



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 6, 2021 – 02:14 am BST

PDB ID : 5M19  
Title : Crystal structure of PBP2a from MRSA in the presence of Oxacillin ligand  
Authors : Molina, R.; Batuecas, M.T.; Hermoso, J.A.  
Deposited on : 2016-10-07  
Resolution : 2.00 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.

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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  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.19  
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) : 2.19

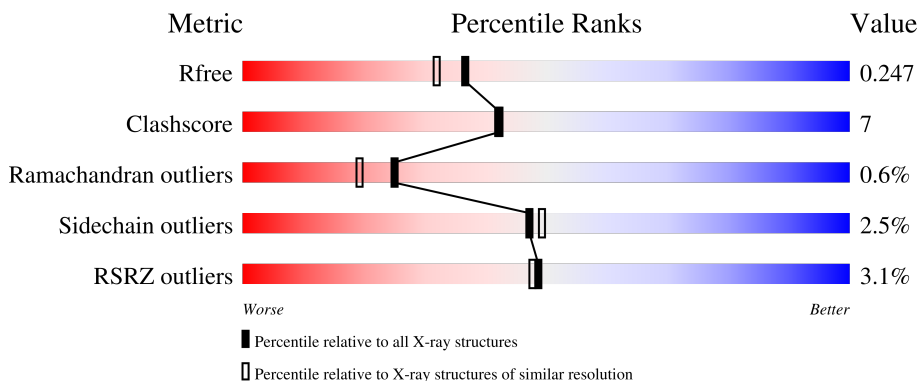
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


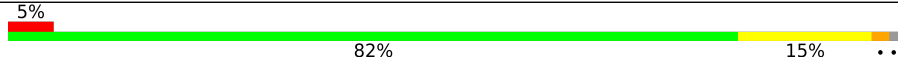
The reported resolution of this entry is 2.00 Å.

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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	642	 87% 11% ..
1	B	642	 82% 15% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CD	B	702	-	-	-	X
3	MUR	A	703	-	-	X	-
3	MUR	B	703	-	-	X	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10946 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.

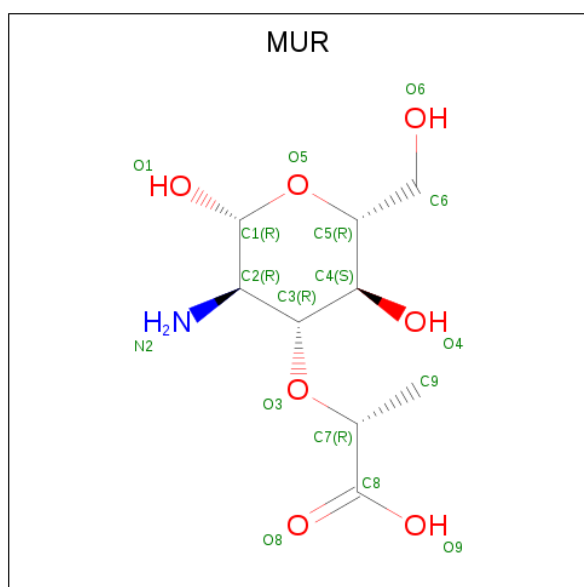
- Molecule 1 is a protein called Penicillin-binding protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	638	Total 5140	C 3243	N 866	O 1015	S 16	0	4	0
1	B	635	Total 5114	C 3224	N 862	O 1013	S 15	0	4	0

- Molecule 2 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total 4	Cd 4	0	0
2	B	2	Total 2	Cd 2	0	0

- Molecule 3 is beta-muramic acid (three-letter code: MUR) (formula: C<sub>9</sub>H<sub>17</sub>NO<sub>7</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	1	7		
3	B	1	Total	C	N	O	0	0
			17	9	1	7		

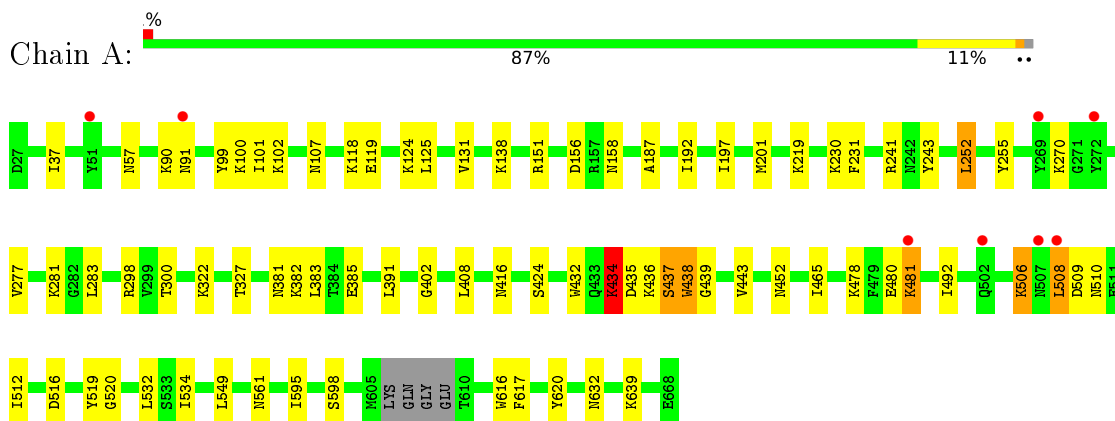
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	348	Total	O	0	0
			348	348		
4	B	304	Total	O	0	0
			304	304		

