



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:04 PM GMT

PDB ID : 1O07
Title : Crystal Structure of the complex between Q120L/Y150E mutant of AmpC and a beta-lactam inhibitor (MXG)
Authors : Meroueh, S.O.; Minasov, G.; Lee, W.; Shoichet, B.K.; Mobashery, S.
Deposited on : 2003-02-20
Resolution : 1.71 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

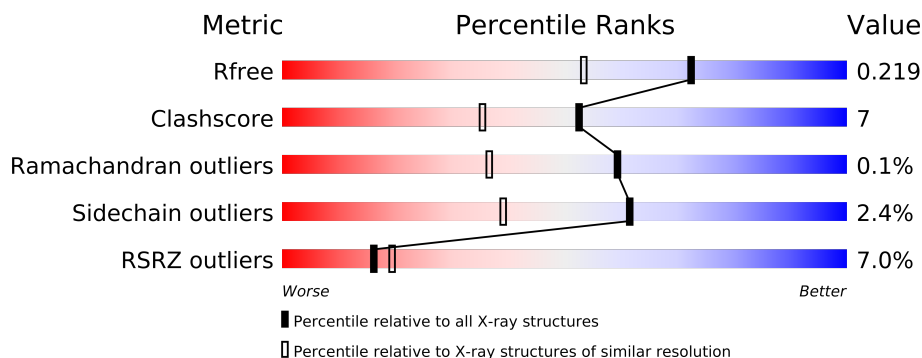
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.71 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	2979 (1.74-1.70)
Clashscore	79885	3506 (1.74-1.70)
Ramachandran outliers	78287	3449 (1.74-1.70)
Sidechain outliers	78261	3449 (1.74-1.70)
RSRZ outliers	66119	2979 (1.74-1.70)

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 ≥ 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	358	
1	B	358	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	MXG	A	400[B]	-	X
3	MXG	B	400[A]	-	X
3	MXG	B	400[B]	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7358 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 Beta-lactamase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	355	Total	C	N	O	S	0	45	0
			3152	2014	543	588	7			
1	B	358	Total	C	N	O	S	0	48	0
			3196	2041	555	593	7			

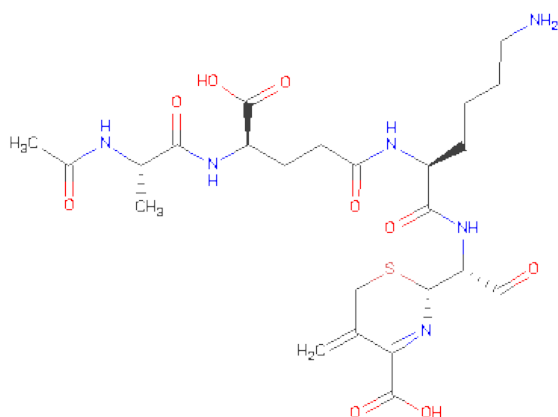
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	120	LEU	GLN	ENGINEERED	UNP P00811
A	150	GLU	TYR	ENGINEERED	UNP P00811
B	120	LEU	GLN	ENGINEERED	UNP P00811
B	150	GLU	TYR	ENGINEERED	UNP P00811

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 3 is 2-(1-{2-[4-(2-ACETYLAMINO-PROPIONYLAMINO)-4-CARBOXY-BUTYRYLAMINO]-6-AMINO-HEXANOYLAMINO}-2-OXO-ETHYL)-5-METHYLENE-5,6-DIHYDRO-2H-[1,3]THIAZINE-4-CARBOXYLICACID (three-letter code: MXG) (formula: C₂₄H₃₆N₆O₉S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	1
			40	24	6	9	1		
3	B	1	Total	C	N	O	S	0	1
			80	48	12	18	2		

- Molecule 4 is water.

