



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 08:26 PM BST

PDB ID : 5M1A  
Title : Crystal structure of PBP2a from MRSA in the presence of Ceftriaxone 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 : 2.13.1  
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) : 2.13.1

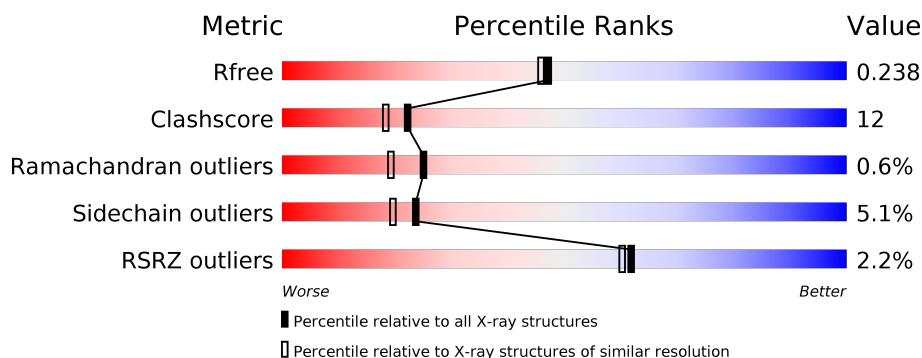
# 1 Overall quality at a glance

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 on 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	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 18%, green 80%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>80%</span> <span>18%</span> <span>•</span> </div> </div>
1	B	642	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 4%, orange 1%, yellow 20%, green 76%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>4%</span> <span>76%</span> <span>20%</span> <span>• •</span> </div> </div>

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
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 10726 atoms, of which 32 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.

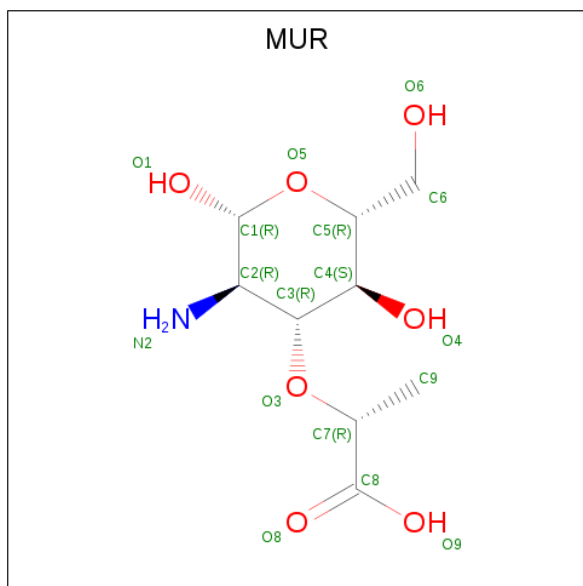
- Molecule 1 is a protein called Penicillin-binding protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	639	Total	C	N	O	S	0	4	0
			5149	3249	868	1016	16			
1	B	635	Total	C	N	O	S	0	3	0
			5105	3218	861	1011	15			

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

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

- 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	H	N	O	0	0
			33	9	16	1	7		
3	B	1	Total	C	H	N	O	0	0
			33	9	16	1	7		

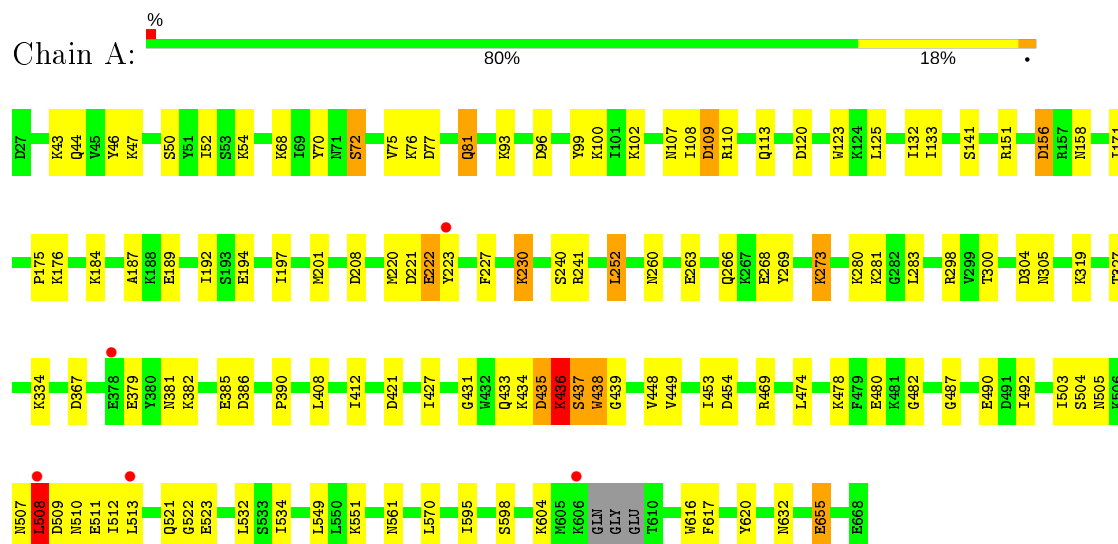
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	211	Total	O	0	0
			211	211		
4	B	189	Total	O	0	0
			189	189		