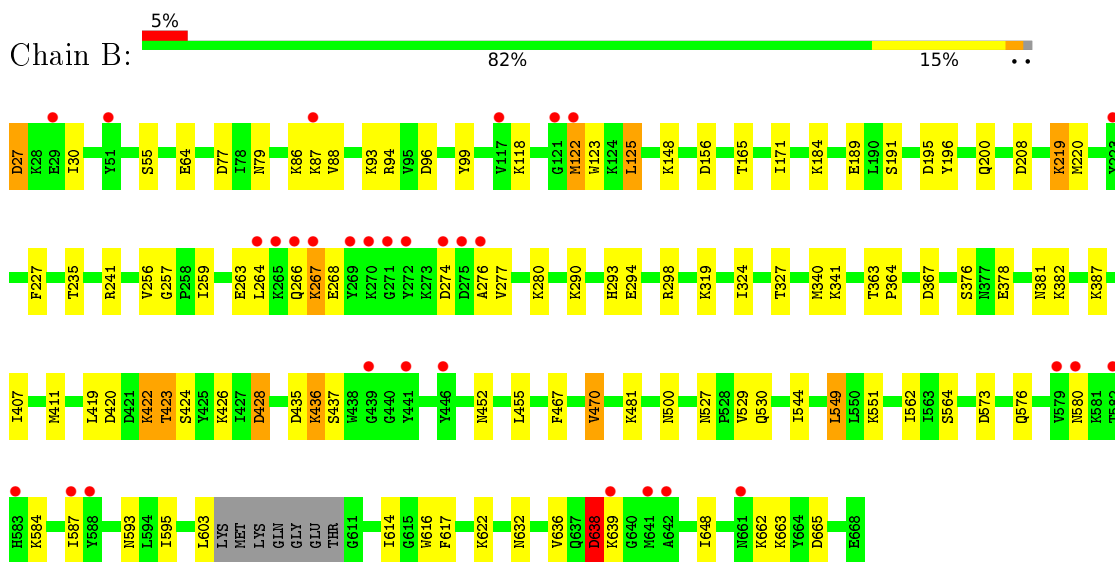
### 3 Residue-property plots [i](#)

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: Penicillin-binding protein 2



- Molecule 1: Penicillin-binding protein 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.50Å 102.19Å 185.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.42 – 2.00 46.42 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.0 (46.42-2.00) 98.8 (46.42-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.03	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.54 (at 2.00Å)	Xtrriage
Refinement program	PHENIX (dev_2420: ???)	Depositor
R, $R_{free}$	0.190 , 0.247 0.190 , 0.247	Depositor DCC
$R_{free}$ test set	1987 reflections (1.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.8	Xtrriage
Anisotropy	0.974	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 47.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10946	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.40	1/5237 (0.0%)	0.56	0/7039
1	B	0.38	0/5211	0.56	1/7008 (0.0%)
All	All	0.39	1/10448 (0.0%)	0.56	1/14047 (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	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	492	ILE	C-N	6.55	1.46	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	125	LEU	CA-CB-CG	5.05	126.91	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	434	LYS	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	5140	0	5154	53	1
1	B	5114	0	5111	83	0
2	A	4	0	0	0	0
2	B	2	0	0	0	0
3	A	17	0	15	10	0
3	B	17	0	15	11	0
4	A	348	0	0	5	0
4	B	304	0	0	15	1
All	All	10946	0	10295	141	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 7.

