



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 6, 2016 – 05:42 PM EDT

PDB ID : 5AA4  
Title : Crystal structure of MltF from *Pseudomonas aeruginosa* in complex with cell-wall tetrapeptide  
Authors : Dominguez-Gil, T.; Acebron, I.; Hermoso, J.A.  
Deposited on : 2015-07-23  
Resolution : 2.40 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.

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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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027939  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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-20027939

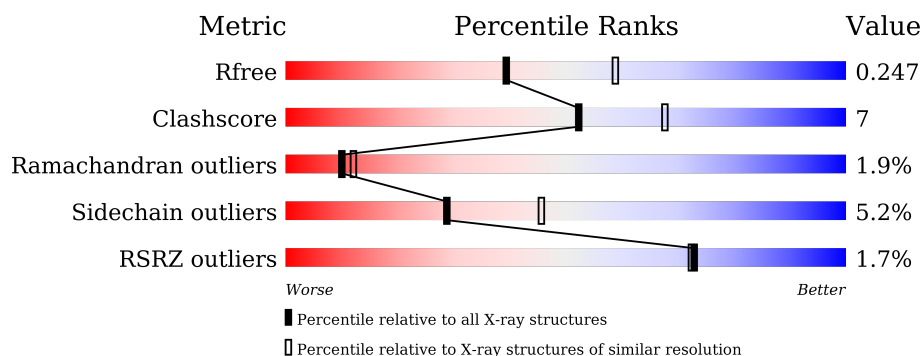
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	451	<div> <div>77%</div> <div>13% .. 7%</div> </div>
1	C	451	<div> <div>%</div> <div>78%</div> <div>11% • 8%</div> </div>
2	B	451	<div> <div>2%</div> <div>82%</div> <div>10% • 8%</div> </div>
2	D	451	<div> <div>3%</div> <div>71%</div> <div>19% • 8%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	6X4	A	1458	X	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 26645 atoms, of which 13109 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 MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	418	Total	C	H	N	O	S	0	0	0
			6623	2112	3274	596	632	9			
1	C	413	Total	C	H	N	O	S	0	0	0
			6552	2087	3240	591	625	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	302	LYS	LEU	CONFLICT	UNP A0A077JMS
C	302	LYS	LEU	CONFLICT	UNP A0A077JMS

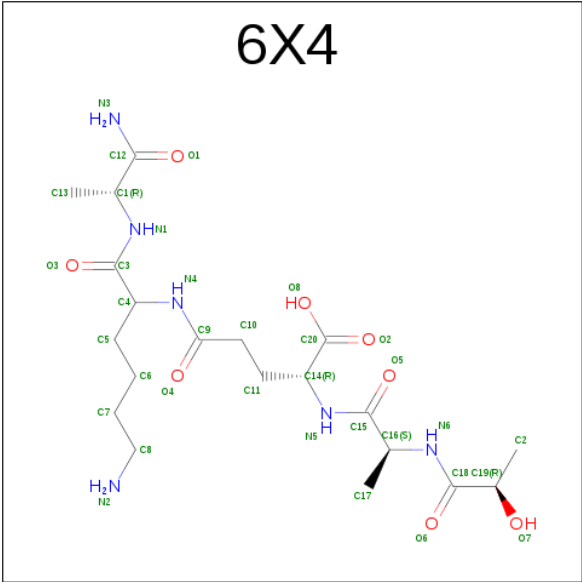
- Molecule 2 is a protein called MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	417	Total	C	H	N	O	S	0	0	0
			6632	2108	3288	595	632	9			
2	D	417	Total	C	H	N	O	S	0	0	0
			6611	2102	3274	594	632	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	281	THR	ALA	CONFLICT	UNP A0A077JMS
B	302	LYS	LEU	CONFLICT	UNP A0A077JMS
D	281	THR	ALA	CONFLICT	UNP A0A077JMS
D	302	LYS	LEU	CONFLICT	UNP A0A077JMS

- Molecule 3 is (2 {R})-5-[[6-AZANYL-1-[(2 {R})-1-AZANYL-1-OXIDANYLIDENE-PROP AN-2-YL]AMINO]-1-OXIDANYLIDENE-HEXAN-2-YL]AMINO]-5-OXIDANYLIDENE-2-[[2 {S}]-2-[[2 {R})-2-OXIDANYLPROPANOYL]AMINO]PROPANOYL]AMINO]PENT ANOIC ACID (three-letter code: 6X4) (formula: C<sub>20</sub>H<sub>36</sub>N<sub>6</sub>O<sub>8</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			67	20	33	6	8		

