



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 10:52 PM GMT

PDB ID : 3A3F  
Title : Crystal structure of penicillin binding protein 4 (dacB) from Haemophilus influenzae, complexed with novel beta-lactam (FMZ)  
Authors : Kawai, F.; Roper, D.I.; Park, S.-Y.; Tame, J.R.H.  
Deposited on : 2009-06-12  
Resolution : 2.10 Å (reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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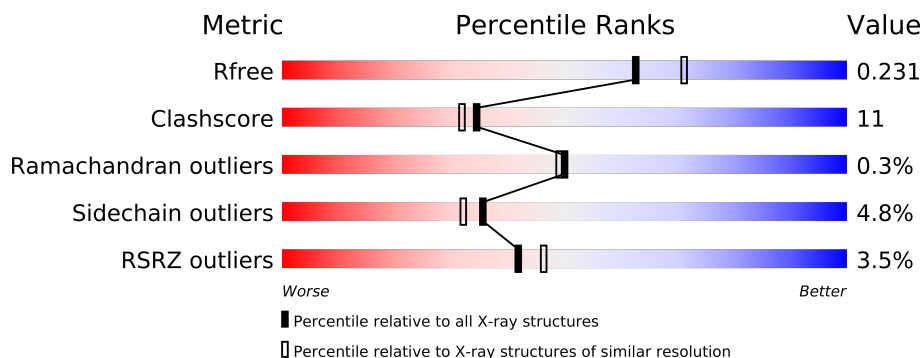
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.10 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))
$R_{free}$	66092	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (2.10-2.10)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	453	
1	B	453	

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 7354 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

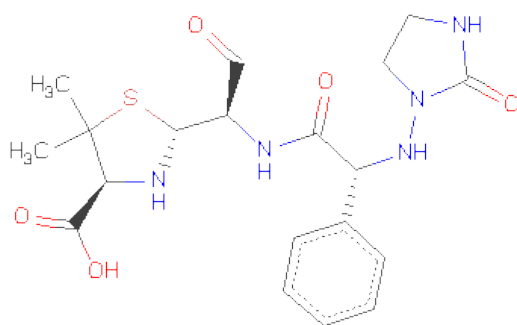
- Molecule 1 is a protein called Penicillin-binding protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	453	Total	C	N	O	S	0	0	0
			3505	2237	605	651	12			
1	B	453	Total	C	N	O	S	0	0	0
			3501	2235	605	649	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	MET	-	EXPRESSION TAG	UNP A8E0K8
B	27	MET	-	EXPRESSION TAG	UNP A8E0K8

- Molecule 2 is (2R,4S)-5,5-DIMETHYL-2-[(1R)-2-OXO-1-({(2R)-2-[(2-OXOIMIDAZOLIDI N-1-YL)AMINO]-2-PHENYLACETYL}AMINO)ETHYL]-1,3-THIAZOLIDINE-4-CARBOXYLICACID (three-letter code: FMZ) (formula: C<sub>19</sub>H<sub>25</sub>N<sub>5</sub>O<sub>5</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 30	C 19	N 5	O 5	S 1	0	0
2	B	1	Total 30	C 19	N 5	O 5	S 1	0	0

- Molecule 3 is water.

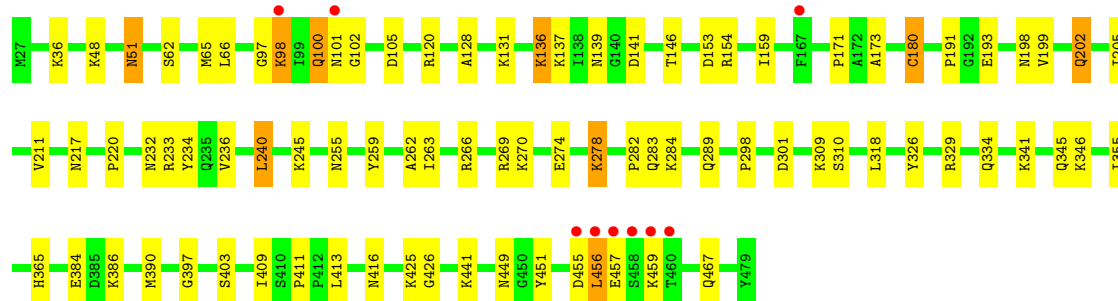
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	176	Total 176	O 176	0	0
3	B	112	Total 112	O 112	0	0

