



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 26, 2018 – 03:42 PM EST

PDB ID : 5M18  
Title : Crystal structure of PBP2a from MRSA in the presence of Cefepime ligand  
Authors : Molina, R.; Batuecas, M.T.; Hermoso, J.A.  
Deposited on : 2016-10-07  
Resolution : 1.98 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030736  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030736

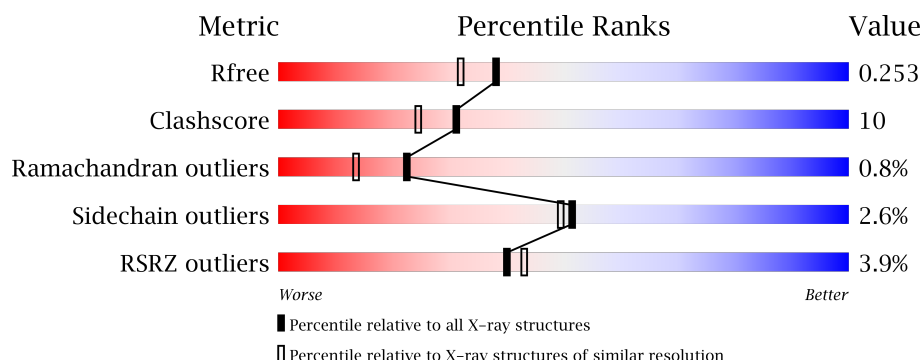
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.98 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))
$R_{free}$	100719	9293 (2.00-1.96)
Clashscore	112137	10621 (2.00-1.96)
Ramachandran outliers	110173	10502 (2.00-1.96)
Sidechain outliers	110143	10501 (2.00-1.96)
RSRZ outliers	101464	9395 (2.00-1.96)

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. 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>2%</div> <div>80%</div> <div>18%</div> <div>.</div> </div>
1	B	642	<div> <div>6%</div> <div>77%</div> <div>21%</div> <div>..</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	X
3	MUR	B	702	-	-	X	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10732 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.

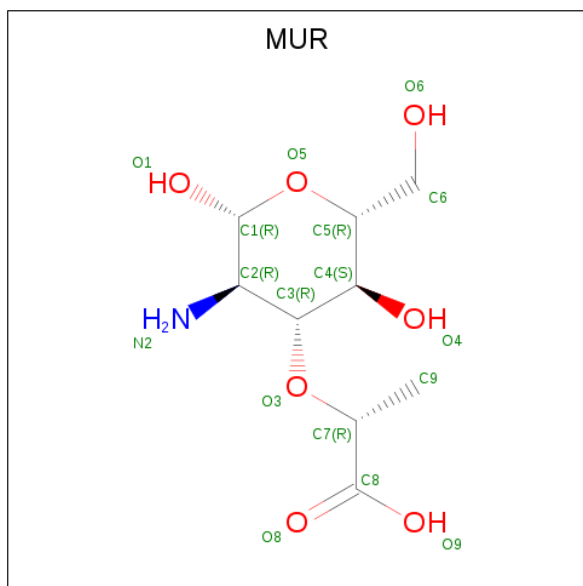
- Molecule 1 is a protein called Penicillin-binding protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	640	Total	C	N	O	S	0	4	0
			5157	3252	868	1021	16			
1	B	635	Total	C	N	O	S	0	5	0
			5125	3232	866	1012	15			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cd	0	0
			1	1		
2	A	4	Total	Cd	0	0
			4	4		