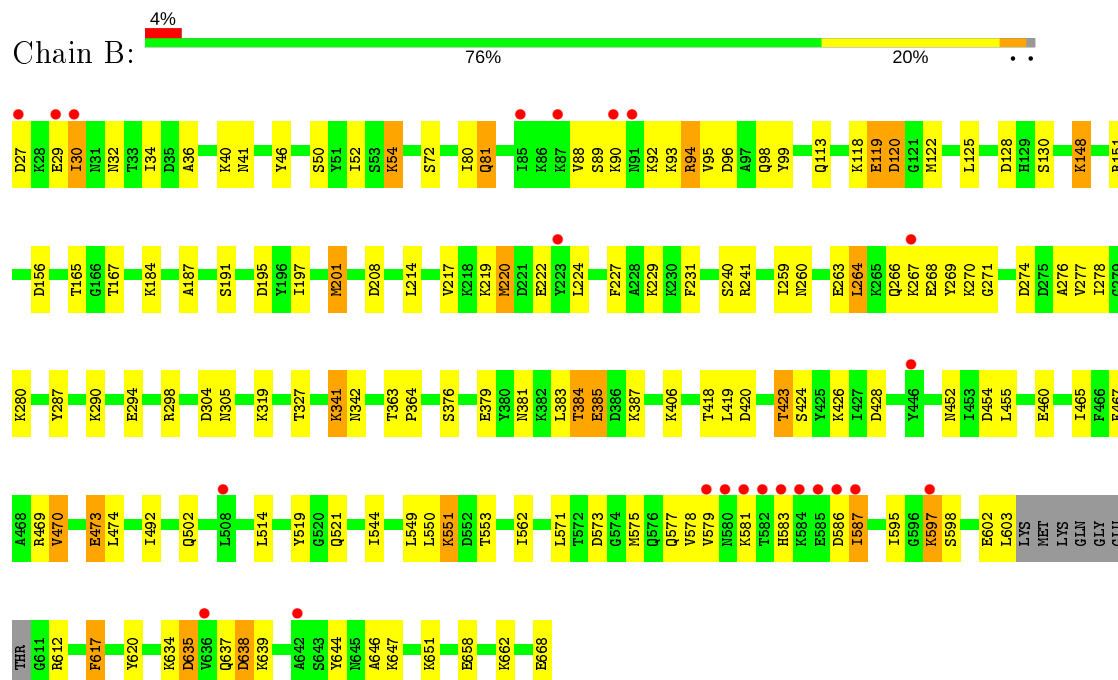
### 3 Residue-property plots

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, $\alpha$ , $\beta$ , $\gamma$	80.74Å 101.91Å 186.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	93.23 – 2.00 93.23 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.6 (93.23-2.00) 97.7 (93.23-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.03	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.52 (at 2.00Å)	Xtriage
Refinement program	PHENIX (dev_2420: ???)	Depositor
R, $R_{free}$	0.203 , 0.238 0.203 , 0.238	Depositor DCC
$R_{free}$ test set	2000 reflections (1.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.6	Xtriage
Anisotropy	0.819	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 46.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10726	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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: MUR, CD

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	0.41	1/5246 (0.0%)	0.55	0/7050
1	B	0.40	1/5199 (0.0%)	0.54	0/6993
All	All	0.40	2/10445 (0.0%)	0.54	0/14043

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	492	ILE	C-N	8.32	1.50	1.34
1	A	492	ILE	C-N	7.67	1.48	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5149	0	5167	109	0
1	B	5105	0	5094	130	1
2	A	4	0	0	0	0
2	B	2	0	0	0	0
3	A	17	16	15	11	0
3	B	17	16	15	10	0
4	A	211	0	0	14	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	189	0	0	7	1
All	All	10694	32	10291	240	2