All (141) 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:B:263:GLU:CA	1:B:266:GLN:OE1	1.79	1.28
1:B:263:GLU:HA	1:B:266:GLN:OE1	1.07	1.23
1:A:241:ARG:HD3	3:A:703:MUR:H61	1.34	1.02
1:B:263:GLU:HA	1:B:266:GLN:CD	1.85	0.96
1:A:241:ARG:H	3:A:703:MUR:H92	1.34	0.91
1:A:100:LYS:HE3	1:A:107:ASN:HB3	1.59	0.84
1:A:508:LEU:O	1:A:510:ASN:N	2.13	0.82
1:A:437:SER:O	1:A:439:GLY:N	2.12	0.81
1:B:263:GLU:C	1:B:266:GLN:OE1	2.20	0.80
1:A:241:ARG:H	3:A:703:MUR:C9	1.96	0.78
1:A:434:LYS:HD3	1:A:436:LYS:HE3	1.65	0.77
1:B:277:VAL:HG11	3:B:703:MUR:H91	1.65	0.77
1:B:277:VAL:CG1	3:B:703:MUR:H91	2.15	0.77
1:A:151:ARG:HB3	3:A:703:MUR:H62	1.66	0.77
1:A:416:ASN:HD21	1:A:481:LYS:NZ	1.85	0.75
1:B:436:LYS:H	1:B:436:LYS:HE2	1.51	0.74
1:B:576:GLN:HB2	1:B:595:ILE:HD12	1.70	0.73
1:B:263:GLU:OE2	1:B:280:LYS:NZ	2.21	0.73
1:B:367[B]:ASP:OD2	4:B:801:HOH:O	2.07	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:561:ASN:ND2	4:A:802:HOH:O	2.25	0.70
1:B:420:ASP:OD1	1:B:422:LYS:HG3	1.91	0.69
1:A:478:LYS:O	1:A:481:LYS:HE3	1.91	0.69
1:A:383:LEU:HB3	1:A:391:LEU:HD21	1.75	0.69
1:B:64:GLU:OE1	4:B:802:HOH:O	2.11	0.69
1:B:603:LEU:HD11	1:B:614:ILE:HG12	1.75	0.68
1:B:298:ARG:HD2	4:B:855:HOH:O	1.95	0.67
1:B:584:LYS:HE3	1:B:587:ILE:HG12	1.77	0.66
1:B:290:LYS:NZ	4:B:812:HOH:O	2.28	0.65
1:B:264:LEU:HD11	1:B:274:ASP:HA	1.79	0.64
1:B:94:ARG:NH1	1:B:96:ASP:OD1	2.32	0.63
1:B:263:GLU:O	1:B:266:GLN:OE1	2.17	0.62
1:B:191:SER:HB3	1:B:376:SER:HB3	1.81	0.62
1:A:416:ASN:HD21	1:A:481:LYS:HZ1	1.48	0.61
3:B:703:MUR:H93	3:B:703:MUR:HN22	1.65	0.61
1:A:158:ASN:HA	1:B:551:LYS:HE3	1.82	0.61
1:A:90:LYS:HG2	1:A:91:ASN:OD1	2.01	0.60
1:A:481:LYS:NZ	4:A:810:HOH:O	2.33	0.60
1:A:598:SER:HB3	1:A:617:PHE:CD2	2.37	0.60
1:B:428:ASP:O	4:B:803:HOH:O	2.16	0.59
1:B:27:ASP:OD1	1:B:93:LYS:NZ	2.29	0.59
1:B:420:ASP:H	1:B:423:THR:CG2	2.16	0.59
1:A:230:LYS:HD3	1:A:231:PHE:CE2	2.37	0.58
1:A:298:ARG:HG2	1:A:300:THR:HG23	1.87	0.57
1:A:438:TRP:HA	1:A:512:ILE:HD11	1.86	0.57
3:A:703:MUR:O9	4:A:801:HOH:O	2.17	0.57
1:B:428:ASP:OD2	4:B:804:HOH:O	2.17	0.56
3:B:703:MUR:O9	4:B:805:HOH:O	2.18	0.56
1:B:93:LYS:HE3	1:B:123:TRP:CZ2	2.41	0.56
1:A:91:ASN:ND2	1:A:118:LYS:HD3	2.20	0.56
1:A:241:ARG:HB2	3:A:703:MUR:H4	1.88	0.56
1:B:378:GLU:O	1:B:382:LYS:HG2	2.06	0.56
1:B:241:ARG:HD3	3:B:703:MUR:H62	1.87	0.56
1:B:419:LEU:HA	1:B:423:THR:HG21	1.87	0.55
1:B:293:HIS:HE2	3:B:703:MUR:C8	2.19	0.55
1:A:595:ILE:HD11	1:A:620:TYR:CZ	2.42	0.54
1:B:118:LYS:HA	1:B:122:MET:O	2.07	0.54
1:B:435:ASP:OD1	1:B:437:SER:HB3	2.08	0.53
1:B:165:THR:HA	3:B:703:MUR:H61	1.91	0.53
1:A:100:LYS:HE2	1:A:102:LYS:HD3	1.89	0.52
1:B:219:LYS:N	1:B:219:LYS:HD3	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:593:ASN:ND2	1:B:622:LYS:HD3	2.25	0.51
1:A:480:GLU:HG2	1:A:508:LEU:HD12	1.93	0.51
1:A:595:ILE:HD11	1:A:620:TYR:OH	2.10	0.50
1:B:340:MET:HG2	1:B:648:ILE:HD13	1.92	0.50
1:A:432:TRP:CZ2	1:A:434:LYS:HA	2.47	0.50
1:A:100:LYS:HD2	1:A:101:ILE:N	2.27	0.50
1:B:259:ILE:HG13	1:B:263:GLU:HG3	1.94	0.50
1:B:376:SER:OG	1:B:378:GLU:HG2	2.12	0.50
1:B:171:ILE:HD11	1:B:220:MET:SD	2.53	0.49
1:B:267:LYS:HG3	1:B:268:GLU:N	2.27	0.48