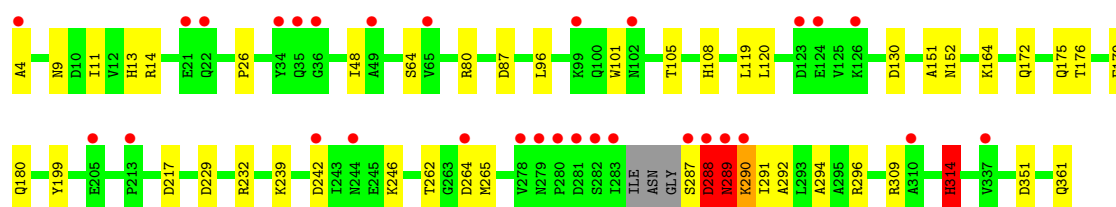
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	398	Total	O	0	62
			436	436		
4	B	408	Total	O	0	68
			452	452		

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.

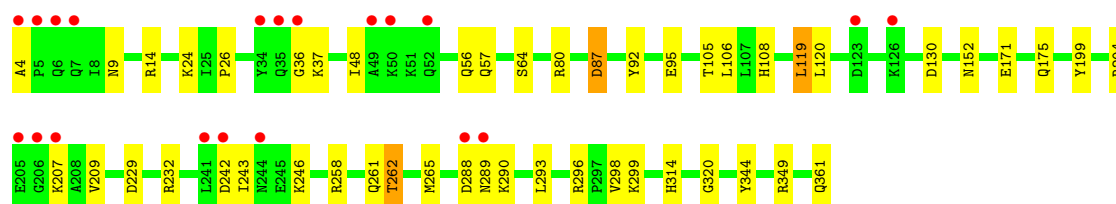
• Molecule 1: Beta-lactamase

Chain A: 



• Molecule 1: Beta-lactamase

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	118.81Å 76.30Å 98.13Å 90.00° 116.21° 90.00°	Depositor
Resolution (Å)	24.77 – 1.71 24.74 – 1.71	Depositor EDS
% Data completeness (in resolution range)	98.1 (24.77-1.71) 94.9 (24.74-1.71)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.82 (at 1.71Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.154 , 0.191 0.193 , 0.219	Depositor DCC
R_{free} test set	4054 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	18.5	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 49.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 80612 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7358	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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: MXG, K

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	0.81	1/3235 (0.0%)	1.07	24/4405 (0.5%)
1	B	0.76	0/3277	0.99	16/4461 (0.4%)
All	All	0.79	1/6512 (0.0%)	1.03	40/8866 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	287	SER	C-N	10.61	1.58	1.34

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	287	SER	CA-C-N	-7.42	100.87	117.20
1	B	242	ASP	CB-CG-OD2	7.29	124.86	118.30
1	B	229	ASP	CB-CG-OD2	7.19	124.77	118.30
1	B	130	ASP	CB-CG-OD2	7.09	124.68	118.30
1	A	232[A]	ARG	NE-CZ-NH2	7.02	123.81	120.30
1	A	232[B]	ARG	NE-CZ-NH2	7.02	123.81	120.30
1	A	232[A]	ARG	NE-CZ-NH1	-6.84	116.88	120.30
1	A	232[B]	ARG	NE-CZ-NH1	-6.84	116.88	120.30
1	B	288	ASP	CB-CG-OD2	6.78	124.40	118.30
1	A	351	ASP	CB-CG-OD2	6.66	124.29	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	242	ASP	CB-CG-OD2	6.44	124.09	118.30
1	A	229	ASP	CB-CG-OD2	6.33	124.00	118.30
1	A	217	ASP	O-C-N	-5.99	113.11	122.70
1	B	87	ASP	CB-CG-OD1	5.88	123.60	118.30
1	A	179	PHE	CB-CG-CD1	5.83	124.88	120.80
1	A	13	HIS	O-C-N	-5.79	113.44	122.70
1	B	232[A]	ARG	NE-CZ-NH2	5.68	123.14	120.30
1	B	232[B]	ARG	NE-CZ-NH2	5.68	123.14	120.30
1	A	264	ASP	CB-CG-OD2	5.67	123.40	118.30
1	B	36	GLY	O-C-N	-5.60	113.74	122.70
1	B	204	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	B	258	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	B	258	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	130	ASP	CB-CG-OD2	5.49	123.24	118.30
1	A	296	ARG	NE-CZ-NH1	-5.32	117.64	120.30
1	B	296[A]	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	B	296[B]	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	80	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	B	80	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	A	288[A]	ASP	O-C-N	-5.19	114.39	122.70
1	A	288[B]	ASP	O-C-N	-5.19	114.39	122.70
1	A	87	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	80	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	A	199	TYR	CB-CG-CD2	5.09	124.06	121.00
1	A	289	ASN	O-C-N	5.08	130.83	122.70
1	B	80	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	A	292	ALA	O-C-N	-5.05	114.61	122.70
1	A	288[A]	ASP	CB-CG-OD2	5.05	122.84	118.30
1	A	288[B]	ASP	CB-CG-OD2	5.05	122.84	118.30
1	B	199	TYR	CB-CG-CD2	5.02	124.01	121.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	288[A]	ASP	Peptide
1	A	288[B]	ASP	Peptide
1	A	314	HIS	Mainchain