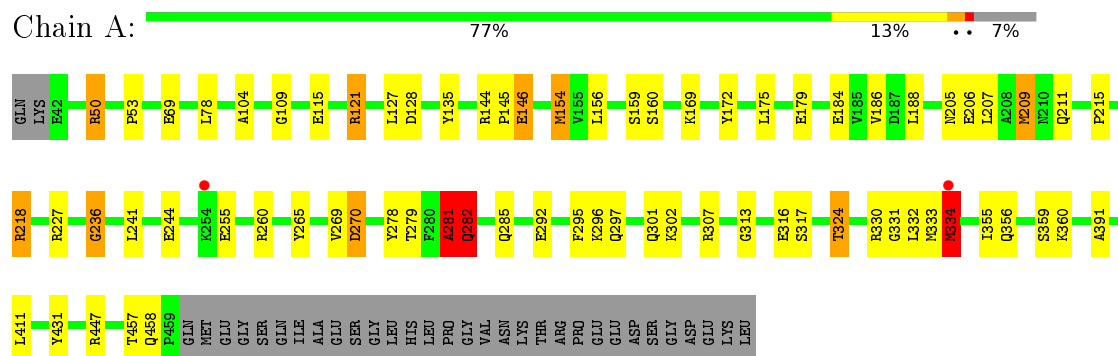
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	73	Total O	0	0
			73 73		
4	B	46	Total O	0	0
			46 46		
4	C	33	Total O	0	0
			33 33		
4	D	8	Total O	0	0
			8 8		

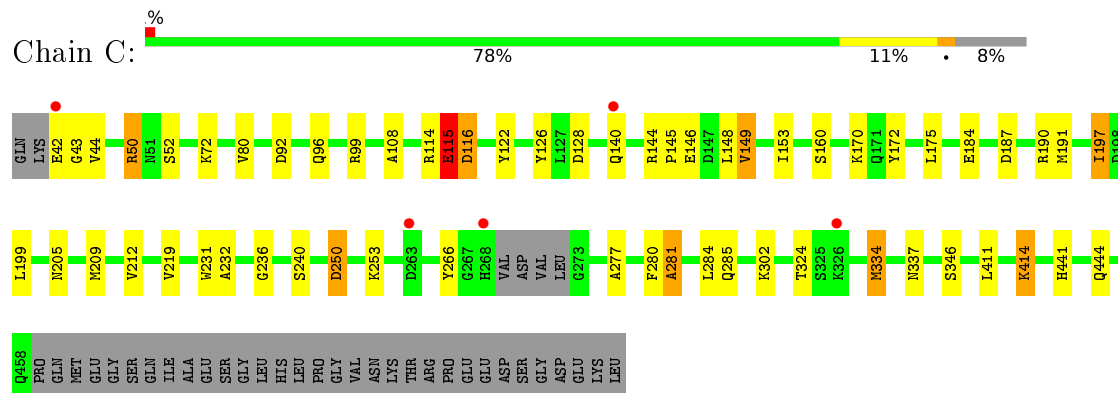
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

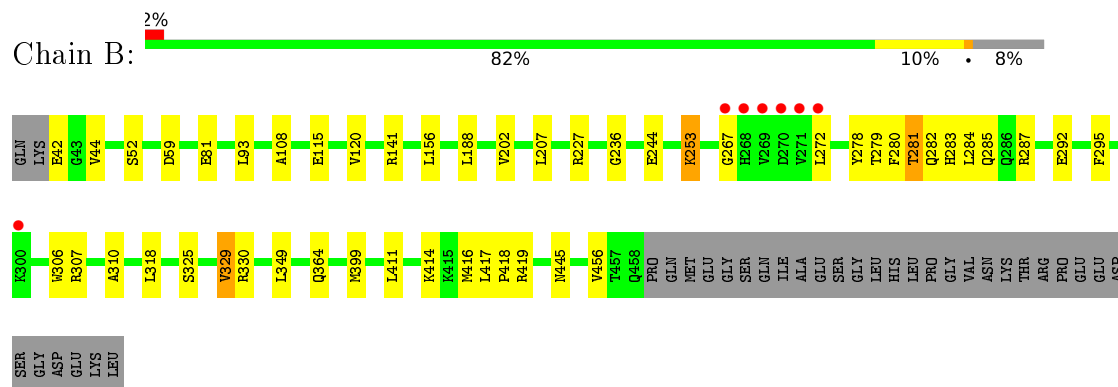
#### • Molecule 1: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F