1:A:277:VAL:HG11	3:A:703:MUR:H7	1.94	0.48
1:A:241:ARG:HD3	3:A:703:MUR:C6	2.25	0.48
1:B:564:SER:HB2	4:B:1074:HOH:O	2.13	0.47
1:B:259:ILE:HG22	1:B:276:ALA:O	2.14	0.47
1:B:327:THR:OG1	1:B:549:LEU:HA	2.14	0.47
1:B:256:VAL:HG21	3:B:703:MUR:H92	1.97	0.47
1:A:281:LYS:NZ	4:A:831:HOH:O	2.48	0.47
1:B:500:ASN:OD1	4:B:806:HOH:O	2.20	0.47
1:B:93:LYS:HE3	1:B:123:TRP:CE2	2.50	0.46
1:B:290:LYS:HD3	1:B:324:ILE:HG12	1.97	0.46
1:B:638:ASP:HB3	1:B:639:LYS:H	1.53	0.46
1:A:408:LEU:HD22	1:A:534:ILE:HG21	1.97	0.46
1:B:662:LYS:O	1:B:663:LYS:HE2	2.15	0.46
1:A:381:ASN:HB3	1:A:385:GLU:OE1	2.15	0.46
1:B:30:ILE:CD1	1:B:93:LYS:HD2	2.46	0.46
1:A:187:ALA:HB1	1:A:192:ILE:O	2.16	0.46
1:B:27:ASP:OD1	1:B:87:LYS:HE3	2.16	0.46
1:B:381:ASN:ND2	4:B:838:HOH:O	2.49	0.45
1:B:93:LYS:HG3	1:B:123:TRP:CH2	2.51	0.45
1:B:267:LYS:CG	1:B:268:GLU:N	2.80	0.45
1:B:527:ASN:HD22	1:B:530:GLN:H	1.64	0.45
1:B:263:GLU:CB	1:B:266:GLN:OE1	2.60	0.45
1:B:544:ILE:HD11	1:B:562:ILE:HD13	1.98	0.45
1:A:327:THR:OG1	1:A:549:LEU:HA	2.17	0.45
1:B:419:LEU:HD21	1:B:455:LEU:HD13	1.99	0.45
1:A:119:GLU:HB2	1:A:124:LYS:HG3	1.98	0.44
3:B:703:MUR:H93	3:B:703:MUR:N2	2.30	0.44
1:B:189:GLU:HG2	1:B:227:PHE:CD2	2.52	0.44
1:B:86:LYS:NZ	1:B:87:LYS:O	2.43	0.44
1:B:481:LYS:HD3	1:B:481:LYS:HA	1.61	0.44
1:B:294:GLU:OE1	1:B:319:LYS:NZ	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:LYS:HB3	1:A:219:LYS:HE3	1.57	0.44
1:B:419:LEU:HD12	1:B:423:THR:HG21	1.99	0.43
1:A:639:LYS:HE2	4:A:1129:HOH:O	2.18	0.43
1:B:467:PHE:HA	1:B:470:VAL:HG13	1.99	0.43
1:A:197:ILE:O	1:A:201:MET:HG2	2.19	0.43
1:B:593:ASN:HD22	1:B:622:LYS:HD3	1.83	0.43
1:A:402:GLY:O	1:A:520:GLY:HA3	2.18	0.43
1:A:506:LYS:O	1:A:506:LYS:HG3	2.19	0.43
1:A:243:TYR:OH	1:A:255:TYR:HA	2.19	0.42
1:B:407:ILE:O	1:B:411:MET:HG3	2.19	0.42
1:B:419:LEU:HD12	1:B:423:THR:CG2	2.49	0.42
1:B:184:LYS:HG3	4:B:989:HOH:O	2.18	0.42
1:B:87:LYS:HD2	1:B:93:LYS:HE2	2.01	0.42
1:B:196:TYR:O	1:B:200:GLN:HG2	2.20	0.42
1:A:616:TRP:CZ3	1:A:632:ASN:HB2	2.55	0.42
1:B:77:ASP:OD2	1:B:79:ASN:ND2	2.48	0.42
1:B:148:LYS:HA	1:B:148:LYS:HD3	1.92	0.42
1:B:86:LYS:NZ	1:B:88:VAL:HA	2.34	0.42
1:B:171:ILE:HD12	1:B:235:THR:HG22	2.02	0.42
1:A:252:LEU:HD22	1:A:283:LEU:HG	2.02	0.42
1:A:516:ASP:HA	1:A:519:TYR:CE1	2.55	0.42
1:B:616:TRP:CZ3	1:B:632:ASN:HB2	2.55	0.42
3:B:703:MUR:H2	4:B:1017:HOH:O	2.19	0.42
1:A:241:ARG:N	3:A:703:MUR:H92	2.17	0.41
1:B:363:THR:HA	1:B:364:PRO:C	2.40	0.41
3:B:703:MUR:H92	4:B:1017:HOH:O	2.20	0.41
1:B:580:ASN:OD1	4:B:807:HOH:O	2.21	0.41
1:A:91:ASN:ND2	1:A:118:LYS:HB3	2.35	0.41
1:B:527:ASN:HD21	1:B:529:VAL:HB	1.85	0.41
1:A:57:ASN:OD1	1:A:138:LYS:NZ	2.53	0.41
1:B:257:GLY:C	1:B:277:VAL:HG13	2.41	0.41
1:B:387:LYS:HD3	1:B:636:VAL:HB	2.03	0.41
1:A:277:VAL:HG11	3:A:703:MUR:C7	2.51	0.41
1:A:322:LYS:HA	1:A:322:LYS:HD3	1.83	0.41
1:B:426:LYS:HD3	1:B:452:ASN:OD1	2.21	0.41
1:B:665:ASP:HA	4:B:895:HOH:O	2.21	0.41
1:A:443:VAL:HG12	1:A:465:ILE:HG12	2.02	0.41
1:A:37:ILE:HD13	1:A:131:VAL:HG13	2.03	0.40
1:A:424:SER:OG	1:A:452:ASN:HB3	2.21	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)
1:A:270:LYS:NZ	4:B:1087:HOH:O[3_545]	1.98	0.22