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 (240) 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:277:VAL:HG11	3:B:703:MUR:H91	1.23	1.20
1:B:578:VAL:HG11	1:B:597:LYS:HA	1.18	1.14
1:B:577:GLN:HB3	1:B:581:LYS:HD3	1.33	1.08
1:A:437:SER:O	1:A:439:GLY:N	1.96	0.99
1:B:587:ILE:HG13	1:B:617:PHE:HE2	1.22	0.98
1:B:277:VAL:CG1	3:B:703:MUR:H91	1.93	0.97
1:B:587:ILE:HG13	1:B:617:PHE:CE2	1.99	0.97
1:B:406:LYS:HE2	1:B:597:LYS:HD2	1.46	0.94
1:B:30:ILE:HD11	1:B:95:VAL:HG21	1.50	0.94
1:B:460:GLU:HG2	1:B:577:GLN:HB2	1.51	0.92
1:A:241:ARG:HD3	3:A:703:MUR:H61	1.49	0.92
1:A:241:ARG:H	3:A:703:MUR:C9	1.86	0.88
1:B:40:LYS:O	4:B:801:HOH:O	1.93	0.87
1:A:508:LEU:O	1:A:510:ASN:N	2.06	0.86
1:B:577:GLN:O	1:B:581:LYS:HG2	1.76	0.86
1:B:658:GLU:HG3	1:B:662:LYS:HD3	1.58	0.85
1:B:578:VAL:CG1	1:B:597:LYS:HA	2.05	0.85
1:A:561:ASN:ND2	4:A:801:HOH:O	2.08	0.85
1:A:151:ARG:HB3	3:A:703:MUR:H62	1.59	0.84
1:A:241:ARG:H	3:A:703:MUR:H92	1.41	0.84
1:B:50:SER:O	1:B:54:LYS:HG2	1.79	0.82
1:A:551[B]:LYS:NZ	4:A:804:HOH:O	2.12	0.81
1:A:434:LYS:HG2	1:A:436:LYS:HE3	1.63	0.81
1:B:420:ASP:H	1:B:423:THR:CG2	1.93	0.81
1:B:553:THR:O	4:B:802:HOH:O	1.99	0.80
1:B:578:VAL:HG11	1:B:597:LYS:CA	2.06	0.79
1:B:406:LYS:HB3	4:B:922:HOH:O	1.84	0.78
1:B:30:ILE:HD11	1:B:95:VAL:CG2	2.13	0.77
1:A:505:ASN:HA	1:A:508:LEU:HD11	1.67	0.77
1:B:27:ASP:OD2	1:B:93:LYS:NZ	2.14	0.76
1:B:298:ARG:HD2	4:B:851:HOH:O	1.85	0.74
1:B:376:SER:OG	1:B:379:GLU:HG3	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:GLU:HA	1:B:32[A]:ASN:OD1	1.88	0.74
3:B:703:MUR:H93	3:B:703:MUR:HN22	1.51	0.74
1:B:381:ASN:HA	1:B:384:THR:HG22	1.68	0.74
1:A:93:LYS:HE3	1:A:123:TRP:CZ2	2.24	0.73
1:B:406:LYS:CE	1:B:597:LYS:HD2	2.20	0.72
1:B:419:LEU:HD12	1:B:423:THR:HG21	1.70	0.72
1:B:263:GLU:HA	1:B:266:GLN:HG3	1.71	0.71
1:B:294:GLU:OE1	1:B:319:LYS:HE3	1.93	0.69
1:B:634:LYS:O	1:B:635:ASP:HB2	1.93	0.69
1:B:290:LYS:NZ	4:B:803:HOH:O	2.13	0.69
1:A:434:LYS:HB3	1:A:435:ASP:HA	1.74	0.69
1:A:504:SER:HB3	1:A:507:ASN:HB2	1.75	0.69
1:B:270:LYS:C	1:B:270:LYS:HE2	2.13	0.69
1:B:419:LEU:HD12	1:B:423:THR:CG2	2.23	0.68
1:B:639:LYS:O	1:B:644:TYR:HB2	1.94	0.68
1:A:522:GLY:O	1:A:604:LYS:NZ	2.22	0.68
1:A:184:LYS:NZ	1:A:194:GLU:OE2	2.18	0.68
1:A:433:GLN:HG3	1:A:435:ASP:HB2	1.76	0.68
1:A:113:GLN:OE1	4:A:803:HOH:O	2.12	0.68
1:A:655:GLU:HG3	4:A:841:HOH:O	1.95	0.67
1:A:454:ASP:OD1	4:A:805:HOH:O	2.12	0.67
1:B:602:GLU:HG2	1:B:603:LEU:H	1.59	0.66
1:A:431:GLY:O	4:A:806:HOH:O	2.12	0.66
1:B:264:LEU:HD11	1:B:274:ASP:HA	1.79	0.65
1:A:305:ASN:HB3	1:B:72[A]:SER:OG	1.96	0.65
1:B:94:ARG:NH1	1:B:96:ASP:OD2	2.30	0.65
3:B:703:MUR:H93	3:B:703:MUR:N2	2.12	0.64
1:B:263:GLU:OE2	1:B:280:LYS:NZ	2.29	0.64
1:B:119:GLU:OE1	1:B:122:MET:N	2.25	0.63
1:B:277:VAL:HG11	3:B:703:MUR:C9	2.15	0.63
1:A:43:LYS:O	1:A:47:LYS:HG3	1.98	0.63
1:B:267:LYS:HG3	1:B:268:GLU:H	1.64	0.63
1:A:334:LYS:NZ	4:A:802:HOH:O	2.10	0.62
1:B:270:LYS:HE2	1:B:271:GLY:N	2.15	0.62
1:A:505:ASN:HA	1:A:508:LEU:CD1	2.30	0.62
1:B:267:LYS:HG3	1:B:268:GLU:N	2.16	0.61
1:B:420:ASP:H	1:B:423:THR:HG22	1.64	0.61
1:A:93:LYS:HG3	1:A:123:TRP:CH2	2.34	0.61
1:A:598:SER:HB3	1:A:617:PHE:CD2	2.36	0.61
1:B:419:LEU:HD21	1:B:455:LEU:HD13	1.82	0.61
1:B:617:PHE:CD2	1:B:646:ALA:HA	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:ILE:HD11	1:A:220:MET:HE1	1.82	0.61
3:A:703:MUR:H2	3:A:703:MUR:H93	1.83	0.60
1:B:467:PHE:HA	1:B:470:VAL:HG13	1.83	0.60
1:A:434:LYS:HB3	1:A:435:ASP:CA	2.32	0.59
1:B:419:LEU:HA	1:B:423:THR:HG21	1.84	0.59