- Molecule 3 is 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		

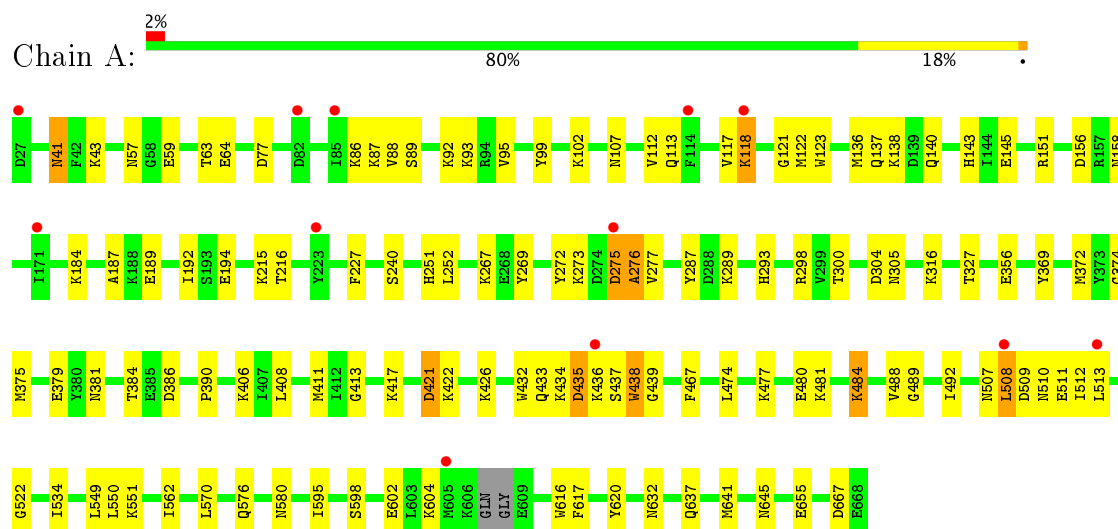
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	232	Total	O	0	0
			232	232		
4	B	179	Total	O	0	0
			179	179		

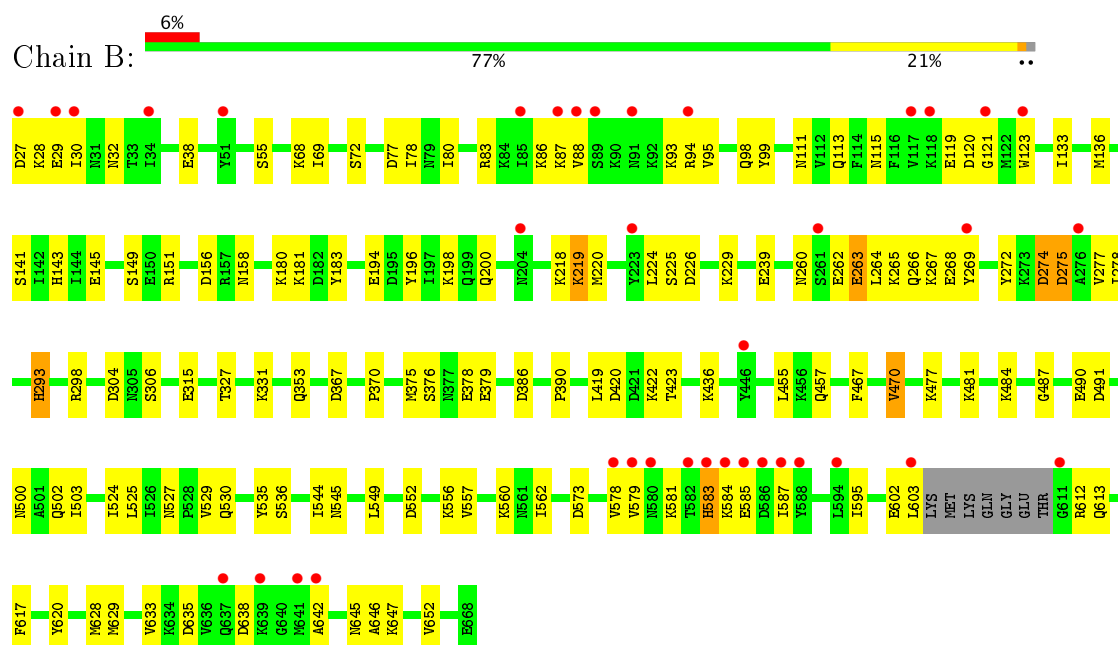
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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, $\alpha$ , $\beta$ , $\gamma$	80.62Å 101.19Å 186.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	93.31 – 1.98 93.31 – 1.98	Depositor EDS
% Data completeness (in resolution range)	93.7 (93.31-1.98) 93.7 (93.31-1.98)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.46 (at 1.98Å)	Xtriage
Refinement program	PHENIX (dev_2420: ???)	Depositor
R, $R_{free}$	0.205 , 0.253 0.205 , 0.253	Depositor DCC
$R_{free}$ test set	1991 reflections (1.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.7	Xtriage
Anisotropy	0.840	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 47.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10732	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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	0.44	1/5254 (0.0%)	0.62	1/7062 (0.0%)
1	B	0.42	0/5223	0.60	1/7023 (0.0%)
All	All	0.43	1/10477 (0.0%)	0.61	2/14085 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	492	ILE	C-N	5.20	1.44	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	275	ASP	CB-CG-OD1	9.13	126.52	118.30
1	B	274	ASP	C-N-CA	6.55	138.08	121.70

