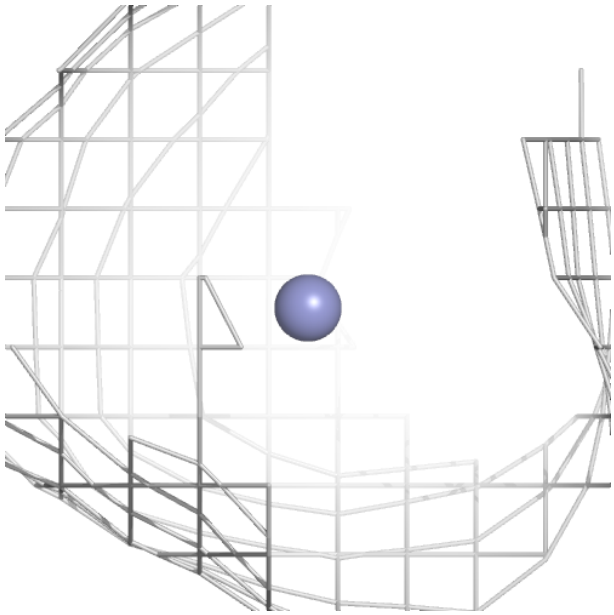
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

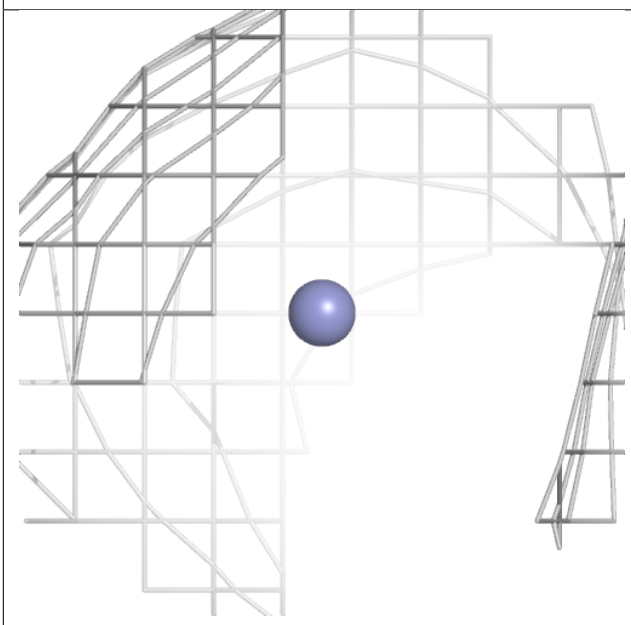
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ZN	C	501	1/1	0.89	0.17	138,138,138,138	0
3	ZN	A	501	1/1	0.96	0.22	94,94,94,94	0
4	PO4	A	502	5/5	0.96	0.22	74,75,81,81	5
4	PO4	C	502	5/5	0.97	0.32	117,118,125,131	5

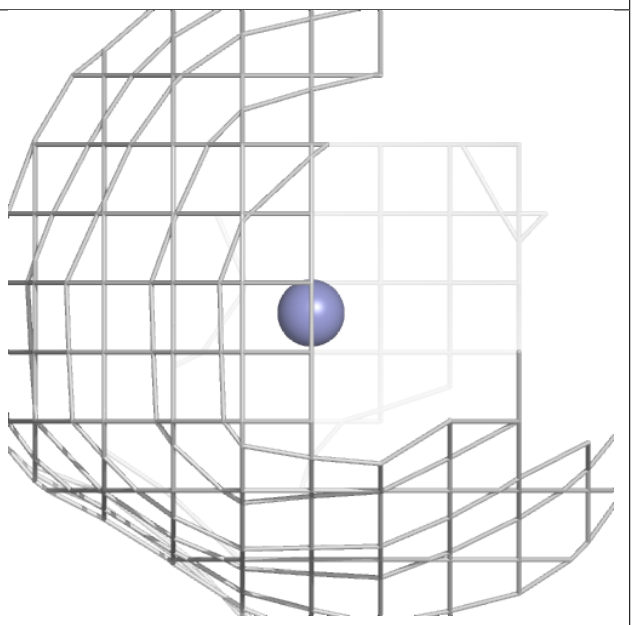
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ZN C 501:

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

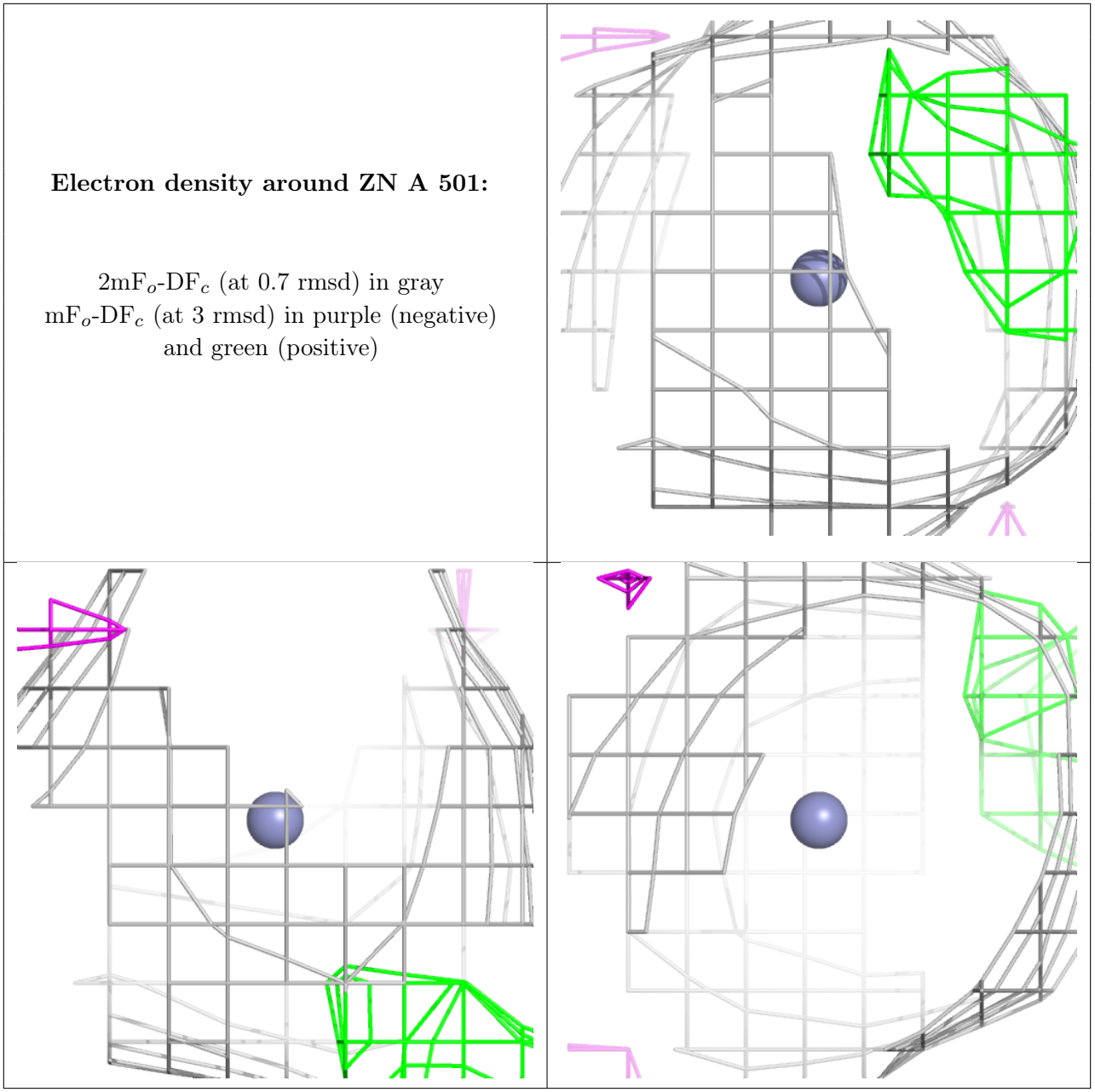






Electron density around ZN A 501:

$2mF_o$-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.