### 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.

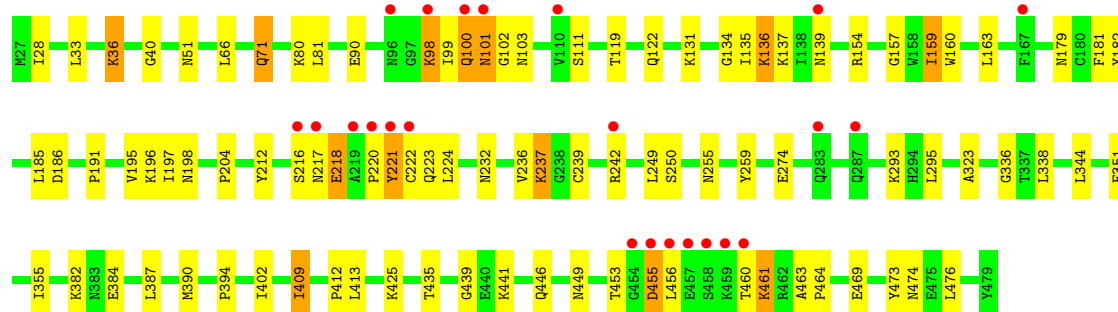
- Molecule 1: Penicillin-binding protein 4

Chain A: 



- Molecule 1: Penicillin-binding protein 4

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.80Å 92.10Å 104.45Å 90.00° 107.95° 90.00°	Depositor
Resolution (Å)	19.87 – 2.10 19.87 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.87-2.10) 95.9 (19.87-2.10)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.62 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, $R_{free}$	0.190 , 0.236 0.187 , 0.231	Depositor DCC
$R_{free}$ test set	3317 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.4	Xtriage
Anisotropy	0.240	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 40.3	EDS
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 65429 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7354	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

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

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	1.11	1/3571 (0.0%)	0.98	3/4830 (0.1%)
1	B	0.98	1/3567 (0.0%)	0.93	0/4825
All	All	1.05	2/7138 (0.0%)	0.96	3/9655 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	180	CYS	CB-SG	-15.14	1.56	1.82
1	B	236	VAL	CB-CG2	5.08	1.63	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	48	LYS	CD-CE-NZ	-5.81	98.34	111.70
1	A	455	ASP	CB-CG-OD2	5.36	123.12	118.30
1	A	455	ASP	CB-CG-OD1	-5.28	113.55	118.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3505	0	3553	79	0
1	B	3501	0	3549	80	0
2	A	30	0	23	2	0
2	B	30	0	23	2	0
3	A	176	0	0	7	0
3	B	112	0	0	3	0
All	All	7354	0	7148	154	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