1:A:252:LEU:HD22	1:A:283:LEU:HG	1.84	0.58
1:B:637:GLN:HG2	1:B:638:ASP:H	1.69	0.58
1:A:273:LYS:N	1:A:273:LYS:HD2	2.18	0.58
1:B:658:GLU:HG3	1:B:662:LYS:CD	2.31	0.57
1:A:100:LYS:HE3	1:A:109:ASP:OD1	2.05	0.57
1:A:319:LYS:NZ	4:A:814:HOH:O	2.38	0.57
1:A:510:ASN:ND2	1:A:513:LEU:HD23	2.20	0.57
1:A:158:ASN:HA	1:B:551:LYS:HE3	1.87	0.57
1:B:603:LEU:CD2	1:B:612:ARG:HB2	2.35	0.56
1:A:189:GLU:HG2	1:A:227:PHE:CE1	2.39	0.56
1:A:44:GLN:HA	1:A:44:GLN:OE1	2.06	0.56
1:A:421:ASP:HB3	1:A:570:LEU:HD21	1.87	0.56
1:B:418:THR:HG21	1:B:474:LEU:HD23	1.88	0.56
1:A:438:TRP:HA	1:A:512:ILE:HD11	1.87	0.56
1:B:658:GLU:CG	1:B:662:LYS:HD3	2.35	0.56
1:A:141:SER:OG	4:A:807:HOH:O	2.17	0.56
1:A:187:ALA:HB1	1:A:192:ILE:O	2.06	0.56
1:B:644:TYR:O	1:B:647:LYS:HB3	2.05	0.56
1:B:220:MET:HA	1:B:220:MET:CE	2.35	0.55
1:A:298:ARG:HG2	1:A:300:THR:HG23	1.89	0.55
1:A:171:ILE:HG12	1:A:220:MET:HE3	1.87	0.55
1:B:80:ILE:HA	1:B:98:GLN:O	2.07	0.55
1:A:221:ASP:OD1	1:A:223:TYR:HB3	2.07	0.54
1:A:480:GLU:OE2	1:A:508:LEU:HD13	2.07	0.54
1:A:230:LYS:HZ2	1:A:230:LYS:HB3	1.72	0.54
1:A:327:THR:OG1	1:A:549:LEU:HA	2.08	0.54
1:B:595:ILE:HD11	1:B:620:TYR:CZ	2.43	0.54
1:A:595:ILE:HD11	1:A:620:TYR:CZ	2.43	0.53
1:A:510:ASN:HD22	1:A:513:LEU:HD23	1.73	0.53
1:A:187:ALA:HB2	1:A:197:ILE:HD12	1.90	0.53
1:A:427:ILE:HD12	1:A:453:ILE:HD12	1.91	0.53
1:B:602:GLU:HG2	1:B:603:LEU:N	2.24	0.53
1:B:603:LEU:HD23	1:B:612:ARG:HB2	1.91	0.53
1:A:241:ARG:HB2	3:A:703:MUR:H4	1.91	0.52
1:B:578:VAL:HG21	1:B:597:LYS:HG2	1.91	0.52
1:A:434:LYS:NZ	1:A:436:LYS:HE3	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:MET:HE1	1:B:224:LEU:HD13	1.90	0.52
1:B:424:SER:OG	1:B:452:ASN:HB3	2.10	0.52
1:B:241:ARG:HD3	3:B:703:MUR:H62	1.91	0.51
3:A:703:MUR:H2	3:A:703:MUR:C9	2.40	0.51
1:B:187:ALA:HB2	1:B:197:ILE:HD12	1.91	0.51
1:B:595:ILE:HD11	1:B:620:TYR:OH	2.09	0.51
1:B:637:GLN:HG2	1:B:638:ASP:N	2.25	0.51
1:A:222:GLU:CD	1:A:222:GLU:H	2.14	0.51
1:A:433:GLN:CG	1:A:435:ASP:HB2	2.40	0.51
1:A:132:ILE:HG22	1:A:133:ILE:HG12	1.93	0.51
1:A:386:ASP:HB3	1:A:390:PRO:HD2	1.92	0.51
1:A:449:VAL:O	1:A:453:ILE:HD11	2.12	0.50
1:A:46:TYR:O	1:A:54:LYS:HD3	2.10	0.50
1:A:241:ARG:HB2	3:A:703:MUR:H92	1.93	0.50
1:A:487:GLY:O	1:A:490:GLU:HG2	2.12	0.50
1:B:418:THR:OG1	1:B:473:GLU:HG2	2.11	0.50
1:B:617:PHE:CE2	1:B:646:ALA:HA	2.47	0.50
1:A:448:VAL:O	1:A:448:VAL:HG13	2.12	0.49
1:B:612:ARG:HG2	1:B:637:GLN:NE2	2.27	0.49
1:B:617:PHE:HD2	1:B:646:ALA:HA	1.77	0.49
1:B:327:THR:OG1	1:B:549:LEU:HA	2.13	0.49
1:A:240:SER:HA	3:A:703:MUR:H93	1.94	0.49
1:A:52:ILE:HG22	4:A:821:HOH:O	2.13	0.49
1:B:191:SER:HB3	1:B:376:SER:HB3	1.94	0.49
1:B:647:LYS:HD3	1:B:651:LYS:HZ1	1.78	0.49
1:B:259:ILE:HG22	1:B:276:ALA:O	2.13	0.48
1:B:46:TYR:CZ	1:B:54:LYS:HE3	2.48	0.48
1:A:379:GLU:OE1	4:A:808:HOH:O	2.20	0.48
1:A:521:GLN:HA	1:A:604:LYS:HZ1	1.77	0.48
1:B:259:ILE:HG13	1:B:263:GLU:HG3	1.94	0.48
1:A:280:LYS:NZ	4:A:824:HOH:O	2.46	0.48
1:A:230:LYS:HZ2	1:A:230:LYS:CB	2.26	0.48
1:A:241:ARG:CB	3:A:703:MUR:H92	2.43	0.48
1:B:363:THR:HA	1:B:364:PRO:C	2.34	0.48
1:B:381:ASN:HA	1:B:384:THR:CG2	2.40	0.48
1:A:175:PRO:HG3	1:A:201:MET:CE	2.44	0.48
1:A:304:ASP:O	1:A:305:ASN:HB2	2.14	0.47
1:A:505:ASN:C	1:A:507:ASN:H	2.18	0.47
1:A:50:SER:O	1:A:54:LYS:HG3	2.13	0.47
1:A:72:SER:HB2	1:B:305:ASN:O	2.14	0.47
1:B:151:ARG:HD2	3:B:703:MUR:O9	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:MET:HE1	1:B:224:LEU:CD1	2.43	0.47
1:A:434:LYS:CB	1:A:435:ASP:HA	2.38	0.47
1:B:418:THR:HG23	4:B:915:HOH:O	2.13	0.47
1:A:474:LEU:O	1:A:478:LYS:HG3	2.14	0.47