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	5157	0	5164	110	0
1	B	5125	0	5126	103	0
2	A	4	0	0	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
3	A	17	0	15	8	0
3	B	17	0	15	8	0
4	A	232	0	0	9	0
4	B	179	0	0	7	0
All	All	10732	0	10320	213	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 10.

All (213) 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:118:LYS:HE3	1:A:122:MET:C	1.70	1.10
1:B:274:ASP:H	1:B:275:ASP:HB3	1.20	1.03
1:A:118:LYS:NZ	1:A:122:MET:N	2.08	0.99
1:B:293:HIS:CE1	3:B:702:MUR:H91	2.02	0.94
1:A:118:LYS:NZ	1:A:121:GLY:C	2.22	0.92
1:A:118:LYS:HZ3	1:A:121:GLY:C	1.76	0.89
1:B:419:LEU:HD12	1:B:423:THR:HG21	1.53	0.87
1:A:437:SER:O	1:A:439:GLY:N	2.08	0.86
1:A:433:GLN:HG3	1:A:435:ASP:HB2	1.57	0.85
1:A:273:LYS:HE3	1:A:275:ASP:HB3	1.58	0.84
1:A:118:LYS:HZ1	1:A:122:MET:N	1.71	0.84
1:A:118:LYS:CE	1:A:122:MET:C	2.47	0.82
1:A:289:LYS:NZ	4:A:803:HOH:O	2.14	0.80
1:B:491:ASP:OD2	4:B:801:HOH:O	2.00	0.80
1:A:118:LYS:CE	1:A:122:MET:N	2.45	0.79
1:A:118:LYS:HZ1	1:A:122:MET:CA	1.96	0.79
1:A:411:MET:HE1	1:A:562:ILE:HD12	1.66	0.76
1:A:118:LYS:HE3	1:A:122:MET:O	1.85	0.76
1:A:277:VAL:HB	3:A:703:MUR:H7	1.66	0.75
1:A:137:GLN:H	1:A:140:GLN:NE2	1.84	0.75
1:A:508:LEU:O	1:A:510:ASN:N	2.20	0.74
1:B:274:ASP:N	1:B:275:ASP:HB3	1.99	0.73
1:B:151:ARG:HB2	3:B:702:MUR:H93	1.69	0.72
1:A:112:VAL:HG22	1:A:113:GLN:H	1.55	0.71
1:B:578:VAL:HG23	1:B:581:LYS:HB2	1.71	0.71
1:A:118:LYS:HE3	1:A:123:TRP:N	2.05	0.71
1:A:184:LYS:HD3	1:A:194:GLU:HG2	1.73	0.70
1:A:57:ASN:OD1	1:A:138:LYS:NZ	2.24	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:LYS:HE3	1:A:88:VAL:HG12	1.73	0.69
1:A:379:GLU:OE2	4:A:801:HOH:O	2.10	0.68
1:A:113:GLN:NE2	4:A:806:HOH:O	2.20	0.67
1:A:417:LYS:HA	1:A:417:LYS:HE2	1.75	0.67
1:A:59:GLU:O	1:A:63:THR:HG22	1.94	0.67
1:B:584:LYS:HE3	1:B:587:ILE:HG12	1.76	0.67
1:A:63:THR:HG23	1:A:64:GLU:HG3	1.77	0.66
1:B:419:LEU:HD12	1:B:423:THR:CG2	2.26	0.66
1:A:386:ASP:O	4:A:802:HOH:O	2.13	0.65
1:B:646:ALA:O	4:B:802:HOH:O	2.15	0.65
1:A:118:LYS:HZ1	1:A:121:GLY:C	1.96	0.64
1:A:434:LYS:NZ	1:A:511:GLU:OE2	2.27	0.64
1:B:467:PHE:HA	1:B:470:VAL:HG13	1.79	0.63
1:B:386:ASP:HB3	1:B:390:PRO:HD3	1.80	0.63
1:A:272:TYR:HE1	1:A:289:LYS:HE2	1.64	0.63
1:A:484:LYS:HD2	1:A:488:VAL:O	1.97	0.63
1:A:406:LYS:HG2	1:A:467:PHE:CD2	2.34	0.62
1:A:484:LYS:HE2	1:A:489:GLY:HA3	1.80	0.62
1:A:118:LYS:HE2	1:A:122:MET:H	1.65	0.62
1:A:369:TYR:HD1	1:A:372:MET:HE2	1.64	0.61