All (154) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:154:ARG:NH1	1:B:163:LEU:HD13	1.48	1.24
1:B:154:ARG:HH11	1:B:163:LEU:CD1	1.63	1.11
1:B:217:ASN:O	1:B:220:PRO:HD2	1.61	1.00
1:B:154:ARG:HH11	1:B:163:LEU:HD13	0.80	0.96
1:A:66:LEU:H	1:A:449:ASN:HD21	1.15	0.93
1:B:66:LEU:H	1:B:449:ASN:HD21	1.13	0.92
1:A:202:GLN:HE21	1:A:202:GLN:N	1.67	0.91
1:B:137:LYS:HB3	1:B:274:GLU:HB3	1.50	0.91
1:B:218:GLU:N	1:B:218:GLU:OE2	2.04	0.90
1:A:202:GLN:NE2	1:A:202:GLN:H	1.69	0.90
1:A:98:LYS:HB3	1:A:98:LYS:HZ3	1.42	0.83
1:B:154:ARG:NH1	1:B:163:LEU:CD1	2.31	0.82
1:A:202:GLN:HE21	1:A:202:GLN:H	0.86	0.82
1:A:232:ASN:HD21	1:A:255:ASN:H	1.24	0.82
1:A:456:LEU:H	1:A:456:LEU:CD1	1.93	0.81
1:B:28:ILE:CD1	1:B:476:LEU:HD23	2.10	0.81
1:A:456:LEU:HG	1:B:355:ILE:HG23	1.62	0.81
1:B:425:LYS:HE2	1:B:456:LEU:HD23	1.64	0.80
1:A:240:LEU:HD23	1:A:240:LEU:N	1.98	0.77
1:B:137:LYS:CB	1:B:274:GLU:HB3	2.15	0.76
1:A:456:LEU:HD12	1:A:456:LEU:H	1.49	0.76
1:B:98:LYS:HD2	1:B:100:GLN:OE1	1.86	0.76
1:B:221:TYR:HD1	1:B:221:TYR:O	1.67	0.75
2:B:1:FMZ:HAVA	3:B:484:HOH:O	1.86	0.75
1:B:232:ASN:HD21	1:B:255:ASN:H	1.35	0.73
1:A:137:LYS:HG3	1:A:274:GLU:HB3	1.70	0.72
1:A:205:ILE:HD12	1:A:205:ILE:C	2.11	0.71
1:A:459:LYS:O	1:A:459:LYS:HG3	1.90	0.71
1:B:51:ASN:ND2	1:B:441:LYS:H	1.88	0.71
1:B:461:LYS:HG3	1:B:463:ALA:H	1.56	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:355:ILE:HD11	1:B:455:ASP:HA	1.73	0.70
1:A:355:ILE:CD1	1:B:455:ASP:HA	2.22	0.69
1:A:198:ASN:HB3	3:A:636:HOH:O	1.92	0.69
1:A:232:ASN:ND2	1:A:255:ASN:H	1.92	0.68
2:B:1:FMZ:CAV	3:B:484:HOH:O	2.42	0.67
1:B:90:GLU:HG2	1:B:295:LEU:HD23	1.77	0.65
1:B:119:THR:OG1	1:B:122:GLN:HG3	1.98	0.64
1:A:51:ASN:ND2	1:A:441:LYS:H	1.95	0.63
1:A:141:ASP:OD1	1:A:278:LYS:HG3	1.98	0.63
1:B:66:LEU:H	1:B:449:ASN:ND2	1.93	0.62
1:A:240:LEU:H	1:A:240:LEU:HD23	1.64	0.62
2:A:1:FMZ:CAV	3:A:13:HOH:O	2.47	0.62
1:A:425:LYS:NZ	1:A:456:LEU:HB3	2.14	0.62
1:A:98:LYS:NZ	1:A:98:LYS:HB3	2.14	0.62
1:A:66:LEU:H	1:A:449:ASN:ND2	1.94	0.62
1:B:28:ILE:HD13	1:B:476:LEU:HD23	1.81	0.62
1:A:326:TYR:OH	1:A:346:LYS:NZ	2.31	0.62
1:B:159:ILE:HD12	3:B:515:HOH:O	1.99	0.62
1:B:137:LYS:HB3	1:B:274:GLU:CB	2.24	0.62
1:B:100:GLN:CG	1:B:100:GLN:O	2.47	0.62
1:A:298:PRO:HD2	1:A:301:ASP:OD2	2.00	0.61
1:B:90:GLU:HG2	1:B:295:LEU:CD2	2.31	0.61
1:B:446:GLN:HE22	1:B:469:GLU:HG2	1.65	0.61