1:B:381:ASN:CA	1:B:384:THR:HG22	2.42	0.47
1:B:240:SER:HA	3:B:703:MUR:O1	2.14	0.47
1:B:201:MET:HE1	1:B:214:LEU:HD21	1.95	0.47
1:A:381:ASN:HB3	1:A:385:GLU:OE1	2.15	0.47
1:B:418:THR:HG21	1:B:474:LEU:CD2	2.44	0.47
1:B:583:HIS:HB3	1:B:586:ASP:HB2	1.97	0.47
1:B:544:ILE:HD11	1:B:562:ILE:HD13	1.97	0.46
1:B:420:ASP:O	1:B:423:THR:HG23	2.16	0.46
1:A:508:LEU:C	1:A:510:ASN:N	2.69	0.46
1:A:81:GLN:HB3	1:A:81:GLN:HE21	1.59	0.45
1:B:598:SER:HB2	1:B:617:PHE:CG	2.51	0.45
1:A:102:LYS:HG2	1:A:107:ASN:OD1	2.15	0.45
1:B:36:ALA:HB1	1:B:41:ASN:HB2	1.98	0.45
1:A:68:LYS:HE2	4:A:1001:HOH:O	2.16	0.45
1:B:227:PHE:CE1	1:B:231:PHE:CE1	3.04	0.45
1:B:612:ARG:HG2	1:B:637:GLN:HE22	1.81	0.45
1:B:165:THR:HA	3:B:703:MUR:H61	1.98	0.45
1:B:577:GLN:HB3	1:B:581:LYS:CD	2.25	0.44
1:B:387:LYS:HE3	1:B:612:ARG:HH22	1.82	0.44
1:A:421:ASP:CB	1:A:570:LEU:HD21	2.46	0.44
1:A:189:GLU:HG2	1:A:227:PHE:CD1	2.53	0.44
1:A:480:GLU:HB3	1:A:505:ASN:OD1	2.17	0.44
1:B:229:LYS:HB2	1:B:229:LYS:HE3	1.59	0.44
1:B:579:VAL:HG21	1:B:595:ILE:HA	1.99	0.44
1:B:579:VAL:HG13	1:B:587:ILE:HG22	1.99	0.44
1:B:587:ILE:CG1	1:B:617:PHE:HE2	2.11	0.43
1:B:519:TYR:CE2	1:B:521:GLN:HG3	2.53	0.43
1:B:381:ASN:OD1	1:B:384:THR:HG21	2.18	0.43
1:B:598:SER:HB2	1:B:617:PHE:CD2	2.53	0.43
1:A:595:ILE:HD11	1:A:620:TYR:OH	2.18	0.43
1:B:220:MET:HA	1:B:220:MET:HE2	2.01	0.43
1:A:70:TYR:CD1	1:A:75:VAL:HG21	2.54	0.43
1:B:128:ASP:OD1	1:B:130:SER:HB2	2.18	0.43
1:B:381:ASN:O	1:B:385:GLU:HB2	2.19	0.43
1:A:171:ILE:HD11	1:A:220:MET:CE	2.46	0.43
1:B:118:LYS:HA	1:B:122:MET:O	2.19	0.43
1:B:571:LEU:O	1:B:575:MET:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:GLU:HA	1:B:266:GLN:CG	2.46	0.43
1:B:420:ASP:H	1:B:423:THR:HG21	1.80	0.43
1:A:268:GLU:HG3	1:A:269:TYR:CD2	2.54	0.42
1:A:386:ASP:HB3	1:A:390:PRO:CD	2.48	0.42
1:B:30:ILE:O	1:B:34:ILE:HG13	2.19	0.42
1:B:465:ILE:O	1:B:469:ARG:HG3	2.19	0.42
1:B:95:VAL:O	1:B:113:GLN:HA	2.19	0.42
1:A:435:ASP:C	1:A:436:LYS:HG3	2.39	0.42
1:B:426:LYS:HG2	1:B:452:ASN:OD1	2.18	0.42
1:B:119:GLU:CD	1:B:120:ASP:N	2.73	0.42
1:B:148:LYS:HD3	1:B:148:LYS:HA	1.79	0.42
1:A:503:ILE:O	1:A:503:ILE:HG23	2.20	0.42
1:B:259:ILE:HD11	1:B:264:LEU:HA	2.01	0.42
1:B:269:TYR:CZ	1:B:278:ILE:HD12	2.54	0.42
1:B:81:GLN:HG2	1:B:81:GLN:H	1.75	0.42
1:A:408:LEU:HD22	1:A:534:ILE:HG21	2.01	0.42
1:B:304:ASP:O	1:B:305:ASN:HB2	2.19	0.42
1:A:100:LYS:HA	1:A:108:ILE:O	2.20	0.41
1:A:434:LYS:HZ2	1:A:436:LYS:HE3	1.85	0.41
1:B:217:VAL:HG21	1:B:220:MET:HE3	2.01	0.41
1:B:260:ASN:OD1	1:B:263:GLU:HG2	2.20	0.41
1:A:184:LYS:HA	1:A:184:LYS:HD2	1.72	0.41
1:B:597:LYS:HB2	1:B:597:LYS:HE3	1.64	0.41
1:B:89:SER:HB2	1:B:92:LYS:HB2	2.02	0.41
1:A:412:ILE:HG23	1:A:482:GLY:HA3	2.02	0.41
1:B:341:LYS:HG2	1:B:342:ASN:N	2.35	0.41
1:A:110:ARG:NH1	4:A:812:HOH:O	2.35	0.41
1:A:334:LYS:HE3	1:A:334:LYS:HB2	1.78	0.41
1:B:220:MET:HA	1:B:220:MET:HE3	2.01	0.41
1:B:454:ASP:HB2	4:B:932:HOH:O	2.20	0.41
1:B:287:TYR:CZ	1:B:550:LEU:HD11	2.55	0.41
3:B:703:MUR:H93	3:B:703:MUR:C2	2.50	0.41
1:A:241:ARG:H	3:A:703:MUR:H93	1.79	0.41
1:A:507:ASN:ND2	1:A:523:GLU:HB2	2.36	0.41
1:A:616:TRP:CZ3	1:A:632:ASN:HB2	2.56	0.41
1:A:260:ASN:OD1	1:A:263:GLU:HG3	2.21	0.41
1:A:434:LYS:NZ	1:A:436:LYS:CE	2.84	0.41
1:A:434:LYS:NZ	1:A:511:GLU:OE2	2.49	0.41
1:A:273:LYS:N	1:A:273:LYS:CD	2.83	0.40
1:A:305:ASN:O	1:B:72[A]:SER:HB3	2.22	0.40
1:A:507:ASN:HD21	1:A:523:GLU:HB2	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:LYS:O	1:A:281:LYS:HG2	2.21	0.40
1:A:156:ASP:OD1	1:A:156:ASP:C	2.60	0.40
1:A:76:LYS:HB2	1:A:77:ASP:H	1.65	0.40