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	3152	0	3105	22	1
1	B	3196	0	3161	67	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	40	0	33	4	0
3	B	80	0	64	28	0
4	A	436	0	0	4	0
4	B	452	0	0	11	1
All	All	7358	0	6363	92	1

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 7.

All (92) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:209[B]:VAL:HG11	3:B:400[B]:MXG:C35	1.49	1.39
1:B:209[B]:VAL:CG1	3:B:400[B]:MXG:H352	1.68	1.22
1:B:293[A]:LEU:HD21	3:B:400[A]:MXG:HC22	1.19	1.17
1:B:293[A]:LEU:HD21	3:B:400[A]:MXG:C2	1.81	1.10
1:B:289[B]:ASN:HB3	1:B:293[B]:LEU:HD23	1.37	1.03
1:B:293[A]:LEU:HD11	3:B:400[A]:MXG:HC21	1.49	0.93
1:B:119[B]:LEU:HD22	1:B:120[B]:LEU:CD1	2.05	0.87
1:B:293[A]:LEU:CD2	3:B:400[A]:MXG:HC22	2.05	0.86
1:B:14[B]:ARG:HD3	4:B:800[B]:HOH:O	1.76	0.84
1:B:293[A]:LEU:HD11	3:B:400[A]:MXG:C2	2.07	0.84
1:A:119[B]:LEU:HD21	3:A:400[B]:MXG:S1	2.18	0.84
1:B:293[B]:LEU:HB3	3:B:400[B]:MXG:HC32	1.63	0.81
1:B:289[B]:ASN:HB3	1:B:293[B]:LEU:CD2	2.11	0.79
3:B:400[B]:MXG:H151	4:B:807[B]:HOH:O	1.83	0.79
1:B:209[B]:VAL:HG11	3:B:400[B]:MXG:H352	0.81	0.78
1:A:4[B]:ALA:HB1	1:A:9[B]:ASN:HD21	1.52	0.75
1:B:119[B]:LEU:HD22	1:B:120[B]:LEU:HD12	1.68	0.74
1:B:57[B]:GLN:HB3	4:B:783:HOH:O	1.87	0.74
1:B:209[B]:VAL:CG1	3:B:400[B]:MXG:C35	2.46	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:293[A]:LEU:CD1	3:B:400[A]:MXG:HC21	2.19	0.72
1:A:180[A]:GLN:NE2	4:A:583[A]:HOH:O	2.24	0.71
1:B:290[A]:LYS:NZ	4:B:789:HOH:O	2.24	0.71
1:B:289[B]:ASN:O	1:B:293[B]:LEU:HG	1.94	0.68
1:A:119[B]:LEU:CD2	3:A:400[B]:MXG:S1	2.82	0.68
1:B:293[A]:LEU:CD2	3:B:400[A]:MXG:C2	2.66	0.67
1:B:289[B]:ASN:CB	1:B:293[B]:LEU:HD23	2.20	0.66
1:B:64[A]:SER:N	3:B:400[A]:MXG:O8A	2.29	0.66
1:B:37[B]:LYS:NZ	4:B:699[B]:HOH:O	2.29	0.66
1:A:4[B]:ALA:HB1	1:A:9[B]:ASN:ND2	2.11	0.66
1:A:11[B]:ILE:HD11	4:A:761[B]:HOH:O	1.96	0.64
1:A:289:ASN:O	1:A:290:LYS:HG2	1.97	0.64
1:B:262[A]:THR:HG23	1:B:265[A]:MET:SD	2.38	0.63
1:A:4[B]:ALA:CB	1:A:9[B]:ASN:HD21	2.12	0.63
1:A:262[A]:THR:O	1:A:265[A]:MET:HG3	2.02	0.60
1:B:207[B]:LYS:O	1:B:209[B]:VAL:HG23	2.02	0.59
1:A:175[A]:GLN:O	1:A:180[A]:GLN:HG2	2.02	0.59
1:B:261[B]:GLN:CD	1:B:299[B]:LYS:HE2	2.22	0.59
1:B:119[B]:LEU:HD23	3:B:400[B]:MXG:S1	2.43	0.58
1:A:11[B]:ILE:HG12	1:A:14[B]:ARG:NH1	2.19	0.57
1:B:119[B]:LEU:HD21	3:B:400[B]:MXG:C3	2.34	0.57
1:A:119[B]:LEU:O	1:A:152[B]:ASN:HB2	2.05	0.57
1:B:119[B]:LEU:CD2	3:B:400[B]:MXG:S1	2.93	0.57