### 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	638/642 (99%)	620 (97%)	12 (2%)	6 (1%)	17 11
1	B	635/642 (99%)	621 (98%)	13 (2%)	1 (0%)	47 44
All	All	1273/1284 (99%)	1241 (98%)	25 (2%)	7 (0%)	25 23

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	434	LYS
1	A	435	ASP
1	A	438	TRP
1	A	508	LEU
1	A	509	ASP
1	A	437	SER
1	B	638	ASP

#### 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	573/572 (100%)	565 (99%)	8 (1%)	67 72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	570/572 (100%)	550 (96%)	20 (4%)	36	35
All	All	1143/1144 (100%)	1115 (98%)	28 (2%)	47	51

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	TYR
1	A	125	LEU
1	A	156	ASP
1	A	252	LEU
1	A	382	LYS
1	A	481	LYS
1	A	506	LYS
1	A	532	LEU
1	B	27	ASP
1	B	55	SER
1	B	99	TYR
1	B	122	MET
1	B	125	LEU
1	B	156	ASP
1	B	195	ASP
1	B	208	ASP
1	B	219	LYS
1	B	267	LYS
1	B	341	LYS
1	B	422	LYS
1	B	423	THR
1	B	424	SER
1	B	428	ASP
1	B	436	LYS
1	B	470	VAL
1	B	549	LEU
1	B	617	PHE
1	B	638	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	A	381	ASN
1	A	416	ASN
1	B	381	ASN

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Mol	Chain	Res	Type
1	B	405	GLN
1	B	433	GLN
1	B	527	ASN

### 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 8 ligands modelled in this entry, 6 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
3	MUR	B	703	-	14,17,17	1.57	3 (21%)	19,24,24	2.35	9 (47%)
3	MUR	A	703	-	14,17,17	1.68	4 (28%)	19,24,24	3.33	8 (42%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MUR	B	703	-	-	3/6/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MUR	A	703	-	-	4/6/30/30	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	703	MUR	O5-C1	3.54	1.51	1.42
3	B	703	MUR	C2-N2	3.17	1.52	1.47
3	A	703	MUR	C2-N2	3.12	1.52	1.47
3	A	703	MUR	C3-C2	-2.43	1.47	1.53
3	B	703	MUR	O5-C1	2.40	1.48	1.42
3	A	703	MUR	O3-C3	2.21	1.49	1.43
3	B	703	MUR	C1-C2	-2.11	1.50	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	703	MUR	C9-C7-C8	-9.87	100.59	113.35
3	A	703	MUR	O5-C1-C2	5.84	116.33	109.51
3	B	703	MUR	O5-C5-C4	5.16	119.07	109.69
3	B	703	MUR	C6-C5-C4	-4.06	103.50	113.00
3	A	703	MUR	O5-C5-C6	-3.78	97.05	106.44
3	A	703	MUR	O3-C3-C4	3.70	117.13	107.28
3	A	703	MUR	O5-C5-C4	3.47	115.99	109.69
3	A	703	MUR	C1-O5-C5	3.16	119.63	113.66
3	B	703	MUR	C9-C7-C8	-3.05	109.40	113.35
3	B	703	MUR	C3-C4-C5	2.96	115.96	109.66
3	A	703	MUR	O3-C7-C9	2.73	114.35	107.33
3	B	703	MUR	O3-C3-C4	-2.69	100.14	107.28
3	B	703	MUR	O3-C7-C8	2.52	118.51	111.85
3	A	703	MUR	C1-C2-C3	2.37	114.46	110.14
3	B	703	MUR	O5-C1-C2	-2.26	106.87	109.51
3	B	703	MUR	O3-C3-C2	2.24	114.37	108.89
3	B	703	MUR	O3-C7-C9	-2.09	101.97	107.33

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	703	MUR	C4-C3-O3-C7
3	A	703	MUR	C9-C7-O3-C3
3	A	703	MUR	O5-C5-C6-O6