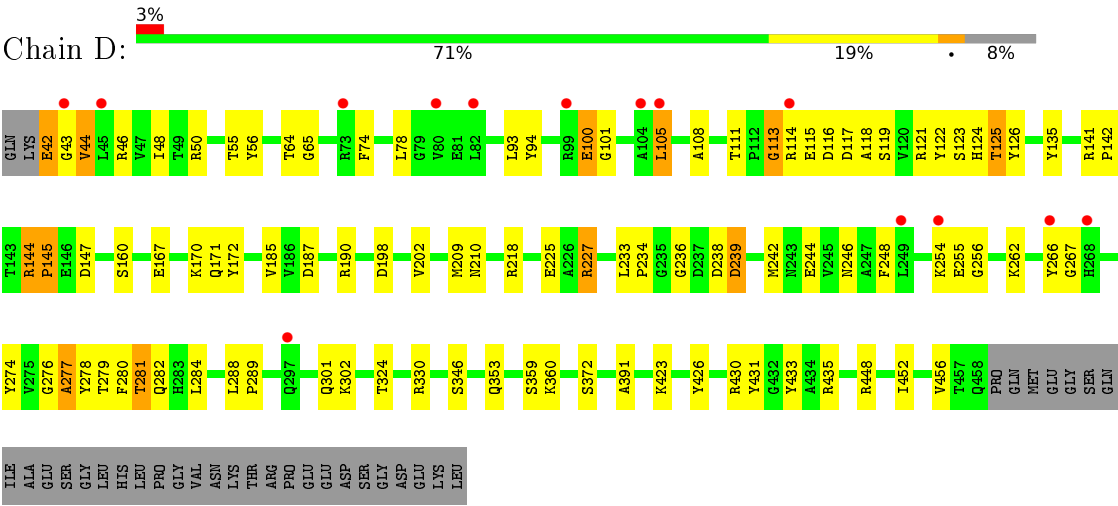
#### • Molecule 1: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F



#### • Molecule 2: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F



● Molecule 2: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.12Å 136.77Å 138.10Å 90.00° 92.34° 90.00°	Depositor
Resolution (Å)	48.57 – 2.40 48.72 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.5 (48.57-2.40) 93.6 (48.72-2.40)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.17 (at 2.39Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.185 , 0.239 0.206 , 0.247	Depositor DCC
$R_{free}$ test set	4681 reflections (5.50%)	DCC
Wilson B-factor (Å <sup>2</sup> )	51.7	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 54.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.013 for -h,l,k 0.019 for -h,-l,-k 0.037 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	26645	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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: 6X4

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	0.82	0/3420	0.86	8/4624 (0.2%)
1	C	0.73	0/3381	0.77	2/4567 (0.0%)
2	B	0.80	1/3414 (0.0%)	0.79	2/4615 (0.0%)
2	D	0.59	0/3407	0.72	0/4607
All	All	0.74	1/13622 (0.0%)	0.78	12/18413 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	202	VAL	CB-CG2	-5.03	1.42	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	50	ARG	NE-CZ-NH2	-8.80	115.90	120.30
1	A	154	MET	CG-SD-CE	-8.74	86.21	100.20
1	A	334	MET	CG-SD-CE	-7.50	88.21	100.20
1	A	281	ALA	C-N-CA	7.42	140.26	121.70
2	B	419	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	A	50	ARG	NE-CZ-NH1	7.35	123.97	120.30
2	B	59	ASP	CB-CG-OD1	6.54	124.19	118.30
1	A	282	GLN	N-CA-CB	6.15	121.67	110.60
1	C	334	MET	CG-SD-CE	-5.44	91.49	100.20
1	A	447	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	A	282	GLN	CA-CB-CG	-5.09	102.20	113.40
1	C	115	GLU	C-N-CA	5.06	134.36	121.70

There are no chirality outliers.

There are no planarity outliers.

## 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	3349	3274	3293	63	0
1	C	3312	3240	3252	36	0
2	B	3344	3288	3288	28	0
2	D	3337	3274	3268	58	0
3	A	34	33	0	9	0
4	A	73	0	0	7	0
4	B	46	0	0	5	0
4	C	33	0	0	1	0
4	D	8	0	0	2	0
All	All	13536	13109	13101	177	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 7.