1:B:293[B]:LEU:HB3	3:B:400[B]:MXG:C3A	2.33	0.57
3:A:400[B]:MXG:H142	4:A:797[B]:HOH:O	2.04	0.56
1:B:262[A]:THR:CG2	1:B:265[A]:MET:SD	2.93	0.56
1:A:314:HIS:CD2	1:A:314:HIS:C	2.78	0.56
1:B:57[B]:GLN:CB	4:B:783:HOH:O	2.49	0.56
1:B:261[B]:GLN:OE1	1:B:299[B]:LYS:HE2	2.07	0.54
1:B:119[B]:LEU:CD2	1:B:120[B]:LEU:HD12	2.37	0.53
1:A:291:ILE:HG21	1:A:294:ALA:HB2	1.91	0.53
1:B:289[B]:ASN:O	1:B:293[B]:LEU:CG	2.56	0.53
1:B:289[B]:ASN:O	1:B:293[B]:LEU:CD2	2.57	0.52
1:B:293[A]:LEU:CD1	3:B:400[A]:MXG:C2	2.84	0.51
1:B:293[A]:LEU:HD21	3:B:400[A]:MXG:HC21	1.87	0.50
1:B:261[B]:GLN:CD	1:B:299[B]:LYS:CE	2.80	0.49
1:B:14[B]:ARG:CD	4:B:800[B]:HOH:O	2.45	0.49
1:B:119[B]:LEU:HD21	3:B:400[B]:MXG:C4	2.42	0.49
1:B:293[A]:LEU:HD11	3:B:400[A]:MXG:C3	2.42	0.49
1:B:289[B]:ASN:O	1:B:293[B]:LEU:HD23	2.12	0.49
3:B:400[A]:MXG:H353	4:B:806[A]:HOH:O	2.12	0.49
3:A:400[B]:MXG:H312	3:A:400[B]:MXG:H23	1.95	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:207[B]:LYS:HG2	1:B:209[B]:VAL:HG22	1.95	0.48
1:B:92:TYR:CE2	1:B:106:LEU:HD11	2.48	0.47
1:A:172[A]:GLN:HE21	1:A:176:THR:HG23	1.79	0.47
1:B:171[A]:GLU:HG2	1:B:175[A]:GLN:NE2	2.30	0.46
1:B:243[B]:ILE:HD11	4:B:756:HOH:O	2.15	0.46
1:B:105:THR:H	1:B:108:HIS:HD2	1.62	0.46
1:B:56[B]:GLN:HG2	1:B:57[B]:GLN:HG3	1.98	0.46
1:A:120:LEU:CD2	1:A:152[B]:ASN:HD22	2.30	0.45
1:A:26:PRO:HB3	1:A:48:ILE:HD11	1.97	0.45
1:B:87:ASP:OD2	1:B:92:TYR:OH	2.32	0.45
1:B:57[B]:GLN:CG	4:B:783:HOH:O	2.64	0.45
1:B:243[B]:ILE:CD1	4:B:756:HOH:O	2.64	0.45
1:B:262[B]:THR:HG22	1:B:298:VAL:HG12	1.99	0.45
1:B:119[B]:LEU:HD21	3:B:400[B]:MXG:S1	2.58	0.44
1:B:293[A]:LEU:CD2	3:B:400[A]:MXG:HC21	2.46	0.44
1:B:171[A]:GLU:O	1:B:175[A]:GLN:HG3	2.17	0.44
1:B:4:ALA:HB3	1:B:9:ASN:ND2	2.33	0.44
1:B:289[B]:ASN:C	1:B:293[B]:LEU:HD23	2.37	0.43
1:A:309[B]:ARG:HD3	1:B:246[B]:LYS:NZ	2.34	0.43
1:B:262[B]:THR:CG2	1:B:298:VAL:HG12	2.49	0.43
1:B:152[B]:ASN:ND2	3:B:400[B]:MXG:O11	2.42	0.42
1:A:119[A]:LEU:HA	1:A:151:ALA:HA	2.02	0.42
1:B:26:PRO:HB3	1:B:48:ILE:HD11	2.01	0.42
1:B:320:GLY:HA3	3:B:400[B]:MXG:H32	1.86	0.41
1:A:4[B]:ALA:HB2	4:A:589:HOH:O	2.19	0.41
1:B:344:TYR:CZ	1:B:349:ARG:HG2	2.55	0.41
1:B:261[B]:GLN:CD	1:B:299[B]:LYS:NZ	2.74	0.41
1:A:105:THR:H	1:A:108:HIS:HD2	1.68	0.41
1:B:119[B]:LEU:HD21	3:B:400[B]:MXG:C2	2.51	0.40
1:B:261[B]:GLN:OE1	1:B:299[B]:LYS:CE	2.68	0.40
1:A:96[A]:LEU:HD21	1:A:101:TRP:CD2	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:4[B]:ALA:O	4:B:584:HOH:O[3_445]	2.06	0.14