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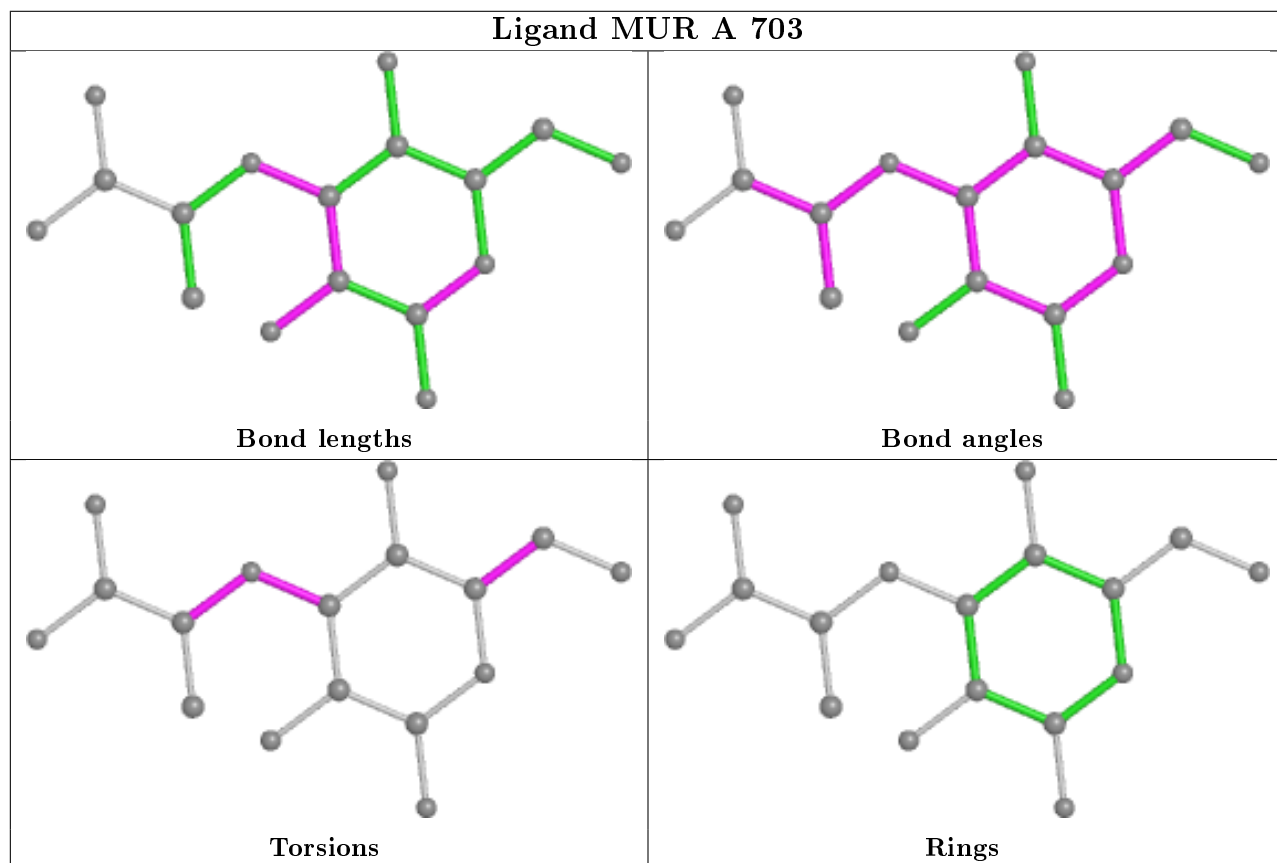
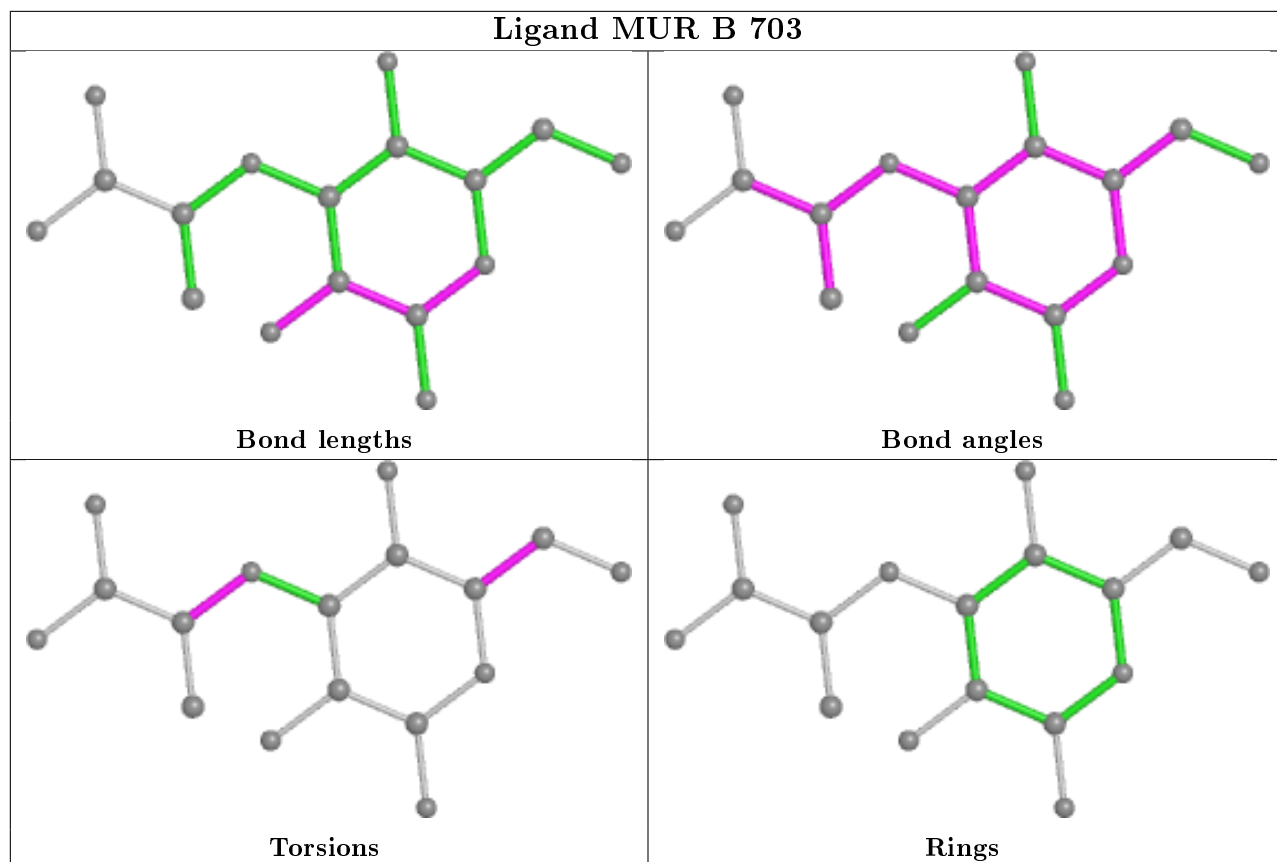
Mol	Chain	Res	Type	Atoms
3	B	703	MUR	O5-C5-C6-O6
3	A	703	MUR	C4-C5-C6-O6
3	B	703	MUR	C4-C5-C6-O6
3	B	703	MUR	C8-C7-O3-C3

There are no ring outliers.

