



# Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2023 – 04:23 am BST

PDB ID : 7Q8E  
Title : Crystal Structure of the MurT-GatD Enzyme Complex from *Staphylococcus aureus* COL strain  
Authors : Leisico, F.; Romao, M.J.; Santos-Silva, T.  
Deposited on : 2021-11-11  
Resolution : 2.90 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Xtrriage (Phenix) : 1.13  
EDS : 2.32.2  
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) : 2.32.2

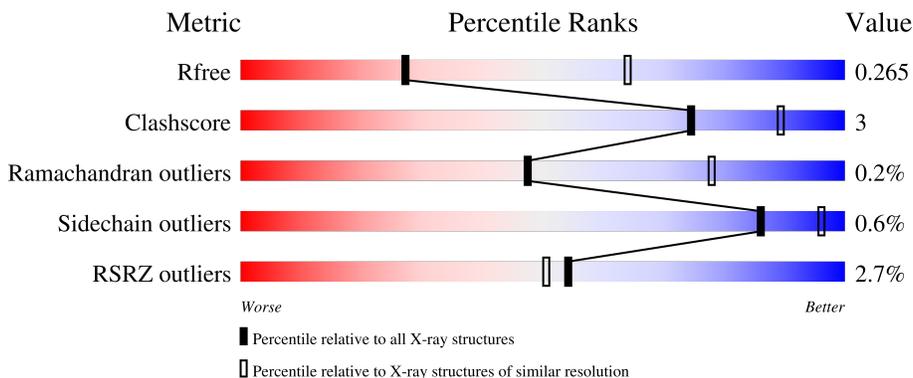
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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  $\geq 3$ , 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	437	 2% 83% 8% 9%
1	C	437	 4% 83% 8% 9%
2	B	251	 % 87% 10% .
2	D	251	 2% 84% 12% .

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 10134 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 Lipid II isoglutaminyl synthase (glutamine-hydrolyzing) subunit MurT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	397	3096	1963	519	598	16	0	0	0
1	C	397	3096	1963	519	598	16	0	0	0

- Molecule 2 is a protein called Lipid II isoglutaminyl synthase (glutamine-hydrolyzing) subunit GatD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	243	1932	1223	327	376	6	0	0	0
2	D	243	1932	1223	327	376	6	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	244	LEU	-	expression tag	UNP A0A0H2WZ38
B	245	GLU	-	expression tag	UNP A0A0H2WZ38
B	246	HIS	-	expression tag	UNP A0A0H2WZ38
B	247	HIS	-	expression tag	UNP A0A0H2WZ38
B	248	HIS	-	expression tag	UNP A0A0H2WZ38
B	249	HIS	-	expression tag	UNP A0A0H2WZ38
B	250	HIS	-	expression tag	UNP A0A0H2WZ38
B	251	HIS	-	expression tag	UNP A0A0H2WZ38
D	244	LEU	-	expression tag	UNP A0A0H2WZ38
D	245	GLU	-	expression tag	UNP A0A0H2WZ38
D	246	HIS	-	expression tag	UNP A0A0H2WZ38
D	247	HIS	-	expression tag	UNP A0A0H2WZ38
D	248	HIS	-	expression tag	UNP A0A0H2WZ38
D	249	HIS	-	expression tag	UNP A0A0H2WZ38
D	250	HIS	-	expression tag	UNP A0A0H2WZ38

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Chain	Residue	Modelled	Actual	Comment	Reference
D	251	HIS	-	expression tag	UNP A0A0H2WZ38

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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Cl 1	0	0

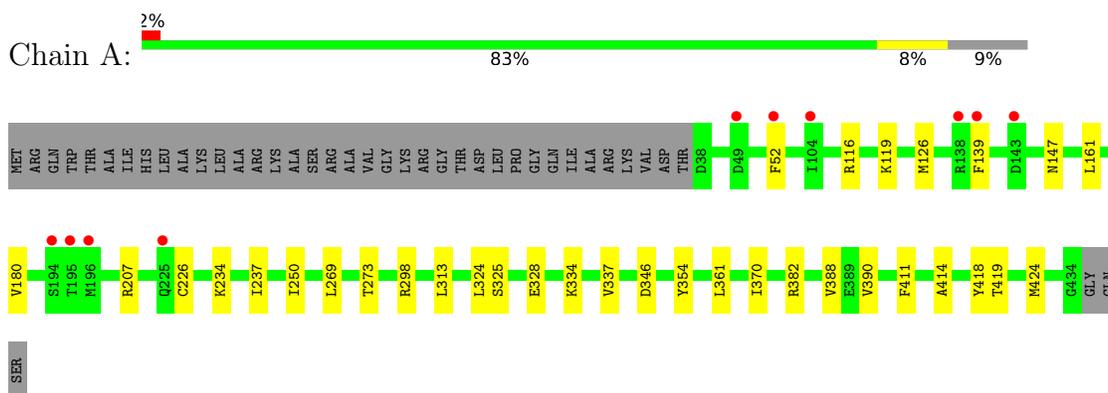
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	30	Total 30	O 30	0	0
5	C	18	Total 18	O 18	0	0
5	B	16	Total 16	O 16	0	0
5	D	11	Total 11	O 11	0	0