All (2) 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:B:88:VAL:O	1:B:184:LYS:NZ[1_655]	2.17	0.03
4:A:818:HOH:O	4:B:926:HOH:O[2_555]	2.17	0.03

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	639/642 (100%)	616 (96%)	17 (3%)	6 (1%)	17	11
1	B	634/642 (99%)	611 (96%)	21 (3%)	2 (0%)	41	37
All	All	1273/1284 (99%)	1227 (96%)	38 (3%)	8 (1%)	25	19

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	437	SER
1	A	438	TRP
1	A	508	LEU
1	B	635	ASP
1	A	120	ASP
1	B	120	ASP
1	A	509	ASP
1	A	436	LYS

### 5.3.2 Protein sidechains ⓘ

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	574/572 (100%)	552 (96%)	22 (4%)	33	31
1	B	568/572 (99%)	532 (94%)	36 (6%)	18	13
All	All	1142/1144 (100%)	1084 (95%)	58 (5%)	24	19

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	SER
1	A	81	GLN
1	A	96	ASP
1	A	99	TYR
1	A	109	ASP
1	A	125	LEU
1	A	156	ASP
1	A	176	LYS
1	A	208	ASP
1	A	222	GLU
1	A	230	LYS
1	A	252	LEU
1	A	266	GLN
1	A	273	LYS
1	A	367	ASP
1	A	382	LYS
1	A	435	ASP
1	A	436	LYS
1	A	469	ARG
1	A	508	LEU
1	A	532	LEU
1	A	655	GLU
1	B	30	ILE
1	B	52	ILE
1	B	54	LYS
1	B	81	GLN
1	B	90	LYS

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Mol	Chain	Res	Type
1	B	94	ARG
1	B	99	TYR
1	B	119	GLU
1	B	125	LEU
1	B	148	LYS
1	B	156	ASP
1	B	167	THR
1	B	195	ASP
1	B	201	MET
1	B	208	ASP
1	B	219	LYS
1	B	220	MET
1	B	222	GLU
1	B	264	LEU
1	B	341	LYS
1	B	383	LEU
1	B	384	THR
1	B	385	GLU
1	B	423	THR
1	B	428	ASP
1	B	470	VAL
1	B	473	GLU
1	B	502	GLN
1	B	514	LEU
1	B	551	LYS
1	B	573	ASP
1	B	587	ILE
1	B	597	LYS
1	B	617	PHE
1	B	638	ASP
1	B	668	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	377	ASN
1	B	81	GLN

### 5.3.3 RNA ⓘ

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	A	703	-	14,17,17	1.78	4 (28%)	19,24,24	2.88	8 (42%)
3	MUR	B	703	-	14,17,17	1.64	4 (28%)	19,24,24	1.91	6 (31%)

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	A	703	-	-	4/6/30/30	0/1/1/1
3	MUR	B	703	-	-	2/6/30/30	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	703	MUR	C2-N2	3.74	1.53	1.47
3	A	703	MUR	O5-C1	3.36	1.51	1.42
3	B	703	MUR	C2-N2	2.90	1.51	1.47
3	B	703	MUR	O5-C1	2.79	1.49	1.42
3	A	703	MUR	O3-C3	2.78	1.51	1.43
3	B	703	MUR	C9-C7	2.46	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	703	MUR	C3-C2	-2.16	1.48	1.53
3	B	703	MUR	C3-C2	-2.02	1.48	1.53

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	703	MUR	C9-C7-C8	-7.68	103.42	113.35
3	A	703	MUR	O5-C1-C2	6.22	116.76	109.51
3	B	703	MUR	O5-C5-C4	4.65	118.14	109.69
3	A	703	MUR	O3-C3-C4	3.78	117.34	107.28
3	B	703	MUR	C6-C5-C4	-3.05	105.86	113.00
3	B	703	MUR	C4-C3-C2	3.01	117.32	111.37
3	A	703	MUR	O5-C5-C4	2.96	115.08	109.69
3	B	703	MUR	C3-C4-C5	2.86	115.76	109.66
3	A	703	MUR	O3-C7-C9	2.66	114.16	107.33
3	B	703	MUR	C1-C2-C3	2.41	114.55	110.14
3	B	703	MUR	C9-C7-C8	-2.27	110.42	113.35
3	A	703	MUR	C1-O5-C5	2.24	117.88	113.66
3	A	703	MUR	O3-C7-C8	2.14	117.52	111.85
3	A	703	MUR	C1-C2-C3	2.04	113.86	110.14

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	703	MUR	C9-C7-O3-C3
3	A	703	MUR	O5-C5-C6-O6
3	A	703	MUR	C4-C5-C6-O6
3	B	703	MUR	O5-C5-C6-O6
3	A	703	MUR	C8-C7-O3-C3
3	B	703	MUR	C4-C5-C6-O6