All (177) 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:333:MET:SD	4:A:2050:HOH:O	2.00	1.20
1:A:281:ALA:HB1	1:C:285:GLN:HB2	1.55	0.87
1:A:179:GLU:OE1	4:A:2019:HOH:O	1.93	0.86
2:D:117:ASP:O	2:D:119:SER:N	2.09	0.86
1:A:281:ALA:HB3	1:A:282:GLN:HB2	1.58	0.85
1:A:301:GLN:OE1	1:A:356:GLN:NE2	2.16	0.79
2:B:244:GLU:OE2	4:B:2034:HOH:O	2.02	0.78
1:C:280:PHE:O	1:C:281:ALA:HB3	1.84	0.78
1:A:356:GLN:OE1	4:A:2058:HOH:O	2.02	0.76
1:A:281:ALA:HB3	1:A:282:GLN:CB	2.17	0.74
1:A:209:MET:HE1	1:A:265:TYR:HB3	1.69	0.74
1:C:414:LYS:NZ	1:C:444:GLN:OE1	2.22	0.72
2:B:292:GLU:OE1	2:D:278:TYR:OH	2.02	0.72
2:D:100:GLU:OE1	2:D:101:GLY:N	2.23	0.72
1:A:282:GLN:HB2	1:C:285:GLN:HG3	1.73	0.70
2:B:253:LYS:CE	4:B:2019:HOH:O	2.39	0.70
1:C:281:ALA:HA	1:C:284:LEU:HB3	1.74	0.68
1:C:334:MET:O	4:C:2005:HOH:O	2.10	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:GLU:OE1	4:A:2037:HOH:O	2.12	0.67
1:C:280:PHE:O	1:C:281:ALA:CB	2.42	0.67
2:D:281:THR:HA	2:D:284:LEU:HD23	1.77	0.65
1:A:324:THR:CG2	1:A:330:ARG:HE	2.09	0.65
2:B:253:LYS:HE2	4:B:2019:HOH:O	1.98	0.64
2:B:253:LYS:HD3	4:B:2019:HOH:O	1.99	0.63
2:B:253:LYS:CD	4:B:2019:HOH:O	2.46	0.63
2:D:279:THR:N	4:D:2006:HOH:O	2.21	0.62
1:A:332:LEU:CD2	1:A:333:MET:HE2	2.30	0.62
1:A:332:LEU:HD22	1:A:333:MET:HE2	1.82	0.62
2:D:225:GLU:O	2:D:227:ARG:NH1	2.29	0.61
2:D:187:ASP:OD1	2:D:190:ARG:NH1	2.35	0.59
2:B:42:GLU:N	2:B:81:GLU:OE2	2.37	0.57
1:A:50:ARG:HD2	1:A:184:GLU:OE2	2.05	0.57
2:B:281:THR:OG1	2:B:282:GLN:N	2.36	0.56
2:B:456:VAL:HG13	2:D:277:ALA:HB2	1.87	0.56
2:D:64:THR:OG1	2:D:65:GLY:N	2.39	0.56
1:C:149:VAL:HG23	1:C:175:LEU:HA	1.88	0.55
1:A:307:ARG:HD3	1:A:457:THR:HG21	1.86	0.55
1:A:331:GLY:O	1:A:334:MET:SD	2.64	0.55
2:D:185:VAL:HG13	2:D:202:VAL:HG11	1.88	0.55
2:B:280:PHE:O	2:B:281:THR:OG1	2.24	0.55
1:A:281:ALA:HB3	1:C:285:GLN:HG3	1.88	0.55
1:A:297:GLN:NE2	4:A:2041:HOH:O	2.33	0.54
2:D:238:ASP:OD1	2:D:239:ASP:N	2.41	0.54
1:A:295:PHE:HE1	1:A:333:MET:CE	2.21	0.54
1:A:50:ARG:HH22	3:A:1458:6X4:C11	2.21	0.54
2:D:280:PHE:O	2:D:281:THR:OG1	2.21	0.54
2:D:42:GLU:N	2:D:43:GLY:HA2	2.24	0.53
2:B:272:LEU:HD22	2:B:318:LEU:HD21	1.89	0.53
1:A:69:GLU:OE2	1:A:265:TYR:OH	2.18	0.53
2:B:280:PHE:O	2:B:281:THR:HG23	2.09	0.53
1:C:187:ASP:OD1	1:C:190:ARG:NH1	2.42	0.52
1:A:156:LEU:HD12	1:A:188:LEU:HD11	1.92	0.52
1:A:278:TYR:O	1:A:281:ALA:HB3	2.10	0.52
2:B:278:TYR:HA	2:D:456:VAL:HG13	1.90	0.52
1:C:153:ILE:HG22	1:C:199:LEU:HB2	1.90	0.52
1:A:302:LYS:HZ1	1:A:359:SER:HB3	1.74	0.52
1:C:115:GLU:CB	1:C:116:ASP:HB2	2.40	0.52
1:A:278:TYR:O	1:A:281:ALA:CB	2.58	0.51