1:B:218:GLU:CA	1:B:218:GLU:OE2	2.49	0.60
1:B:80:LYS:HE3	1:B:387:LEU:O	2.02	0.60
1:A:51:ASN:HD21	1:A:441:LYS:H	1.49	0.59
1:A:211:VAL:HG23	1:A:236:VAL:HG23	1.85	0.58
1:B:196:LYS:CE	1:B:198:ASN:HD21	2.16	0.58
1:B:232:ASN:ND2	1:B:255:ASN:H	2.01	0.58
1:B:221:TYR:O	1:B:221:TYR:CD1	2.52	0.57
1:A:159:ILE:HD13	1:B:157:GLY:HA2	1.85	0.57
1:A:137:LYS:HD2	1:A:274:GLU:OE1	2.05	0.57
1:A:102:GLY:O	1:A:136:LYS:HD2	2.05	0.57
1:A:240:LEU:N	1:A:240:LEU:CD2	2.67	0.57
2:A:1:FMZ:CAU	3:A:13:HOH:O	2.53	0.56
1:A:51:ASN:H	1:A:51:ASN:HD22	1.52	0.55
1:B:453:THR:OG1	1:B:460:THR:HB	2.06	0.55
1:B:36:LYS:O	1:B:464:PRO:HB3	2.06	0.55
1:B:344:LEU:HD12	1:B:351:PHE:HZ	1.72	0.55
1:A:105:ASP:HA	1:A:139:ASN:HD22	1.70	0.55
1:A:309:LYS:HE2	1:A:309:LYS:HA	1.89	0.55
1:B:100:GLN:HG2	1:B:100:GLN:O	2.06	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:384:GLU:OE1	1:B:390:MET:HG2	2.07	0.53
1:B:100:GLN:O	1:B:101:ASN:HB2	2.09	0.52
1:B:137:LYS:HE2	1:B:139:ASN:ND2	2.24	0.52
1:A:269:ARG:HH11	1:A:269:ARG:HG3	1.75	0.52
1:A:120:ARG:HH21	1:A:120:ARG:HG2	1.75	0.52
1:A:193:GLU:HG3	3:A:615:HOH:O	2.09	0.52
1:A:51:ASN:N	1:A:51:ASN:HD22	2.08	0.52
1:B:216:SER:O	1:B:220:PRO:HD3	2.09	0.51
1:B:196:LYS:HE2	1:B:198:ASN:HD21	1.74	0.51
1:A:65:MET:HB3	1:A:449:ASN:ND2	2.25	0.51
1:A:205:ILE:HD12	1:A:205:ILE:O	2.10	0.50
1:B:453:THR:H	1:B:460:THR:CG2	2.25	0.50
1:B:51:ASN:HD21	1:B:441:LYS:H	1.56	0.50
1:B:409:ILE:H	1:B:409:ILE:HD12	1.77	0.50
1:A:425:LYS:HZ1	1:A:456:LEU:HB3	1.75	0.50
1:B:435:THR:CG2	1:B:439:GLY:HA2	2.42	0.50
1:A:100:GLN:HG2	1:A:100:GLN:O	2.11	0.50
1:B:412:PRO:HD2	1:B:474:ASN:HD21	1.78	0.49
1:A:384:GLU:OE1	1:A:390:MET:HG2	2.12	0.48
1:B:102:GLY:O	1:B:136:LYS:N	2.24	0.48
1:B:185:LEU:HG	1:B:197:ILE:HG12	1.95	0.48
1:B:204:PRO:HD2	1:B:259:TYR:CE1	2.48	0.48
1:A:341:LYS:O	1:A:345:GLN:HB2	2.13	0.48
1:A:397:GLY:HA2	1:A:403:SER:O	2.14	0.47
1:A:233:ARG:HD3	3:A:511:HOH:O	2.13	0.47
1:A:128:ALA:O	1:A:131:LYS:HB2	2.14	0.47
1:B:99:ILE:HD11	1:B:135:ILE:HD11	1.95	0.47
1:A:154:ARG:HG3	1:B:160:TRP:CE2	2.51	0.46
1:A:411:PRO:HA	3:A:608:HOH:O	2.14	0.46
1:A:234:TYR:CD2	1:A:234:TYR:N	2.82	0.46
1:A:98:LYS:CB	1:A:98:LYS:NZ	2.76	0.46
1:B:99:ILE:HA	1:B:103:ASN:O	2.16	0.46
1:A:425:LYS:HZ2	1:A:456:LEU:HB3	1.81	0.46
1:A:120:ARG:HD2	3:A:541:HOH:O	2.15	0.46
1:B:131:LYS:O	1:B:134:GLY:N	2.39	0.46