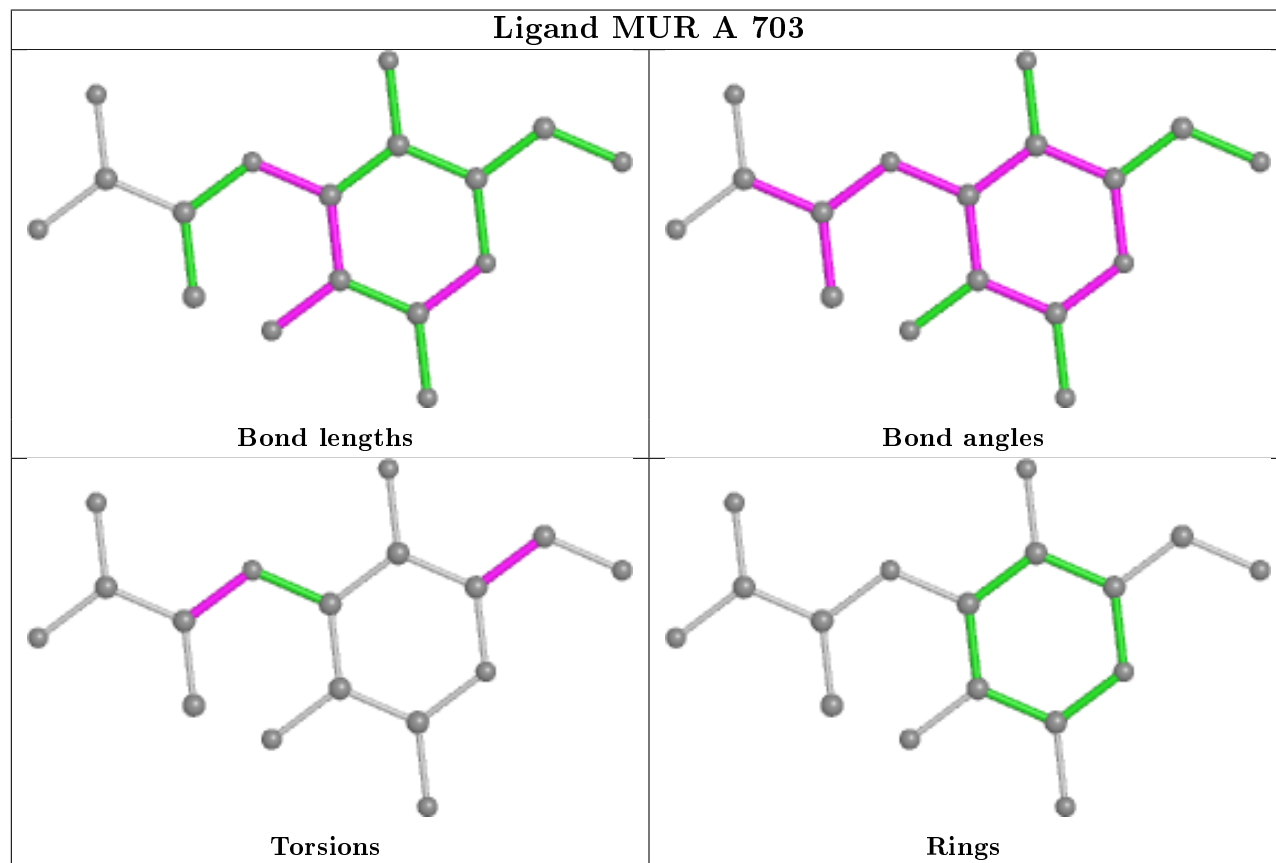
There are no ring outliers.

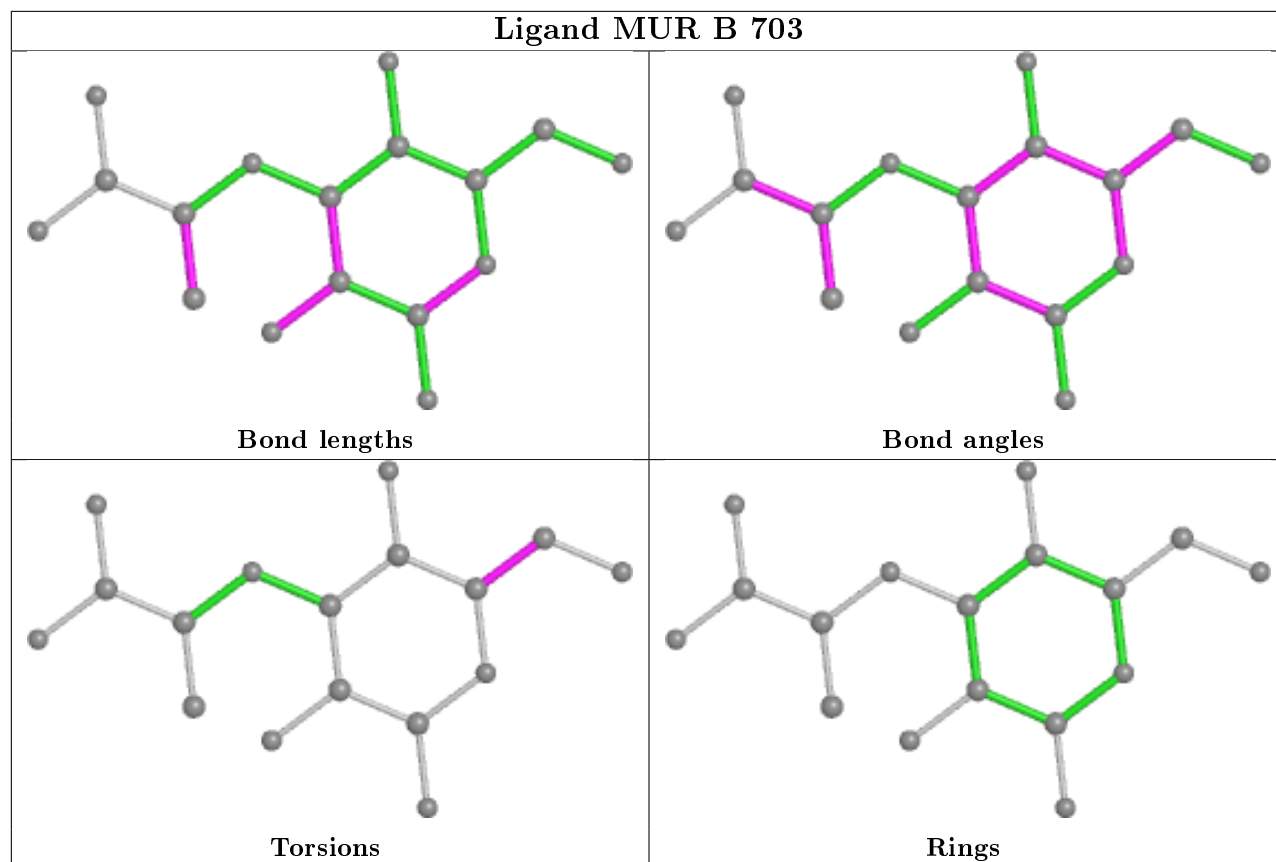
2 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	703	MUR	11	0
3	B	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	639/642 (99%)	0.17	5 (0%) 86 85	29, 49, 77, 107	0
1	B	635/642 (98%)	0.28	23 (3%) 42 42	30, 53, 89, 118	0
All	All	1274/1284 (99%)	0.23	28 (2%) 62 60	29, 51, 84, 118	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	606	LYS	5.1
1	B	587	ILE	5.0
1	A	508	LEU	4.0
1	B	585	GLU	3.8
1	B	223	TYR	3.5
1	B	446	TYR	3.5
1	B	642	ALA	3.4
1	B	580	ASN	3.4
1	B	586	ASP	3.3
1	B	582	THR	3.2
1	B	29	GLU	3.2
1	B	267	LYS	3.0
1	B	27	ASP	2.9
1	B	583	HIS	2.8
1	B	584	LYS	2.8
1	B	30	ILE	2.8
1	B	87	LYS	2.7
1	B	85	ILE	2.6
1	B	579	VAL	2.5
1	B	90	LYS	2.5
1	B	91	ASN	2.3
1	B	508	LEU	2.2
1	A	223	TYR	2.2
1	A	513	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	636	VAL	2.2
1	B	581	LYS	2.1
1	B	597	LYS	2.1
1	A	378	GLU	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](#)