1:A:333:MET:HE3	1:A:355:ILE:HG12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:GLU:OE2	1:A:296:LYS:NZ	2.39	0.51
1:A:295:PHE:CE1	1:A:333:MET:CE	2.93	0.51
2:B:280:PHE:O	2:B:281:THR:CB	2.59	0.51
2:D:125:THR:HG22	2:D:126:TYR:N	2.26	0.51
2:D:115:GLU:O	2:D:117:ASP:N	2.45	0.50
2:D:280:PHE:O	2:D:281:THR:CB	2.60	0.50
1:C:115:GLU:HB2	1:C:116:ASP:HB2	1.94	0.49
1:A:207:LEU:HG	1:A:211:GLN:HG2	1.93	0.49
1:A:50:ARG:HH22	3:A:1458:6X4:C10	2.25	0.49
1:A:121:ARG:NH1	1:A:236:GLY:HA2	2.26	0.49
2:D:144:ARG:HG3	2:D:145:PRO:CD	2.43	0.49
1:A:281:ALA:CB	1:C:285:GLN:HG3	2.43	0.49
1:A:324:THR:HG23	1:A:330:ARG:HG3	1.95	0.48
1:A:169:LYS:HD2	1:A:175:LEU:O	2.13	0.48
2:D:113:GLY:HA3	2:D:114:ARG:HB2	1.95	0.48
2:D:227:ARG:HH11	2:D:227:ARG:CG	2.26	0.48
2:D:281:THR:OG1	2:D:282:GLN:N	2.47	0.48
1:A:302:LYS:HZ2	1:A:302:LYS:HB2	1.79	0.48
2:D:135:TYR:CE1	2:D:141:ARG:HG3	2.48	0.48
1:A:295:PHE:HE1	1:A:333:MET:HE3	1.79	0.48
2:B:330:ARG:HD3	2:B:349:LEU:HD21	1.95	0.48
1:A:260:ARG:HG3	1:A:260:ARG:HH11	1.79	0.47
2:D:135:TYR:CE1	2:D:218:ARG:HB2	2.50	0.47
2:D:233:LEU:HD13	2:D:242:MET:HE1	1.96	0.47
1:C:144:ARG:NE	1:C:146:GLU:HG3	2.29	0.47
2:D:94:TYR:HE1	2:D:122:TYR:HH	1.61	0.47
2:B:283:HIS:CD2	2:B:287:ARG:NH1	2.83	0.47
1:A:205:ASN:ND2	3:A:1458:6X4:O8	2.43	0.47
1:A:279:THR:O	1:A:282:GLN:HB3	2.15	0.47
2:D:274:TYR:CE2	2:D:276:GLY:HA2	2.50	0.47
2:B:272:LEU:O	2:B:445:ASN:ND2	2.47	0.46
2:D:144:ARG:NE	2:D:145:PRO:HD2	2.29	0.46
2:D:324:THR:HG21	2:D:330:ARG:HE	1.81	0.46
1:A:115:GLU:N	4:A:2011:HOH:O	2.48	0.46
1:C:205:ASN:HB2	1:C:266:TYR:CE1	2.50	0.46
1:A:159:SER:HA	3:A:1458:6X4:C13	2.46	0.46
2:D:209:MET:HE2	2:D:266:TYR:CE1	2.50	0.46
1:A:269:VAL:O	1:A:270:ASP:HB3	2.16	0.46
1:A:316:GLU:HB3	1:A:334:MET:HG2	1.96	0.46
2:B:417:LEU:N	2:B:418:PRO:CD	2.78	0.46
1:C:114:ARG:O	1:C:115:GLU:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:115:GLU:C	2:D:117:ASP:H	2.18	0.46
1:A:135:TYR:CE1	1:A:218:ARG:HB3	2.50	0.46
1:C:115:GLU:CB	1:C:116:ASP:CB	2.94	0.46
2:D:142:PRO:HB3	2:D:147:ASP:HB2	1.97	0.46
1:C:115:GLU:HB2	1:C:116:ASP:CB	2.47	0.45
2:B:399:MET:SD	2:B:416:MET:SD	3.13	0.45
2:D:302:LYS:HZ1	2:D:359:SER:HB3	1.80	0.45
2:D:266:TYR:CD1	2:D:266:TYR:N	2.84	0.45
1:A:109:GLY:HA3	3:A:1458:6X4:C14	2.46	0.45
1:A:78:LEU:HD21	1:A:244:GLU:HG2	1.99	0.45
1:C:191:MET:HB3	1:C:197:ILE:HB	1.99	0.45
2:D:280:PHE:CE2	2:D:284:LEU:HD21	2.52	0.45
1:A:317:SER:HB3	1:A:334:MET:SD	2.56	0.45
2:D:254:LYS:O	2:D:256:GLY:N	2.50	0.45
1:A:206:GLU:OE2	3:A:1458:6X4:C10	2.65	0.44
1:C:115:GLU:N	1:C:116:ASP:HB3	2.33	0.44
2:D:198:ASP:O	4:D:2004:HOH:O	2.21	0.44