2 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	703	MUR	11	0
3	A	703	MUR	10	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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	638/642 (99%)	-0.01	8 (1%) 77 76	25, 43, 70, 99	0
1	B	635/642 (98%)	0.24	31 (4%) 29 28	28, 47, 81, 111	0
All	All	1273/1284 (99%)	0.11	39 (3%) 49 48	25, 45, 76, 111	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	588	TYR	5.8
1	B	269	TYR	4.4
1	B	272	TYR	4.4
1	B	580	ASN	4.3
1	B	266	GLN	4.0
1	B	446	TYR	3.6
1	B	270	LYS	3.6
1	A	91	ASN	3.6
1	B	267	LYS	3.5
1	B	274	ASP	3.3
1	B	587	ILE	3.2
1	B	264	LEU	3.1
1	B	223	TYR	2.9
1	B	122	MET	2.9
1	B	51	TYR	2.8
1	B	121	GLY	2.8
1	B	275	ASP	2.7
1	B	29	GLU	2.7
1	A	269	TYR	2.6
1	B	265	LYS	2.6
1	A	502	GLN	2.6
1	B	639	LYS	2.5
1	A	51	TYR	2.5
1	B	87	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	642	ALA	2.5
1	A	508	LEU	2.4
1	B	582	THR	2.4
1	A	481	LYS	2.4
1	B	661	ASN	2.4
1	B	583	HIS	2.2
1	B	441	TYR	2.2
1	B	117	VAL	2.2
1	A	272	TYR	2.2
1	A	507	ASN	2.2
1	B	579	VAL	2.1
1	B	439	GLY	2.1
1	B	641	MET	2.1
1	B	276	ALA	2.1
1	B	271	GLY	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](#)

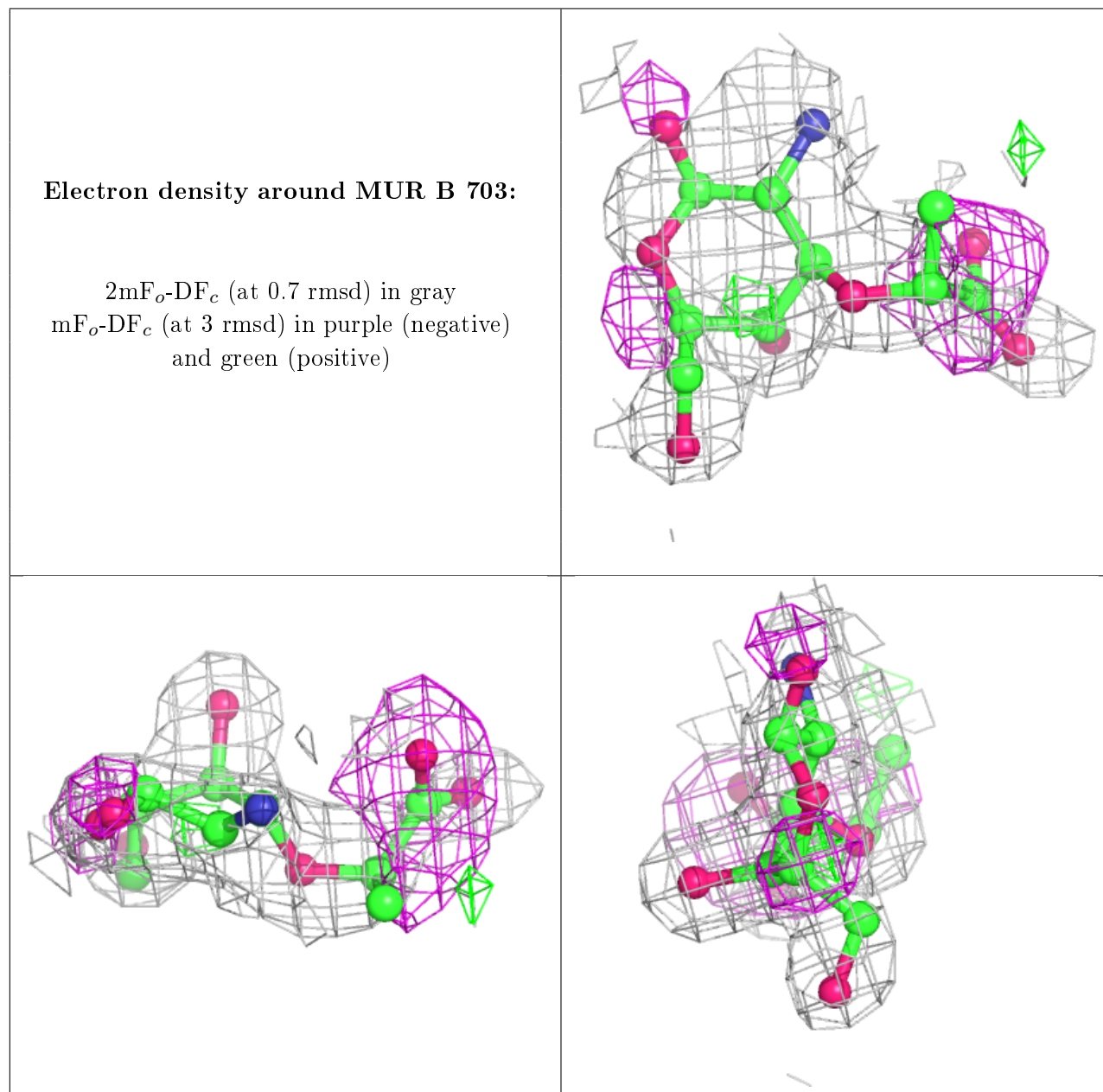
There are no monosaccharides in this entry.