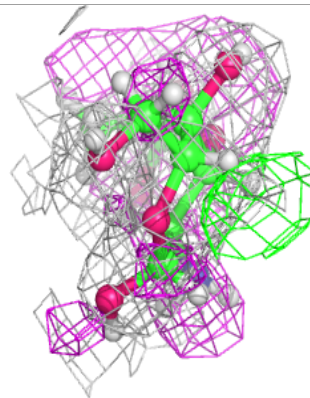
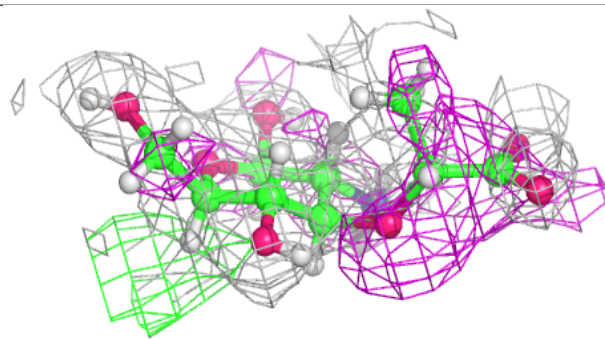
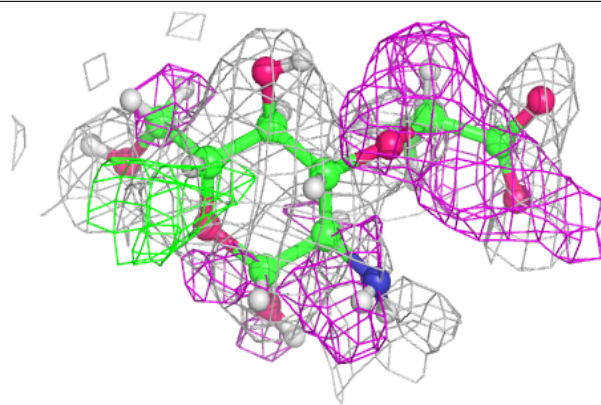
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MUR	A	703	17/17	0.76	0.32	42,60,75,78	0
3	MUR	B	703	17/17	0.81	0.27	39,65,87,90	0
2	CD	B	701	1/1	0.84	0.08	123,123,123,123	0
2	CD	B	702	1/1	0.98	0.04	83,83,83,83	0
2	CD	A	701	1/1	1.00	0.19	37,37,37,37	0
2	CD	A	705	1/1	1.00	0.19	40,40,40,40	0
2	CD	A	702	1/1	1.00	0.18	46,46,46,46	0
2	CD	A	704	1/1	1.00	0.19	37,37,37,37	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 MUR A 703:**

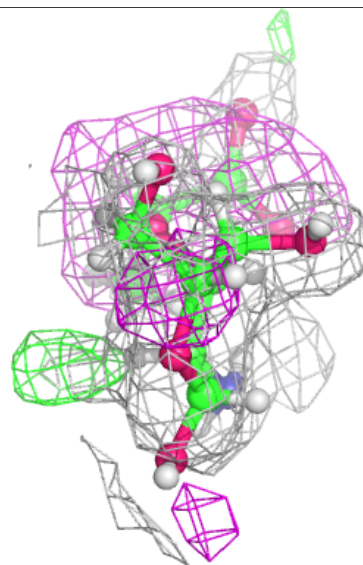
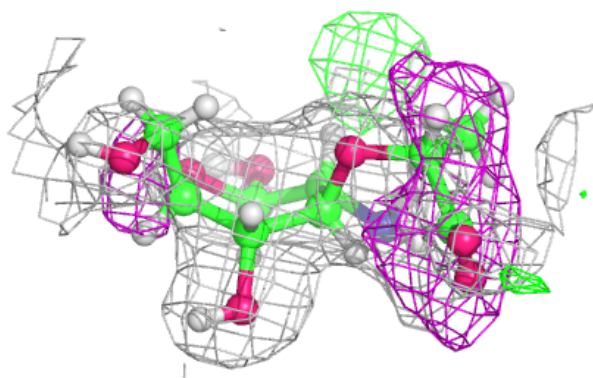
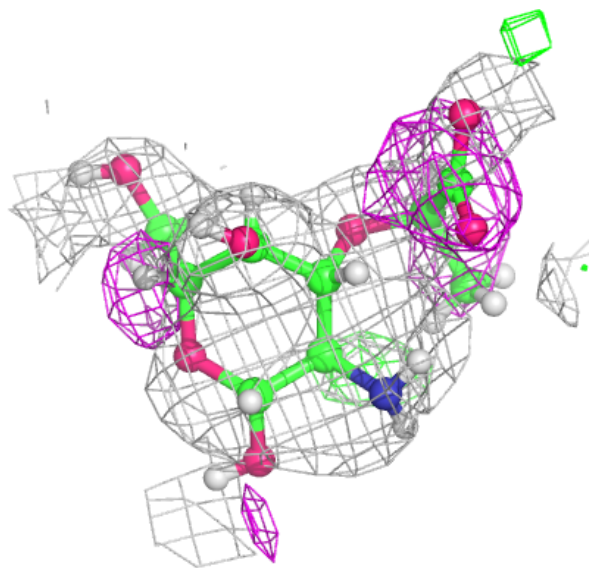
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around MUR B 703:**

$2mF_o-DF_c$  (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.