1:A:259:TYR:O	1:A:263:ILE:HG12	2.16	0.46
1:A:413:LEU:O	1:A:416:ASN:HB3	2.16	0.46
1:B:196:LYS:HE3	1:B:198:ASN:HD21	1.81	0.45
1:B:181:PHE:O	1:B:250:SER:HA	2.17	0.45
1:B:186:ASP:O	1:B:195:VAL:HG13	2.16	0.45
1:B:102:GLY:HA2	1:B:134:GLY:O	2.16	0.45
1:A:205:ILE:HG22	1:A:232:ASN:HB3	1.97	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:456:LEU:HD12	1:A:456:LEU:N	2.24	0.45
1:A:426:GLY:HA2	1:A:451:TYR:O	2.16	0.45
1:A:36:LYS:HE3	1:A:467:GLN:OE1	2.17	0.45
1:B:212:TYR:CZ	1:B:239:CYS:HB3	2.52	0.44
1:B:182:TYR:HA	1:B:249:LEU:O	2.18	0.44
1:A:205:ILE:CD1	1:A:205:ILE:C	2.82	0.44
1:A:217:ASN:O	1:A:220:PRO:HD2	2.17	0.44
1:A:97:GLY:C	1:A:98:LYS:HD2	2.38	0.43
1:A:141:ASP:OD1	1:A:278:LYS:CG	2.67	0.43
1:B:453:THR:OG1	1:B:460:THR:CB	2.67	0.43
1:B:33:LEU:O	1:B:36:LYS:HD2	2.19	0.43
1:A:262:ALA:O	1:A:266:ARG:HG3	2.19	0.43
1:A:365:HIS:NE2	1:B:159:ILE:HD13	2.34	0.43
1:B:154:ARG:HD3	1:B:163:LEU:HD22	2.01	0.42
1:A:199:VAL:HG11	1:A:205:ILE:HD11	1.99	0.42
1:A:62:SER:O	1:B:40:GLY:HA2	2.20	0.42
1:B:28:ILE:HD13	1:B:476:LEU:CD2	2.48	0.42
1:A:309:LYS:HE2	1:A:309:LYS:CA	2.46	0.42
1:B:455:ASP:N	1:B:455:ASP:OD1	2.51	0.42
1:A:154:ARG:HG3	1:B:160:TRP:CZ2	2.54	0.42
1:A:141:ASP:CG	1:A:278:LYS:HG3	2.40	0.42
1:B:323:ALA:HB2	1:B:336:GLY:HA2	2.02	0.42
1:B:71:GLN:HG3	1:B:71:GLN:O	2.20	0.41
1:A:153:ASP:O	1:A:171:PRO:HD2	2.20	0.41
1:A:456:LEU:N	1:A:456:LEU:CD1	2.74	0.41
1:A:269:ARG:NH1	1:A:269:ARG:HG3	2.35	0.41
1:A:101:ASN:HD22	1:A:101:ASN:HA	1.71	0.41
1:B:102:GLY:HA3	1:B:136:LYS:HE2	2.02	0.41
1:B:179:ASN:HA	1:B:179:ASN:HD22	1.52	0.41
1:B:237:LYS:HB2	1:B:237:LYS:HE2	1.94	0.41
1:A:289:GLN:O	1:A:289:GLN:HG3	2.21	0.41
1:B:394:PRO:HB2	1:B:402:ILE:HG12	2.02	0.41
1:B:425:LYS:NZ	1:B:456:LEU:HA	2.36	0.41
1:A:282:PRO:O	1:A:283:GLN:HB2	2.20	0.41
1:B:413:LEU:HD13	1:B:473:TYR:HB2	2.03	0.41
1:B:36:LYS:HB3	1:B:36:LYS:HE3	1.49	0.40
1:A:318:LEU:HD23	1:A:318:LEU:HA	1.92	0.40
1:A:146:THR:HB	1:A:173:ALA:HB3	2.03	0.40
1:A:334:GLN:HE21	1:B:223:GLN:CD	2.24	0.40
1:B:81:LEU:HD23	1:B:81:LEU:HA	1.86	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	451/453 (100%)	443 (98%)	8 (2%)	0	100	100
1	B	451/453 (100%)	433 (96%)	15 (3%)	3 (1%)	30	23
All	All	902/906 (100%)	876 (97%)	23 (2%)	3 (0%)	50	49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	100	GLN
1	B	191	PRO
1	B	101	ASN