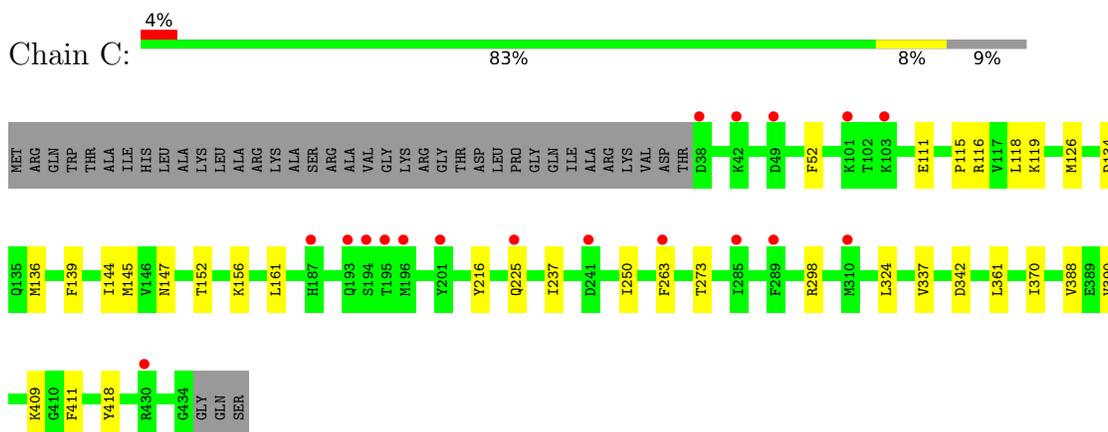
### 3 Residue-property plots [i](#)

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.

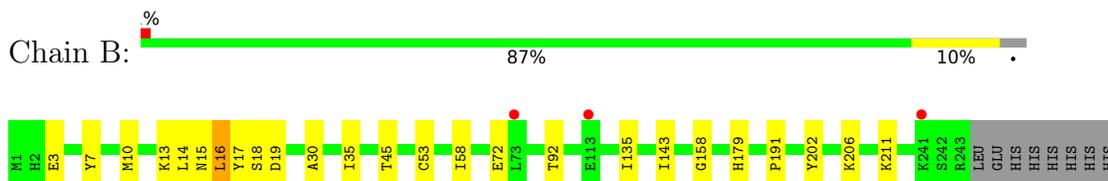
- Molecule 1: Lipid II isoglutaminyll synthase (glutamine-hydrolyzing) subunit MurT



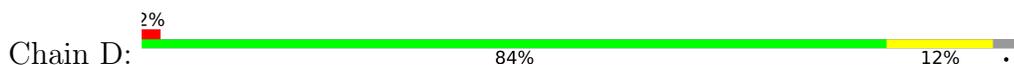
- Molecule 1: Lipid II isoglutaminyll synthase (glutamine-hydrolyzing) subunit MurT

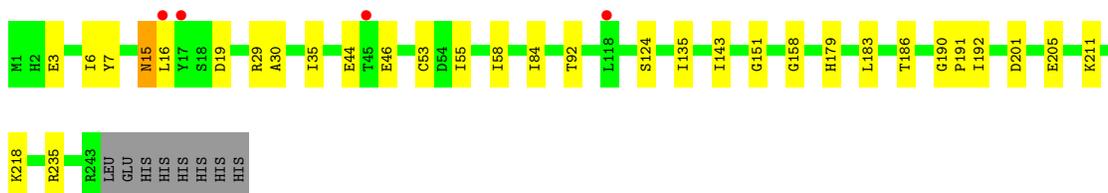


- Molecule 2: Lipid II isoglutaminyll synthase (glutamine-hydrolyzing) subunit GatD