2:D:227:ARG:HG2	2:D:227:ARG:HH11	1.83	0.44
1:A:295:PHE:CE1	1:A:333:MET:HE3	2.52	0.44
2:B:325:SER:HB3	2:B:329:VAL:HG12	1.98	0.44
2:B:285:GLN:HG3	2:D:282:GLN:HG2	2.00	0.44
2:B:295:PHE:CZ	2:B:310:ALA:HA	2.53	0.44
2:D:266:TYR:HD1	2:D:266:TYR:N	2.14	0.43
1:A:313:GLY:HA3	1:A:333:MET:HE1	2.00	0.43
2:B:93:LEU:C	2:B:93:LEU:HD23	2.39	0.43
1:C:126:TYR:CE2	1:C:231:TRP:CD1	3.06	0.43
2:D:288:LEU:N	2:D:289:PRO:CD	2.82	0.43
1:C:92:ASP:O	1:C:96:GLN:HG2	2.17	0.43
2:D:274:TYR:CE1	2:D:448:ARG:HG2	2.54	0.43
2:D:391:ALA:HB1	2:D:431:TYR:CE2	2.53	0.43
2:B:156:LEU:HD12	2:B:188:LEU:HD11	2.01	0.43
2:D:111:THR:CG2	2:D:227:ARG:HD3	2.48	0.42
2:D:144:ARG:CZ	2:D:145:PRO:HD2	2.49	0.42
1:C:250:ASP:HA	1:C:253:LYS:HB3	2.01	0.42
2:D:115:GLU:C	2:D:117:ASP:N	2.73	0.42
1:C:146:GLU:O	1:C:149:VAL:HG12	2.19	0.42
2:D:124:HIS:CE1	2:D:246:ASN:ND2	2.87	0.42
2:D:55:THR:OG1	2:D:56:TYR:N	2.52	0.42
1:A:146:GLU:N	1:A:146:GLU:OE1	2.52	0.42
1:C:205:ASN:N	1:C:205:ASN:OD1	2.53	0.42
1:C:277:ALA:O	1:C:280:PHE:O	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:210:ASN:OD1	2:D:435:ARG:NH2	2.50	0.42
1:A:146:GLU:HG3	1:A:172:TYR:CE1	2.54	0.42
1:C:42:GLU:N	1:C:44:VAL:H	2.17	0.42
1:A:302:LYS:NZ	1:A:302:LYS:HB2	2.34	0.42
1:A:295:PHE:CE1	1:A:333:MET:HE1	2.54	0.42
2:D:433:TYR:C	2:D:433:TYR:CD1	2.92	0.42
1:C:144:ARG:HE	1:C:146:GLU:HG3	1.84	0.42
1:C:146:GLU:OE2	1:C:172:TYR:OH	2.37	0.42
1:C:302:LYS:NZ	1:C:302:LYS:HB2	2.35	0.42
1:A:127:LEU:HD22	3:A:1458:6X4:C17	2.50	0.42
1:A:281:ALA:HB1	1:C:285:GLN:CB	2.38	0.42
1:A:53:PRO:HG3	1:A:186:VAL:HG21	2.02	0.41
1:C:122:TYR:CE1	1:C:232:ALA:HB2	2.55	0.41
1:A:391:ALA:HB1	1:A:431:TYR:CE2	2.54	0.41
2:B:279:THR:HG22	2:B:283:HIS:CE1	2.55	0.41
2:B:283:HIS:CD2	2:B:287:ARG:CZ	3.03	0.41
1:C:42:GLU:N	1:C:43:GLY:HA2	2.34	0.41
2:D:423:LYS:HA	2:D:426:TYR:CE2	2.55	0.41
1:A:104:ALA:HB1	1:A:241:LEU:HD21	2.01	0.41
1:A:278:TYR:HB2	4:A:2034:HOH:O	2.21	0.41
2:D:74:PHE:CD1	2:D:248:PHE:CD2	3.08	0.41
1:A:206:GLU:OE2	3:A:1458:6X4:C11	2.69	0.41
3:A:1458:6X4:C9	3:A:1458:6X4:O2	2.68	0.41
2:B:280:PHE:O	2:B:281:THR:CG2	2.69	0.41
1:A:324:THR:HG21	1:A:330:ARG:HE	1.82	0.41
2:D:42:GLU:CB	2:D:44:VAL:H	2.34	0.41
1:A:215:PRO:O	1:A:218:ARG:NH2	2.54	0.41
2:B:306:TRP:CE2	2:B:307:ARG:HG3	2.56	0.41
1:C:50:ARG:HD2	1:C:184:GLU:OE2	2.20	0.41
2:D:42:GLU:HB3	2:D:44:VAL:H	1.85	0.41
1:C:209:MET:HE3	1:C:266:TYR:CE1	2.55	0.41
2:D:452:ILE:O	2:D:456:VAL:HG23	2.22	0.40
2:D:121:ARG:HD3	2:D:234:PRO:O	2.20	0.40
2:D:144:ARG:HG3	2:D:145:PRO:N	2.37	0.40
2:D:105:LEU:HD12	2:D:105:LEU:N	2.37	0.40
2:D:135:TYR:CZ	2:D:141:ARG:HG3	2.56	0.40