### 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	378/378 (100%)	360 (95%)	18 (5%)	35	32
1	B	377/378 (100%)	359 (95%)	18 (5%)	35	32
All	All	755/756 (100%)	719 (95%)	36 (5%)	35	32

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	98	LYS
1	A	100	GLN
1	A	136	LYS
1	A	180	CYS
1	A	191	PRO

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Mol	Chain	Res	Type
1	A	202	GLN
1	A	240	LEU
1	A	245	LYS
1	A	270	LYS
1	A	278	LYS
1	A	284	LYS
1	A	310	SER
1	A	329	ARG
1	A	386	LYS
1	A	409	ILE
1	A	456	LEU
1	A	457	GLU
1	B	36	LYS
1	B	71	GLN
1	B	98	LYS
1	B	111	SER
1	B	136	LYS
1	B	159	ILE
1	B	218	GLU
1	B	221	TYR
1	B	222	CYS
1	B	224	LEU
1	B	237	LYS
1	B	242	ARG
1	B	293	LYS
1	B	338	LEU
1	B	382	LYS
1	B	409	ILE
1	B	455	ASP
1	B	461	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	51	ASN
1	A	101	ASN
1	A	139	ASN
1	A	152	HIS
1	A	198	ASN
1	A	202	GLN
1	A	206	GLN

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Mol	Chain	Res	Type
1	A	223	GLN
1	A	232	ASN
1	A	283	GLN
1	A	334	GLN
1	A	446	GLN
1	A	449	ASN
1	B	35	GLN
1	B	51	ASN
1	B	71	GLN
1	B	103	ASN
1	B	139	ASN
1	B	179	ASN
1	B	198	ASN
1	B	223	GLN
1	B	232	ASN
1	B	276	ASN
1	B	283	GLN
1	B	334	GLN
1	B	446	GLN
1	B	449	ASN
1	B	474	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

2 ligands are 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
2	FMZ	A	1	1	32,32,32	2.98	6 (18%)	46,46,46	3.11	15 (32%)
2	FMZ	B	1	1	32,32,32	3.02	7 (21%)	46,46,46	2.92	19 (41%)

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
2	FMZ	A	1	1	-	0/21/51/51	0/3/3/3
2	FMZ	B	1	1	-	0/21/51/51	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FMZ	NAL-NAI	-13.08	1.25	1.41
2	A	1	FMZ	NAL-NAI	-12.87	1.25	1.41
2	A	1	FMZ	OAR-CAM	6.68	1.36	1.23
2	B	1	FMZ	OAR-CAM	6.11	1.35	1.23
2	B	1	FMZ	C14-C15	5.36	1.55	1.50
2	A	1	FMZ	C6-S1	-3.86	1.77	1.85
2	B	1	FMZ	C6-S1	-3.57	1.78	1.85
2	A	1	FMZ	CAU-CAV	3.39	1.59	1.52
2	A	1	FMZ	CAS-CAK	-3.13	1.47	1.52
2	A	1	FMZ	CAU-NAI	-2.97	1.43	1.47
2	B	1	FMZ	CAU-CAV	2.45	1.57	1.52
2	B	1	FMZ	CAS-CAK	-2.06	1.49	1.52
2	B	1	FMZ	C12-C2	-2.03	1.49	1.52