- Molecule 2: Lipid II isoglutaminyll synthase (glutamine-hydrolyzing) subunit GatD





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.09Å 111.09Å 112.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.31 – 2.90 49.31 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.31-2.90) 99.7 (49.31-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.81 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, $R_{free}$	0.240 , 0.265 0.240 , 0.265	Depositor DCC
$R_{free}$ test set	1492 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	62.9	Xtriage
Anisotropy	0.821	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 27.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.003 for -h,l,k 0.000 for -l,-k,-h 0.005 for k,h,-l 0.000 for k,l,h 0.000 for l,h,k	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	10134	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.56% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CL

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	0/3150	0.42	0/4260
1	C	0.24	0/3150	0.42	0/4260
2	B	0.24	0/1967	0.44	0/2646
2	D	0.25	0/1967	0.43	0/2646
All	All	0.24	0/10234	0.43	0/13812

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
2	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	190	GLY	Peptide

### 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	3096	0	3021	21	0
1	C	3096	0	3021	22	0
2	B	1932	0	1913	12	0
2	D	1932	0	1913	16	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	1	0	0	0	0
5	A	30	0	0	1	0
5	B	16	0	0	0	0
5	C	18	0	0	0	0
5	D	11	0	0	0	0
All	All	10134	0	9868	64	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 (64) 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:298:ARG:NH2	1:C:139:PHE:O	2.22	0.73
2:D:135:ILE:HB	2:D:143:ILE:HB	1.75	0.68
2:B:10:MET:HB2	2:B:14:LEU:HD22	1.76	0.67
2:B:17:TYR:O	2:B:19:ASP:N	2.28	0.67
1:C:116:ARG:HA	1:C:119:LYS:HE2	1.77	0.66
1:A:237:ILE:HG12	1:A:250:ILE:HG12	1.79	0.65
2:D:15:ASN:O	2:D:15:ASN:ND2	2.31	0.63
1:C:324:LEU:HD22	1:C:361:LEU:HD21	1.82	0.61
1:A:116:ARG:HA	1:A:119:LYS:HE2	1.84	0.59
1:A:207:ARG:HH21	1:A:226:CYS:HB3	1.67	0.58
2:D:84:ILE:HD13	2:D:183:LEU:HD22	1.89	0.55
1:A:313:LEU:HD22	1:C:144:ILE:HD11	1.89	0.54
1:C:115:PRO:HA	1:C:152:THR:HG21	1.90	0.54
1:A:334:LYS:NZ	5:A:601:HOH:O	2.38	0.54
2:B:58:ILE:HB	2:B:92:THR:HG22	1.91	0.53
2:D:44:GLU:HB3	2:D:46:GLU:OE2	2.08	0.53
2:B:158:GLY:O	2:B:179:HIS:N	2.35	0.53