1:A:240:SER:HA	3:A:703:MUR:O5	2.00	0.61
1:A:158:ASN:HD21	1:A:667:ASP:HA	1.64	0.61
1:B:535:TYR:C	1:B:628:MET:HE1	2.21	0.61
1:A:551:LYS:HE3	1:B:158:ASN:HA	1.82	0.61
1:A:273:LYS:HZ2	1:A:275:ASP:H	1.48	0.60
1:B:226:ASP:OD1	1:B:229:LYS:NZ	2.34	0.60
1:B:269:TYR:HA	1:B:272:TYR:CD1	2.36	0.60
1:A:273:LYS:CE	1:A:275:ASP:HB3	2.30	0.60
1:A:655:GLU:OE1	4:A:804:HOH:O	2.16	0.59
1:B:436:LYS:N	1:B:436:LYS:HD2	2.17	0.59
1:B:264:LEU:HD11	1:B:274:ASP:HA	1.84	0.58
1:B:80:ILE:HA	1:B:98:GLN:O	2.03	0.58
1:A:305:ASN:ND2	1:B:68:LYS:C	2.56	0.58
1:B:94:ARG:HG3	1:B:94:ARG:HH11	1.68	0.58
1:B:151:ARG:CB	3:B:702:MUR:H93	2.34	0.58
1:A:421:ASP:HB3	1:A:570:LEU:HD21	1.86	0.57
1:A:434:LYS:HD3	1:A:436:LYS:HZ3	1.68	0.57
1:B:544:ILE:HD11	1:B:562:ILE:HD13	1.85	0.57
1:B:151:ARG:HB2	3:B:702:MUR:C9	2.34	0.57
1:B:263:GLU:HB2	1:B:266:GLN:HE22	1.69	0.57
1:A:598:SER:HB3	1:A:617:PHE:CD2	2.40	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:GLY:O	1:A:604:LYS:NZ	2.32	0.56
1:A:273:LYS:NZ	1:A:275:ASP:H	2.03	0.56
1:A:272:TYR:CE1	1:A:289:LYS:HE2	2.41	0.56
1:B:527:ASN:ND2	1:B:529:VAL:H	2.03	0.56
1:A:293:HIS:NE2	3:A:703:MUR:O8	2.39	0.55
1:A:304:ASP:O	1:A:305:ASN:HB2	2.06	0.55
1:A:118:LYS:CE	1:A:118:LYS:HA	2.36	0.55
1:A:118:LYS:HZ3	1:A:121:GLY:CA	2.20	0.55
1:B:260:ASN:OD1	1:B:263:GLU:N	2.36	0.55
1:B:180:LYS:HD3	1:B:183:TYR:CE2	2.42	0.55
1:B:94:ARG:CG	1:B:94:ARG:HH11	2.20	0.55
1:B:29:GLU:HB2	1:B:32[B]:ASN:HB2	1.89	0.54
1:A:143:HIS:HB3	1:A:145:GLU:OE1	2.07	0.54
1:B:260:ASN:OD1	1:B:263:GLU:HG3	2.08	0.54
1:B:420:ASP:O	1:B:423:THR:HG22	2.07	0.54
1:A:305:ASN:HB3	1:B:72[A]:SER:OG	2.07	0.54
1:B:98:GLN:NE2	1:B:111:ASN:OD1	2.38	0.53
1:B:467:PHE:HA	1:B:470:VAL:CG1	2.39	0.53
1:A:381:ASN:HA	1:A:384:THR:OG1	2.09	0.52
1:B:633:VAL:HG12	1:B:642:ALA:HB2	1.92	0.52
1:A:374:GLY:O	4:A:805:HOH:O	2.19	0.52
1:A:375:MET:HE2	1:A:379:GLU:HB3	1.92	0.52
1:A:602:GLU:H	1:A:602:GLU:CD	2.13	0.52
1:A:136:MET:HG3	1:A:140:GLN:HE21	1.75	0.52
1:B:27:ASP:O	1:B:30:ILE:HG22	2.10	0.52
1:A:432:TRP:CZ2	1:A:434:LYS:HA	2.45	0.51
1:B:375:MET:HB2	1:B:379:GLU:HG3	1.92	0.51
1:B:277:VAL:HB	3:B:702:MUR:H7	1.93	0.51
1:B:353:GLN:O	1:B:545:ASN:ND2	2.43	0.51
1:A:215:LYS:HG3	1:A:216:THR:N	2.25	0.51
1:A:93:LYS:HG3	1:A:123:TRP:CH2	2.46	0.51
1:B:298:ARG:HD3	1:B:315:GLU:OE1	2.11	0.51
1:B:535:TYR:HB3	1:B:628:MET:HE1	1.92	0.51
1:A:118:LYS:CE	1:A:122:MET:O	2.57	0.50
1:A:41:ASN:HD22	1:A:41:ASN:C	2.15	0.50
1:B:264:LEU:HD23	1:B:264:LEU:O	2.11	0.50