There are no symmetry-related clashes.

## 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	416/451 (92%)	395 (95%)	15 (4%)	6 (1%)	14	19
1	C	409/451 (91%)	381 (93%)	21 (5%)	7 (2%)	11	14
2	B	415/451 (92%)	397 (96%)	14 (3%)	4 (1%)	19	28
2	D	415/451 (92%)	379 (91%)	21 (5%)	15 (4%)	4	3
All	All	1655/1804 (92%)	1552 (94%)	71 (4%)	32 (2%)	10	12

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	255	GLU
1	A	282	GLN
2	B	281	THR
1	C	149	VAL
2	D	113	GLY
2	D	118	ALA
2	D	123	SER
2	D	171	GLN
2	D	281	THR
1	A	270	ASP
1	C	115	GLU
1	C	116	ASP
1	C	281	ALA
2	D	108	ALA
2	B	236	GLY
1	C	108	ALA
1	C	145	PRO
1	C	236	GLY
2	D	116	ASP
2	D	145	PRO
2	D	170	LYS
2	D	255	GLU

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Mol	Chain	Res	Type
1	A	236	GLY
1	A	281	ALA
2	B	108	ALA
2	D	78	LEU
2	D	236	GLY
2	D	125	THR
2	D	277	ALA
1	A	145	PRO
2	B	267	GLY
2	D	267	GLY

### 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	348/376 (93%)	333 (96%)	15 (4%)	35	55
1	C	343/376 (91%)	321 (94%)	22 (6%)	22	34
2	B	348/377 (92%)	335 (96%)	13 (4%)	41	62
2	D	346/377 (92%)	324 (94%)	22 (6%)	22	34
All	All	1385/1506 (92%)	1313 (95%)	72 (5%)	29	45

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	ARG
1	A	128	ASP
1	A	144	ARG
1	A	146	GLU
1	A	154	MET
1	A	160	SER
1	A	209	MET
1	A	218	ARG
1	A	227	ARG
1	A	285	GLN
1	A	324	THR

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Mol	Chain	Res	Type
1	A	334	MET
1	A	360	LYS
1	A	411	LEU
1	A	458	GLN
2	B	44	VAL
2	B	52	SER
2	B	115	GLU
2	B	120	VAL
2	B	141	ARG
2	B	207	LEU
2	B	227	ARG
2	B	253	LYS
2	B	284	LEU
2	B	329	VAL
2	B	364	GLN
2	B	411	LEU
2	B	414	LYS
1	C	50	ARG
1	C	52	SER
1	C	72	LYS
1	C	80	VAL
1	C	99	ARG
1	C	115	GLU
1	C	128	ASP
1	C	140	GLN
1	C	148	LEU
1	C	160	SER
1	C	170	LYS
1	C	197	ILE
1	C	212	VAL
1	C	219	VAL
1	C	240	SER
1	C	250	ASP
1	C	324	THR
1	C	337	ASN
1	C	346	SER
1	C	411	LEU
1	C	414	LYS
1	C	441	HIS
2	D	42	GLU
2	D	44	VAL
2	D	46	ARG

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Mol	Chain	Res	Type
2	D	48	ILE
2	D	50	ARG
2	D	93	LEU
2	D	100	GLU
2	D	105	LEU
2	D	144	ARG
2	D	160	SER
2	D	167	GLU
2	D	172	TYR
2	D	227	ARG
2	D	239	ASP
2	D	244	GLU
2	D	262	LYS
2	D	301	GLN
2	D	346	SER
2	D	353	GLN
2	D	360	LYS
2	D	372	SER
2	D	430	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	356	GLN
2	B	282	GLN
2	B	285	GLN
1	C	140	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

1 ligand is modelled in this entry.