1:A:388:VAL:HG12	1:A:390:VAL:HG22	1.93	0.51
1:A:147:ASN:HB3	1:C:418:TYR:CZ	2.46	0.51
2:B:135:ILE:HB	2:B:143:ILE:HB	1.92	0.51
1:A:237:ILE:HD11	1:A:269:LEU:HB2	1.93	0.50
1:A:324:LEU:HD22	1:A:361:LEU:HD21	1.92	0.50
2:B:3:GLU:O	2:B:211:LYS:NZ	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:30:ALA:HB1	2:D:35:ILE:HB	1.94	0.50
1:A:418:TYR:CZ	1:C:147:ASN:HB3	2.48	0.49
1:C:237:ILE:HG12	1:C:250:ILE:HG12	1.93	0.49
1:A:346:ASP:OD2	1:A:419:THR:OG1	2.22	0.49
1:C:225:GLN:NE2	2:B:16:LEU:HD13	2.28	0.49
1:C:388:VAL:HG12	1:C:390:VAL:HG22	1.96	0.48
2:B:202:TYR:O	2:B:206:LYS:HG2	2.13	0.48
1:C:118:LEU:HB3	1:C:156:LYS:HZ3	1.78	0.47
2:D:58:ILE:HB	2:D:92:THR:HG22	1.96	0.47
1:C:52:PHE:HB2	1:C:126:MET:HG3	1.95	0.47
1:C:342:ASP:OD2	2:D:235:ARG:NH1	2.38	0.46
2:D:3:GLU:O	2:D:211:LYS:NZ	2.47	0.46
1:A:139:PHE:O	1:C:298:ARG:NH2	2.31	0.46
1:C:216:TYR:CE2	1:C:263:PHE:HE1	2.34	0.46
1:A:161:LEU:HD13	1:A:273:THR:HG22	1.97	0.45
1:C:134:ASP:O	1:C:136:MET:N	2.39	0.45
2:D:158:GLY:O	2:D:179:HIS:N	2.41	0.45
2:D:205:GLU:OE2	2:D:218:LYS:NZ	2.39	0.44
1:C:111:GLU:HG3	1:C:145:MET:SD	2.58	0.43
1:A:337:VAL:HG22	1:A:370:ILE:HB	2.00	0.43
2:D:29:ARG:NH2	2:D:201:ASP:OD2	2.42	0.43
2:B:45:THR:OG1	2:B:72:GLU:O	2.26	0.42
2:D:7:TYR:CE2	2:D:53:CYS:HB2	2.54	0.42
1:A:325:SER:O	1:A:328:GLU:HG2	2.19	0.42
1:A:180:VAL:HG13	1:A:234:LYS:HD3	2.01	0.42
2:B:7:TYR:CE2	2:B:53:CYS:HB2	2.54	0.42
2:B:13:LYS:HD2	2:B:13:LYS:HA	1.78	0.42
1:A:414:ALA:HB1	1:A:424:MET:SD	2.60	0.42
2:D:124:SER:HA	2:D:151:GLY:HA2	2.02	0.42
2:D:15:ASN:OD1	2:D:19:ASP:N	2.52	0.42
1:C:161:LEU:HD13	1:C:273:THR:HG22	2.02	0.42
1:C:409:LYS:N	1:C:409:LYS:HD2	2.35	0.41
1:C:225:GLN:H	1:C:225:GLN:HG2	1.74	0.41
1:C:337:VAL:HA	1:C:370:ILE:O	2.21	0.41
2:D:6:ILE:HG12	2:D:55:ILE:HB	2.03	0.41
1:A:354:TYR:HA	1:A:382:ARG:NE	2.36	0.41
1:A:237:ILE:HG13	1:A:269:LEU:HD22	2.03	0.40
2:D:186:THR:HG21	2:D:192:ILE:HD12	2.03	0.40
2:B:30:ALA:HB1	2:B:35:ILE:HB	2.04	0.40
1:C:118:LEU:HB3	1:C:156:LYS:NZ	2.37	0.40
1:A:52:PHE:HB2	1:A:126:MET:HG3	2.04	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	395/437 (90%)	383 (97%)	12 (3%)	0	100	100
1	C	395/437 (90%)	380 (96%)	15 (4%)	0	100	100
2	B	241/251 (96%)	222 (92%)	17 (7%)	2 (1%)	19	51
2	D	241/251 (96%)	224 (93%)	16 (7%)	1 (0%)	34	66
All	All	1272/1376 (92%)	1209 (95%)	60 (5%)	3 (0%)	47	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	18	SER
2	D	191	PRO
2	B	191	PRO