1:A:408:LEU:HD22	1:A:534:ILE:HG21	1.93	0.50
1:A:151:ARG:HB2	3:A:703:MUR:O8	2.10	0.50
1:A:436:LYS:HE2	1:A:511:GLU:OE2	2.12	0.50
1:B:635:ASP:OD2	1:B:642:ALA:HB3	2.12	0.50
1:A:287:TYR:CZ	1:A:550:LEU:HD11	2.46	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:557:VAL:HG11	1:B:560:LYS:HD3	1.94	0.50
1:B:629:MET:CE	1:B:652:VAL:HG11	2.42	0.50
1:A:438:TRP:HA	1:A:512:ILE:HD11	1.94	0.50
1:B:629:MET:HE1	1:B:652:VAL:HG11	1.93	0.50
1:A:118:LYS:HE2	1:A:122:MET:N	2.20	0.49
3:A:703:MUR:H92	3:A:703:MUR:HN22	1.76	0.49
1:A:251:HIS:HE1	1:A:390:PRO:O	1.93	0.49
1:A:477:LYS:O	1:A:481:LYS:HG3	2.13	0.49
1:B:265:LYS:N	4:B:816:HOH:O	2.42	0.49
1:B:268:GLU:OE2	1:B:269:TYR:CZ	2.66	0.49
1:B:500:ASN:ND2	4:B:819:HOH:O	2.44	0.49
1:A:118:LYS:NZ	1:A:122:MET:CA	2.68	0.48
1:B:595:ILE:HD11	1:B:620:TYR:OH	2.13	0.48
1:A:102:LYS:HD2	1:A:102:LYS:HA	1.50	0.48
3:A:703:MUR:H92	3:A:703:MUR:N2	2.29	0.48
1:B:375:MET:HE2	1:B:379:GLU:HG3	1.96	0.47
1:B:477:LYS:CG	1:B:481:LYS:HE3	2.44	0.47
1:B:557:VAL:HG11	1:B:560:LYS:CD	2.44	0.47
1:A:595:ILE:HD11	1:A:620:TYR:CZ	2.49	0.47
1:B:527:ASN:HD21	1:B:529:VAL:HB	1.78	0.47
1:B:620:TYR:HB3	1:B:628:MET:HG3	1.97	0.47
3:B:702:MUR:H4	4:B:956:HOH:O	2.14	0.47
1:A:272:TYR:OH	1:A:289:LYS:HG2	2.15	0.47
1:A:273:LYS:HD3	1:A:276:ALA:H	1.80	0.47
1:A:616:TRP:CZ3	1:A:632:ASN:HB2	2.50	0.46
1:A:298:ARG:HG2	1:A:300:THR:HG23	1.97	0.46
1:B:94:ARG:CG	1:B:94:ARG:NH1	2.77	0.46
1:A:118:LYS:CE	1:A:122:MET:CA	2.94	0.46
1:A:189:GLU:HG2	1:A:227:PHE:CE1	2.50	0.46
3:B:702:MUR:H92	3:B:702:MUR:H3	1.26	0.46
1:A:327:THR:OG1	1:A:549:LEU:HA	2.16	0.46
1:A:59:GLU:HG2	1:A:63:THR:HG21	1.96	0.46
1:B:269:TYR:CZ	1:B:278:ILE:HD12	2.49	0.46
1:A:215:LYS:NZ	4:A:810:HOH:O	2.49	0.46
1:A:484:LYS:HD2	1:A:484:LYS:HA	1.82	0.45
1:B:224:LEU:HD12	1:B:224:LEU:HA	1.80	0.45
1:B:38:GLU:OE1	1:B:83:ARG:NH2	2.48	0.45
1:B:119:GLU:O	1:B:121:GLY:N	2.48	0.45
1:B:95:VAL:O	1:B:113:GLN:HA	2.16	0.45
1:B:225:SER:O	1:B:229:LYS:HG3	2.16	0.45
1:B:93:LYS:HG3	1:B:123:TRP:CH2	2.50	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:LYS:HD3	1:B:181:LYS:N	2.32	0.45
1:B:583[B]:HIS:NE2	1:B:585:GLU:OE1	2.43	0.45
1:B:196:TYR:O	1:B:200:GLN:HG2	2.17	0.45
1:B:218:LYS:HB3	1:B:219:LYS:HD3	1.99	0.45
1:B:457:GLN:OE1	1:B:579:VAL:HG23	2.17	0.45
1:B:419:LEU:HD21	1:B:455:LEU:HD23	2.00	0.44
1:A:369:TYR:HD1	1:A:372:MET:CE	2.28	0.44
1:A:637:GLN:HA	1:A:641:MET:SD	2.58	0.44
1:B:133:ILE:HB	1:B:136:MET:HE2	2.00	0.44
1:B:573:ASP:OD1	1:B:583[A]:HIS:NE2	2.50	0.44