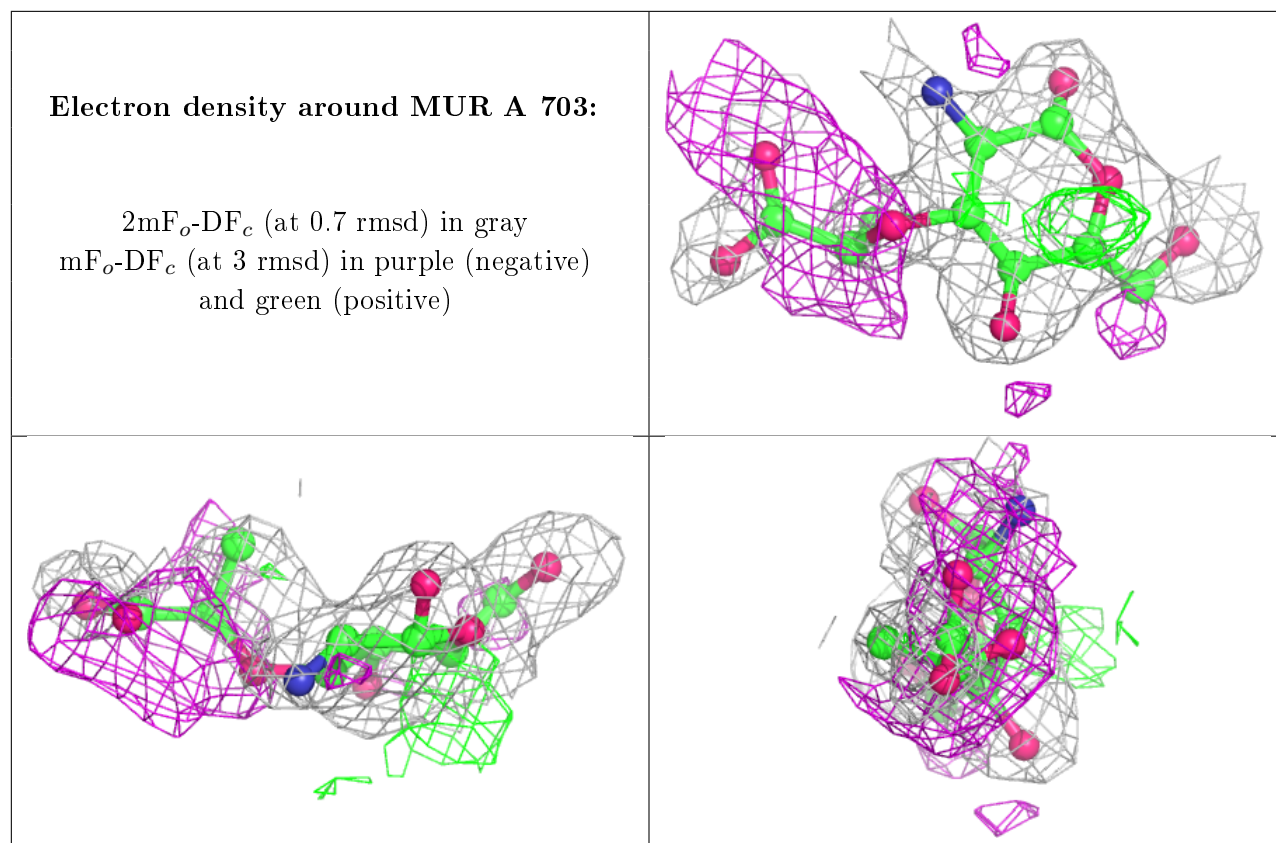
## 6.4 Ligands [i](#)

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
2	CD	B	702	1/1	0.72	0.56	252,252,252,252	0
3	MUR	B	703	17/17	0.79	0.28	27,45,66,68	0
3	MUR	A	703	17/17	0.87	0.28	27,38,63,64	0
2	CD	B	701	1/1	0.87	0.08	121,121,121,121	0
2	CD	A	701	1/1	0.99	0.13	31,31,31,31	0
2	CD	A	704	1/1	1.00	0.15	32,32,32,32	0
2	CD	A	705	1/1	1.00	0.14	34,34,34,34	0
2	CD	A	702	1/1	1.00	0.10	40,40,40,40	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.