### 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	326/371 (88%)	325 (100%)	1 (0%)	92	98
1	C	326/371 (88%)	325 (100%)	1 (0%)	92	98
2	B	208/216 (96%)	206 (99%)	2 (1%)	76	92
2	D	208/216 (96%)	206 (99%)	2 (1%)	76	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1068/1174 (91%)	1062 (99%)	6 (1%)	86 96

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	411	PHE
1	C	411	PHE
2	B	15	ASN
2	B	16	LEU
2	D	15	ASN
2	D	16	LEU

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 3 ligands modelled in this entry, 3 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

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	397/437 (90%)	0.29	10 (2%) 57 55	46, 69, 103, 128	0
1	C	397/437 (90%)	0.40	18 (4%) 33 29	54, 74, 102, 134	0
2	B	243/251 (96%)	0.23	3 (1%) 79 79	46, 70, 106, 117	0
2	D	243/251 (96%)	0.22	4 (1%) 72 71	51, 70, 92, 100	0
All	All	1280/1376 (93%)	0.30	35 (2%) 54 50	46, 72, 102, 134	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	225	GLN	4.4
1	C	195	THR	4.2
1	A	196	MET	3.9
2	D	16	LEU	3.6
1	A	194	SER	3.6
1	C	194	SER	3.5
1	C	101	LYS	3.2
1	C	310	MET	3.2
1	A	225	GLN	3.0
1	C	196	MET	3.0
1	C	42	LYS	2.9
1	C	38	ASP	2.9
1	A	195	THR	2.8
1	C	285	ILE	2.5
1	C	289	PHE	2.5
2	D	45	THR	2.4
2	B	113	GLU	2.4
2	B	73	LEU	2.4
2	D	17	TYR	2.3
1	C	263	PHE	2.3
1	C	103	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	49	ASP	2.2
2	D	118	LEU	2.2
1	A	52	PHE	2.2
1	A	104	ILE	2.2
1	A	139	PHE	2.2
2	B	241	LYS	2.2
1	C	201	TYR	2.1
1	A	143	ASP	2.1
1	C	241	ASP	2.1
1	C	193	GLN	2.0
1	C	187	HIS	2.0
1	C	430	ARG	2.0
1	A	49	ASP	2.0
1	A	138	ARG	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](#)

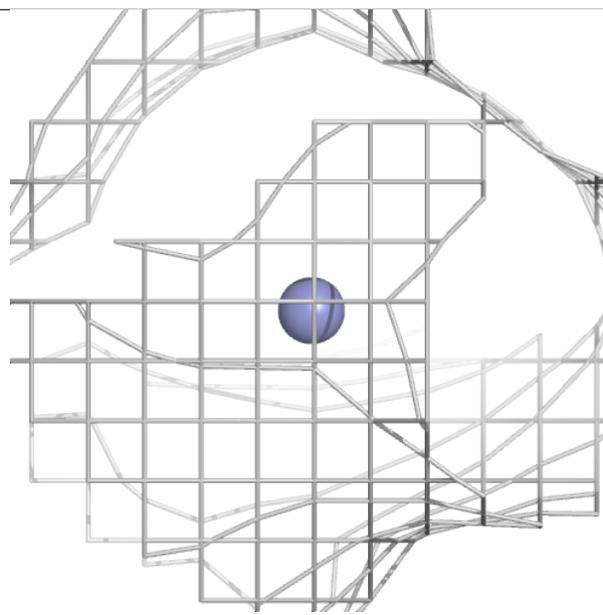
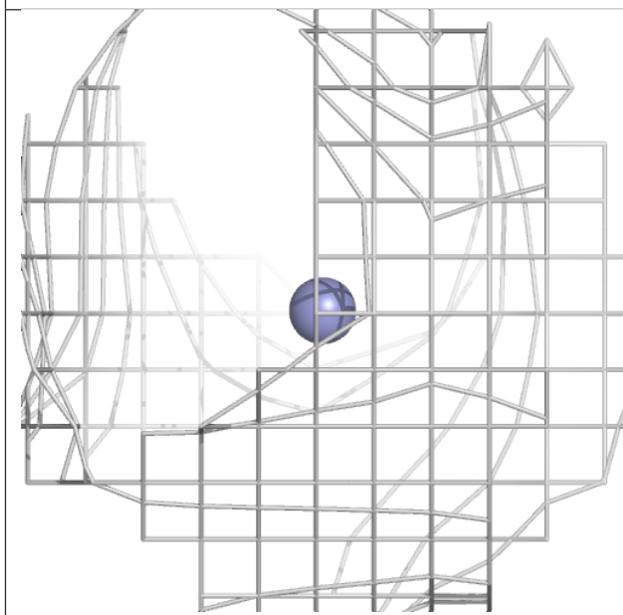
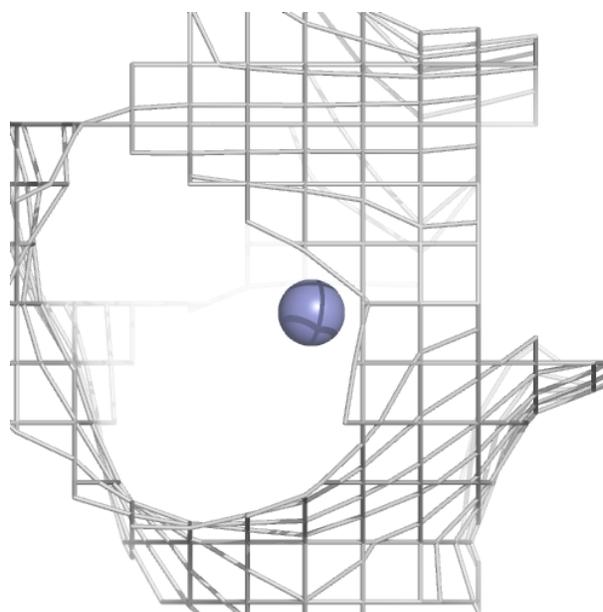
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