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	395/358 (110%)	381 (96%)	14 (4%)	0	100	100
1	B	404/358 (113%)	396 (98%)	6 (2%)	2 (0%)	38	17
All	All	799/716 (112%)	777 (97%)	20 (2%)	2 (0%)	59	28

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	119[A]	LEU
1	B	119[B]	LEU

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	334/292 (114%)	321 (96%)	13 (4%)	43	17
1	B	339/292 (116%)	332 (98%)	7 (2%)	66	45
All	All	673/584 (115%)	653 (97%)	20 (3%)	61	28

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64[A]	SER
1	A	64[B]	SER
1	A	164[A]	LYS
1	A	164[B]	LYS
1	A	239	LYS
1	A	246[A]	LYS
1	A	246[B]	LYS

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Mol	Chain	Res	Type
1	A	288[A]	ASP
1	A	288[B]	ASP
1	A	289	ASN
1	A	290	LYS
1	A	314	HIS
1	A	361	GLN
1	B	24	LYS
1	B	95[A]	GLU
1	B	95[B]	GLU
1	B	262[A]	THR
1	B	262[B]	THR
1	B	314	HIS
1	B	361	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	102	ASN
1	A	108	HIS
1	A	137	ASN
1	A	249	GLN
1	A	361	GLN
1	B	9	ASN
1	B	108	HIS
1	B	137	ASN
1	B	172	GLN
1	B	249	GLN
1	B	253	GLN
1	B	358	ASN
1	B	361	GLN