1:A:645:ASN:HD22	1:A:645:ASN:H	1.65	0.44
1:A:92:LYS:CD	1:A:117:VAL:HG12	2.47	0.44
1:B:331:LYS:HE2	4:B:832:HOH:O	2.17	0.44
1:B:536:SER:N	1:B:628:MET:HE1	2.32	0.44
1:A:480:GLU:HG2	1:A:508:LEU:HD12	1.99	0.44
1:A:293:HIS:CD2	3:A:703:MUR:O8	2.71	0.44
1:B:527:ASN:ND2	1:B:529:VAL:N	2.66	0.44
1:B:552:ASP:OD1	4:B:805:HOH:O	2.21	0.44
1:A:92:LYS:HA	1:A:92:LYS:HD3	1.87	0.43
1:B:77:ASP:OD1	1:B:78:ILE:N	2.51	0.43
1:B:86:LYS:HZ1	1:B:87:LYS:HG2	1.82	0.43
1:B:535:TYR:HB3	1:B:628:MET:CE	2.48	0.43
1:B:527:ASN:HD22	1:B:530:GLN:H	1.65	0.43
1:B:93:LYS:HE3	1:B:123:TRP:CZ2	2.53	0.43
1:B:149:SER:C	1:B:293:HIS:HD2	2.22	0.43
1:B:143:HIS:HB3	1:B:145:GLU:OE2	2.19	0.43
1:B:602:GLU:OE2	1:B:613:GLN:HG2	2.19	0.43
1:B:603:LEU:HD12	1:B:612:ARG:O	2.19	0.42
1:B:239:GLU:HB3	3:B:702:MUR:O6	2.19	0.42
1:B:86:LYS:NZ	1:B:87:LYS:HG2	2.33	0.42
1:B:327:THR:OG1	1:B:549:LEU:HA	2.20	0.42
1:A:187:ALA:HB1	1:A:192:ILE:O	2.19	0.42
1:A:305:ASN:HD21	1:B:69:ILE:N	2.17	0.42
1:B:436:LYS:H	1:B:436:LYS:HD2	1.82	0.42
1:A:269:TYR:HA	1:A:272:TYR:CD1	2.55	0.42
1:A:426:LYS:NZ	4:A:809:HOH:O	2.53	0.42
1:A:95:VAL:O	1:A:113:GLN:HA	2.20	0.42
1:A:118:LYS:HA	1:A:118:LYS:HE2	2.00	0.42
1:B:304:ASP:O	1:B:306:SER:N	2.51	0.42
1:B:29:GLU:HA	1:B:32[B]:ASN:HB2	2.00	0.41
1:B:86:LYS:HZ2	1:B:87:LYS:H	1.69	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:GLU:O	1:B:198:LYS:HG3	2.20	0.41
1:B:502:GLN:HB2	1:B:525:LEU:HB2	2.03	0.41
1:B:573:ASP:OD2	1:B:583[A]:HIS:NE2	2.53	0.41
1:A:484:LYS:CD	1:A:488:VAL:O	2.66	0.41
1:A:43:LYS:NZ	1:A:63:THR:HG21	2.35	0.41
1:B:367:ASP:HB3	1:B:370:PRO:HD2	2.02	0.41
1:B:484:LYS:HB2	1:B:484:LYS:HE3	1.65	0.41
1:A:118:LYS:HZ3	1:A:121:GLY:HA2	1.84	0.41
1:A:316:LYS:NZ	4:A:821:HOH:O	2.41	0.41
1:A:595:ILE:HD11	1:A:620:TYR:OH	2.20	0.41
3:A:703:MUR:H92	3:A:703:MUR:H3	1.53	0.41
1:A:413:GLY:HA2	1:A:474:LEU:HD21	2.03	0.41
1:A:576:GLN:HG2	1:A:580:ASN:ND2	2.35	0.41
1:A:327:THR:HB	1:A:356:GLU:HB3	2.02	0.40
1:A:507:ASN:O	1:A:513:LEU:HD13	2.21	0.40
1:A:102:LYS:HD3	1:A:107:ASN:OD1	2.21	0.40
1:B:503:ILE:HD12	1:B:524:ILE:HD13	2.04	0.40
1:B:376:SER:OG	1:B:378:GLU:HG2	2.21	0.40
1:B:487:GLY:O	1:B:490:GLU:HG2	2.20	0.40
1:B:86:LYS:HG3	1:B:87:LYS:O	2.21	0.40
1:A:305:ASN:HD22	1:B:68:LYS:C	2.23	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	640/642 (100%)	616 (96%)	20 (3%)	4 (1%)	28	20
1	B	636/642 (99%)	604 (95%)	26 (4%)	6 (1%)	20	11
All	All	1276/1284 (99%)	1220 (96%)	46 (4%)	10 (1%)	22	13