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	6X4	A	1458	-	29,33,33	2.65	7 (24%)	38,43,43	3.57	20 (52%)

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	6X4	A	1458	-	1/1/14/15	1/42/46/46	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1458	6X4	O7-C19	-6.38	1.20	1.42
3	A	1458	6X4	C1-N1	-2.01	1.41	1.46
3	A	1458	6X4	C12-N3	3.96	1.40	1.32
3	A	1458	6X4	C3-N1	4.20	1.43	1.34
3	A	1458	6X4	C18-N6	5.14	1.45	1.34
3	A	1458	6X4	C9-N4	5.40	1.45	1.34
3	A	1458	6X4	C15-N5	7.06	1.50	1.34

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1458	6X4	O3-C3-N1	-6.71	109.85	122.91
3	A	1458	6X4	O5-C15-C16	-3.63	111.72	120.45
3	A	1458	6X4	O1-C12-N3	-3.35	117.52	123.06
3	A	1458	6X4	O6-C18-C19	-3.33	112.62	119.59
3	A	1458	6X4	O4-C9-C10	-3.02	116.73	121.97
3	A	1458	6X4	C11-C14-N5	-2.88	105.43	109.92
3	A	1458	6X4	C13-C1-C12	-2.22	104.78	109.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1458	6X4	C6-C5-C4	-2.08	107.62	113.94
3	A	1458	6X4	C16-C15-N5	2.36	122.57	116.86
3	A	1458	6X4	C10-C9-N4	2.42	119.91	115.85
3	A	1458	6X4	C19-C18-N6	2.77	127.05	117.82
3	A	1458	6X4	C20-C14-N5	2.77	118.47	112.93
3	A	1458	6X4	C1-N1-C3	3.16	128.49	121.25
3	A	1458	6X4	C3-C4-N4	3.58	121.43	111.28
3	A	1458	6X4	C16-N6-C18	4.89	132.45	121.25
3	A	1458	6X4	C5-C4-C3	7.12	127.81	110.34
3	A	1458	6X4	C4-C3-N1	7.18	133.53	116.80
3	A	1458	6X4	C10-C11-C14	7.67	127.64	113.05
3	A	1458	6X4	C11-C10-C9	7.99	131.52	113.26
3	A	1458	6X4	C14-N5-C15	8.00	137.62	123.43

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1458	6X4	C4

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1458	6X4	C19-C18-N6-C16

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1458	6X4	9	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	418/451 (92%)	-0.08	2 (0%) 91 91	37, 55, 90, 148	0
1	C	413/451 (91%)	-0.04	5 (1%) 81 81	40, 67, 100, 148	0
2	B	417/451 (92%)	0.01	7 (1%) 73 72	40, 63, 96, 186	0
2	D	417/451 (92%)	0.20	14 (3%) 49 49	56, 80, 109, 128	0
All	All	1665/1804 (92%)	0.02	28 (1%) 73 72	37, 68, 102, 186	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	270	ASP	8.0
2	B	271	VAL	7.1
2	B	269	VAL	5.7
1	A	254	LYS	3.7
2	B	272	LEU	3.5
1	C	268	HIS	3.4
2	D	249	LEU	3.1
2	D	45	LEU	3.0
2	D	266	TYR	3.0
2	D	297	GLN	2.8
2	D	254	LYS	2.8
1	C	42	GLU	2.7
2	D	99	ARG	2.7
1	C	263	ASP	2.6
2	B	300	LYS	2.6
2	D	268	HIS	2.5
1	C	140	GLN	2.5
2	D	73	ARG	2.4
2	D	80	VAL	2.4
2	D	43	GLY	2.3
1	A	334	MET	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	268	HIS	2.2
2	D	105	LEU	2.2
2	D	114	ARG	2.2
2	D	82	LEU	2.1
1	C	326	LYS	2.1
2	B	267	GLY	2.0
2	D	104	ALA	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	6X4	A	1458	34/34	0.77	0.44	9.84	56,77,94,104	67

## 6.5 Other polymers [i](#)

There are no such residues in this entry.