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 ⓘ

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	MXG	A	400[B]	-	40,40,40	0.88	3 (7%)	51,53,53	2.02	13 (25%)
3	MXG	B	400[A]	-	40,40,40	0.93	2 (5%)	51,53,53	3.05	19 (37%)
3	MXG	B	400[B]	-	40,40,40	1.11	4 (10%)	51,53,53	2.34	13 (25%)

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	MXG	A	400[B]	-	-	0/42/61/61	0/0/1/1
3	MXG	B	400[A]	-	-	0/42/61/61	0/0/1/1
3	MXG	B	400[B]	-	-	0/42/61/61	0/0/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	400[B]	MXG	C7-C8	3.17	1.53	1.50
3	A	400[B]	MXG	C7-C8	2.70	1.53	1.50
3	B	400[A]	MXG	C6-S1	-2.60	1.76	1.82
3	B	400[A]	MXG	C2-S1	-2.40	1.76	1.82
3	A	400[B]	MXG	C6-S1	-2.38	1.77	1.82
3	B	400[B]	MXG	C6-S1	-2.22	1.77	1.82
3	B	400[B]	MXG	C4-N5	-2.12	1.26	1.28
3	B	400[B]	MXG	C2-S1	-2.10	1.77	1.82
3	A	400[B]	MXG	C2-S1	-2.09	1.77	1.82

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	400[A]	MXG	C23-N27-C28	8.90	141.32	121.63
3	B	400[A]	MXG	C7-C6-S1	-7.50	99.11	112.76
3	B	400[B]	MXG	C23-N27-C28	7.12	137.37	121.63
3	A	400[B]	MXG	C3-C4-N5	-6.12	116.77	124.23
3	B	400[A]	MXG	C12-N18-C19	6.09	137.87	121.53
3	B	400[A]	MXG	C13-C12-N18	-5.88	99.64	110.83
3	B	400[B]	MXG	C6-N5-C4	5.79	124.86	116.66
3	B	400[A]	MXG	C7-C6-N5	5.46	116.82	111.19
3	A	400[B]	MXG	C22-C23-N27	-5.27	100.80	110.83
3	B	400[A]	MXG	C3-C4-N5	-5.26	117.82	124.23
3	B	400[B]	MXG	C7-N9-C10	5.04	131.55	123.09
3	B	400[A]	MXG	C6-N5-C4	4.65	123.23	116.66
3	B	400[B]	MXG	C7-C6-N5	-4.49	106.56	111.19
3	B	400[A]	MXG	C8-C7-N9	4.44	118.11	109.61
3	B	400[B]	MXG	C21-C22-C23	4.44	121.69	112.99
3	B	400[B]	MXG	C30-C28-N27	4.43	127.44	116.89
3	B	400[A]	MXG	C30-C28-N27	4.38	127.33	116.89
3	A	400[B]	MXG	C8-C7-N9	4.30	117.83	109.61
3	B	400[A]	MXG	C7-N9-C10	4.13	130.03	123.09
3	B	400[B]	MXG	C22-C23-N27	-4.03	103.16	110.83
3	A	400[B]	MXG	C23-N27-C28	4.03	130.53	121.63
3	B	400[A]	MXG	C2-S1-C6	3.87	102.19	94.48
3	B	400[A]	MXG	C24-C23-N27	3.75	120.21	110.53
3	B	400[B]	MXG	C3-C4-N5	-3.60	119.84	124.23
3	A	400[B]	MXG	C7-C6-N5	3.59	114.90	111.19
3	B	400[A]	MXG	C22-C23-N27	-3.57	104.02	110.83
3	B	400[A]	MXG	C21-C19-N18	-3.55	109.08	115.83
3	B	400[A]	MXG	C4A-C4-N5	3.36	120.47	115.74
3	B	400[A]	MXG	C10-C12-N18	3.30	120.56	111.28
3	B	400[A]	MXG	O29-C28-N27	-3.28	116.61	122.93
3	B	400[B]	MXG	C12-N18-C19	3.27	130.29	121.53
3	A	400[B]	MXG	C4A-C4-N5	3.16	120.18	115.74
3	A	400[B]	MXG	C30-C28-N27	3.03	124.12	116.89
3	B	400[B]	MXG	O20-C19-C21	-2.82	116.31	121.92
3	B	400[A]	MXG	C13-C12-C10	2.79	116.78	110.31
3	A	400[B]	MXG	C6-N5-C4	2.71	120.49	116.66
3	B	400[B]	MXG	C8-C7-N9	2.68	114.73	109.61
3	B	400[B]	MXG	O29-C28-C30	-2.63	114.20	120.42
3	A	400[B]	MXG	C7-N9-C10	2.60	127.45	123.09
3	A	400[B]	MXG	C12-N18-C19	2.52	128.30	121.53
3	B	400[A]	MXG	O20-C19-N18	2.41	127.27	123.08
3	B	400[B]	MXG	O29-C28-N27	-2.38	118.35	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	400[B]	MXG	C31-C30-C28	2.31	114.89	110.22
3	A	400[B]	MXG	C7-C6-S1	-2.18	108.79	112.76
3	A	400[B]	MXG	O20-C19-C21	-2.13	117.69	121.92