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	FMZ	CAK-NAL-NAI	16.46	131.95	112.56
2	B	1	FMZ	CAK-NAL-NAI	12.35	127.12	112.56
2	B	1	FMZ	CAV-CAU-NAI	-5.38	95.16	102.17
2	B	1	FMZ	S1-C13-N3	-5.37	99.42	106.66
2	A	1	FMZ	CAV-CAU-NAI	-4.58	96.21	102.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FMZ	CAU-CAV-NAO	4.55	108.81	102.65
2	A	1	FMZ	CAU-CAV-NAO	4.04	108.13	102.65
2	B	1	FMZ	C6-S1-C13	3.89	102.40	94.01
2	B	1	FMZ	C14-C13-N3	-3.67	104.66	112.69
2	A	1	FMZ	C13-C14-C15	-3.54	106.53	112.03
2	B	1	FMZ	C1-C6-S1	3.53	115.13	109.15
2	B	1	FMZ	C3-CAK-NAL	-3.43	98.32	108.19
2	A	1	FMZ	C14-C13-S1	3.41	119.87	110.25
2	B	1	FMZ	C14-C13-S1	3.27	119.46	110.25
2	B	1	FMZ	C6-C12-C2	3.24	117.08	112.55
2	B	1	FMZ	CAS-CAK-C3	3.21	114.89	107.77
2	B	1	FMZ	C1-C6-C16	-3.16	105.58	110.90
2	A	1	FMZ	C14-C13-N3	-3.07	105.97	112.69
2	B	1	FMZ	C13-N3-C12	3.00	116.77	109.62
2	A	1	FMZ	CAM-NAI-NAL	-2.91	118.04	123.99
2	A	1	FMZ	C6-C12-C2	2.85	116.54	112.55
2	A	1	FMZ	CBA-CAS-CAZ	2.83	122.09	118.33
2	A	1	FMZ	C1-C6-C16	-2.67	106.41	110.90
2	A	1	FMZ	C3-CAK-NAL	-2.63	100.63	108.19
2	A	1	FMZ	OAR-CAM-NAI	-2.59	124.07	126.07
2	B	1	FMZ	CAU-NAI-CAM	2.53	118.58	113.07
2	B	1	FMZ	C12-C6-S1	-2.46	99.65	104.00
2	A	1	FMZ	CAU-NAI-NAL	2.45	125.13	115.44
2	B	1	FMZ	OAR-CAM-NAI	2.44	127.95	126.07
2	A	1	FMZ	CAS-CAK-C3	2.37	113.04	107.77
2	B	1	FMZ	OAR-CAM-NAO	-2.35	123.31	127.12
2	B	1	FMZ	CAM-NAI-NAL	-2.26	119.39	123.99
2	B	1	FMZ	C13-C14-C15	-2.09	108.79	112.03
2	A	1	FMZ	C13-C14-N1	2.05	113.10	109.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	453/453 (100%)	-0.16	9 (1%) 62 67	13, 25, 43, 68	0
1	B	453/453 (100%)	0.15	23 (5%) 27 30	15, 31, 59, 77	0
All	All	906/906 (100%)	-0.01	32 (3%) 42 46	13, 28, 53, 77	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	220	PRO	8.3
1	B	457	GLU	7.7
1	B	454	GLY	7.4
1	B	460	THR	7.3
1	B	458	SER	7.2
1	B	455	ASP	7.2
1	B	459	LYS	6.3
1	B	456	LEU	5.8
1	A	458	SER	5.2
1	B	216	SER	5.1
1	A	457	GLU	5.0
1	A	456	LEU	4.9
1	A	459	LYS	4.1
1	B	287	GLN	3.8
1	B	219	ALA	3.7
1	A	455	ASP	3.7
1	B	222	CYS	3.7
1	B	217	ASN	3.6
1	B	283	GLN	3.4
1	B	221	TYR	3.1
1	B	96	ASN	3.0
1	A	460	THR	2.8
1	B	242	ARG	2.8
1	B	101	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	167	PHE	2.7
1	B	100	GLN	2.7
1	B	98	LYS	2.6
1	A	98	LYS	2.6
1	B	139	ASN	2.4
1	B	167	PHE	2.4
1	A	101	ASN	2.3
1	B	110	VAL	2.3

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	FMZ	A	1	30/30	0.10	-0.15	13,23,41,44	0
2	FMZ	B	1	30/30	0.10	-0.30	19,26,48,49	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.