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	438	TRP
1	A	508	LEU
1	B	88	VAL
1	B	267	LYS
1	B	275	ASP
1	A	276	ALA
1	A	509	ASP
1	B	28	LYS
1	B	638	ASP
1	B	262	GLU

### 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	575/572 (100%)	562 (98%)	13 (2%)	56	55
1	B	571/572 (100%)	553 (97%)	18 (3%)	44	40
All	All	1146/1144 (100%)	1115 (97%)	31 (3%)	51	48

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	77	ASP
1	A	87	LYS
1	A	89	SER
1	A	99	TYR
1	A	118	LYS
1	A	156	ASP
1	A	252	LEU
1	A	267	LYS
1	A	421	ASP
1	A	422	LYS
1	A	435	ASP
1	A	484	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	55	SER
1	B	99	TYR
1	B	115	ASN
1	B	120	ASP
1	B	141	SER
1	B	156	ASP
1	B	219	LYS
1	B	220	MET
1	B	263	GLU
1	B	293	HIS
1	B	422	LYS
1	B	470	VAL
1	B	556	LYS
1	B	583[A]	HIS
1	B	583[B]	HIS
1	B	617	PHE
1	B	645	ASN
1	B	647	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	140	GLN
1	A	158	ASN
1	A	251	HIS
1	A	305	ASN
1	A	381	ASN
1	A	567	ASN
1	A	624	ASN
1	A	645	ASN
1	B	293	HIS
1	B	442	ASN
1	B	527	ASN
1	B	530	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 5 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	2.02	3 (21%)	19,24,24	1.64	6 (31%)
3	MUR	B	702	-	14,17,17	1.81	2 (14%)	19,24,24	2.32	7 (36%)