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, 95th 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 ²)	Q < 0.9
1	A	355/358 (99%)	0.42	30 (8%)	11 13	4, 10, 26, 58	0
1	B	358/358 (100%)	0.28	20 (5%)	24 27	5, 10, 23, 30	0
All	All	713/716 (99%)	0.35	50 (7%)	16 19	4, 10, 23, 58	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	289	ASN	8.2
1	A	287	SER	6.3
1	A	279	ASN	5.5
1	A	288[A]	ASP	5.4
1	A	290	LYS	4.8
1	B	4	ALA	4.6
1	A	4[A]	ALA	4.5
1	B	244	ASN	4.5
1	A	281	ASP	4.3
1	B	49	ALA	4.3
1	B	242	ASP	3.5
1	A	126	LYS	3.5
1	A	244	ASN	3.4
1	A	22	GLN	3.4
1	B	6	GLN	3.4
1	A	36	GLY	3.3
1	B	126	LYS	3.2
1	A	34	TYR	3.1
1	A	278	VAL	3.0
1	B	289[A]	ASN	3.0
1	B	206	GLY	2.9
1	A	282	SER	2.8
1	A	242	ASP	2.8
1	A	123	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	102	ASN	2.7
1	B	5	PRO	2.7
1	A	35	GLN	2.6
1	B	7	GLN	2.6
1	B	52[A]	GLN	2.6
1	B	288	ASP	2.6
1	B	35	GLN	2.4
1	A	283	ILE	2.4
1	A	205[A]	GLU	2.4
1	B	241	LEU	2.3
1	A	124[A]	GLU	2.3
1	B	50	LYS	2.3
1	B	34	TYR	2.3
1	B	36	GLY	2.3
1	A	213[A]	PRO	2.3
1	A	99	LYS	2.2
1	A	49	ALA	2.2
1	A	21[A]	GLU	2.2
1	B	207[A]	LYS	2.2
1	B	205[A]	GLU	2.1
1	A	65	VAL	2.1
1	A	264	ASP	2.1
1	A	310	ALA	2.1
1	A	280	PRO	2.1
1	B	123	ASP	2.0
1	A	337	VAL	2.0

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, 95th 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(\AA^2)	Q<0.9
3	MXG	B	400[B]	40/40	0.34	4.40	17,44,50,52	40
3	MXG	B	400[A]	40/40	0.34	3.89	29,46,54,55	40
3	MXG	A	400[B]	40/40	0.42	3.03	14,41,48,49	40
2	K	B	1	1/1	0.10	1.16	40,40,40,40	0
2	K	A	2	1/1	0.09	0.41	42,42,42,42	0

6.5 Other polymers ⓘ

There are no such residues in this entry.