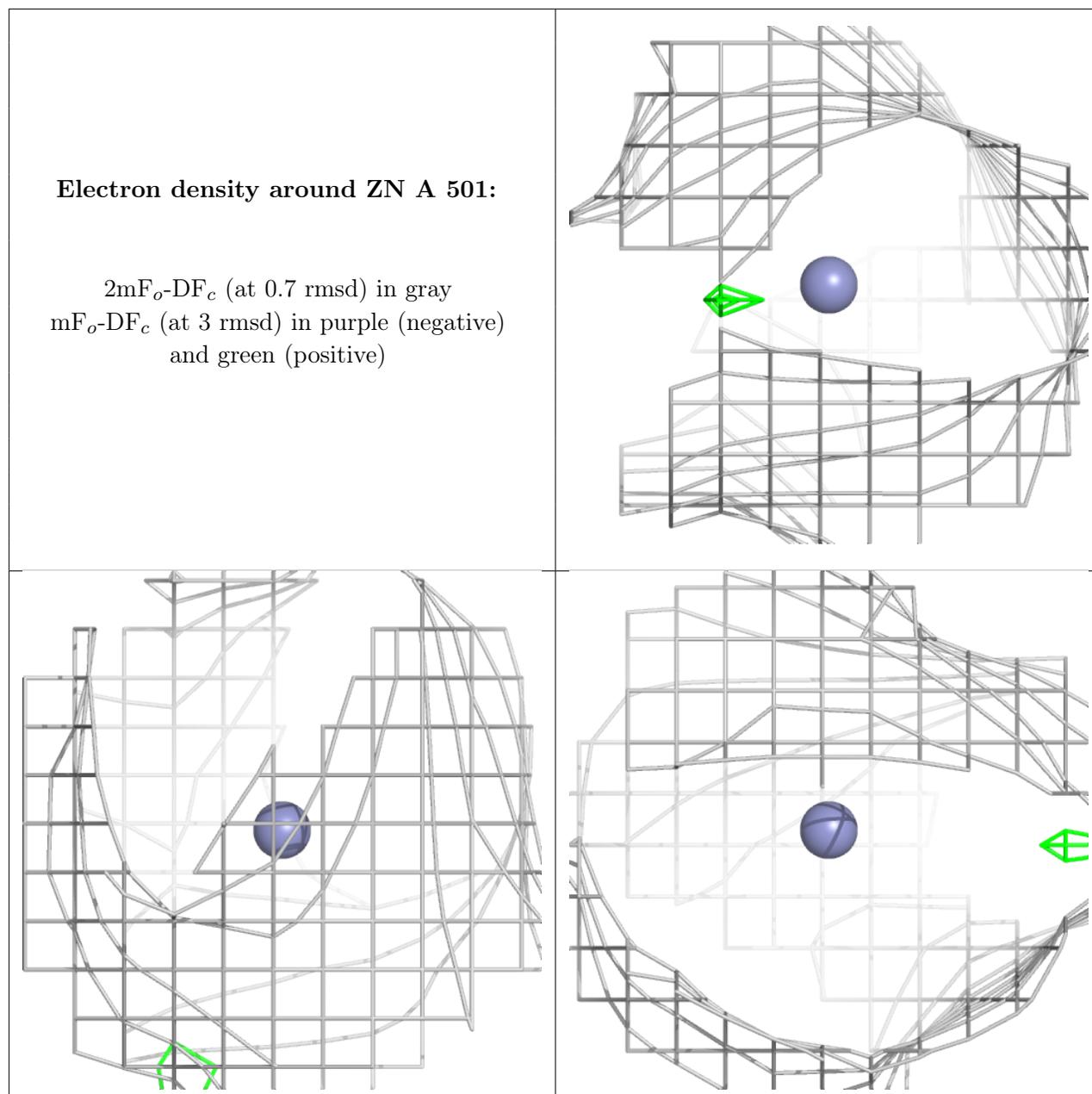
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	CL	A	502	1/1	0.79	0.15	95,95,95,95	0
3	ZN	C	501	1/1	0.95	0.15	71,71,71,71	0
3	ZN	A	501	1/1	0.97	0.16	67,67,67,67	0

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.

**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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.