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	-	-	0/6/30/30	0/1/1/1
3	MUR	B	702	-	-	0/6/30/30	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	703	MUR	C9-C7	2.24	1.56	1.51
3	B	702	MUR	C2-N2	3.22	1.52	1.47
3	A	703	MUR	C2-N2	3.43	1.52	1.47
3	B	702	MUR	O5-C1	5.02	1.52	1.43
3	A	703	MUR	O5-C1	5.53	1.53	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	703	MUR	C3-C4-C5	-3.25	102.71	109.67
3	B	702	MUR	C9-C7-C8	-2.71	109.89	113.35
3	B	702	MUR	C6-C5-C4	-2.45	107.26	113.00
3	A	703	MUR	O3-C3-C2	2.06	113.34	108.57
3	A	703	MUR	C4-C3-C2	2.11	114.78	111.09
3	A	703	MUR	O3-C7-C9	2.18	113.03	107.38
3	B	702	MUR	O3-C7-C8	2.39	118.18	111.85
3	A	703	MUR	C1-C2-C3	2.47	114.64	110.14
3	A	703	MUR	O5-C5-C6	2.60	112.64	106.41
3	B	702	MUR	O5-C5-C6	3.04	113.68	106.41
3	B	702	MUR	C4-C3-C2	3.31	116.88	111.09
3	B	702	MUR	C1-C2-C3	3.72	116.92	110.14
3	B	702	MUR	O5-C1-C2	5.63	116.08	109.51

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	703	MUR	8	0
3	B	702	MUR	8	0

## 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	640/642 (99%)	0.39	12 (1%) 67 69	27, 49, 82, 115	0
1	B	635/642 (98%)	0.57	38 (5%) 23 25	28, 52, 97, 137	0
All	All	1275/1284 (99%)	0.48	50 (3%) 40 43	27, 50, 88, 137	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	580	ASN	5.4
1	B	587	ILE	4.6
1	B	579	VAL	4.6
1	B	446	TYR	4.5
1	B	269	TYR	4.4
1	B	588	TYR	3.8
1	B	578	VAL	3.8
1	B	118	LYS	3.7
1	B	30	ILE	3.7
1	B	642	ALA	3.5
1	B	603	LEU	3.4
1	B	582	THR	3.4
1	B	641	MET	3.3
1	B	223	TYR	3.0
1	B	87	LYS	3.0
1	B	586	ASP	3.0
1	B	585	GLU	2.9
1	B	121	GLY	2.9
1	B	639	LYS	2.9
1	A	605	MET	2.9
1	B	91	ASN	2.9
1	B	261	SER	2.8
1	A	275	ASP	2.8
1	A	27	ASP	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	117	VAL	2.7
1	B	34	ILE	2.6
1	B	27	ASP	2.6
1	B	29	GLU	2.6
1	A	85	ILE	2.6
1	A	223	TYR	2.5
1	A	118	LYS	2.3
1	B	583[A]	HIS	2.3
1	B	204	ASN	2.3
1	B	51	TYR	2.2
1	A	508	LEU	2.2
1	B	637	GLN	2.2
1	B	611	GLY	2.2
1	A	82	ASP	2.2
1	A	114	PHE	2.2
1	B	94	ARG	2.2
1	B	89	SER	2.2
1	A	513	LEU	2.2
1	B	85	ILE	2.1
1	A	171	ILE	2.1
1	B	584	LYS	2.1
1	B	594	LEU	2.1
1	B	276	ALA	2.1
1	B	88	VAL	2.1
1	B	123	TRP	2.0
1	A	436	LYS	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MUR	B	702	17/17	0.81	0.33	15.00	55,85,96,97	0
3	MUR	A	703	17/17	0.83	0.32	9.63	40,75,89,95	0
2	CD	A	701	1/1	1.00	0.14	1.24	31,31,31,31	0
2	CD	A	705	1/1	1.00	0.17	0.71	37,37,37,37	0
2	CD	A	704	1/1	0.99	0.14	0.37	31,31,31,31	0
2	CD	A	702	1/1	1.00	0.12	-0.50	38,38,38,38	0
2	CD	B	701	1/1	0.88	0.08	-4.39	122,122,122,122	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.