



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2024 – 06:39 PM EST

PDB ID : 3R2U  
Title : 2.1 Angstrom Resolution Crystal Structure of Metallo-beta-lactamase from Staphylococcus aureus subsp. aureus COL  
Authors : Minasov, G.; Wawrzak, Z.; Halavaty, A.; Shuvalova, L.; Dubrovskaya, I.; Winsor, J.; Kiryukhina, O.; Papazisi, L.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)  
Deposited on : 2011-03-14  
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

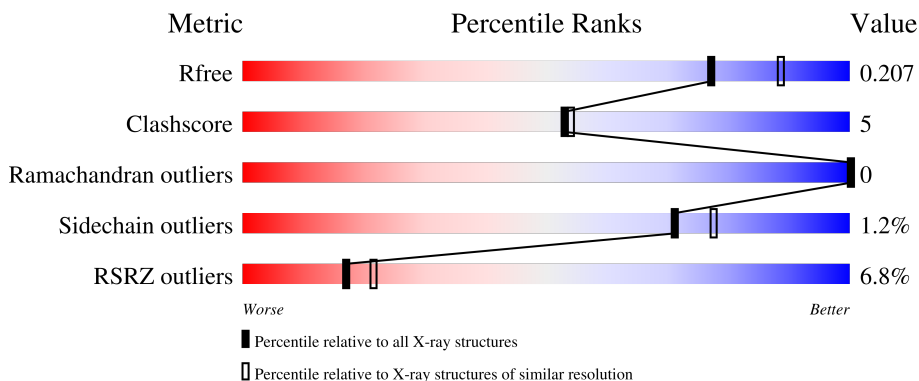
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	466	 5% 68% 6% 25%
1	B	466	 5% 65% 6% 28%
1	C	466	 5% 64% 9% 27%
1	D	466	 5% 65% 7% 28%

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 12459 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 Metallo-beta-lactamase family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	348	Total 2862	C 1819	N 483	O 551	S 9	0	14	0
1	B	336	Total 2810	C 1782	N 477	O 543	S 8	0	18	0
1	C	338	Total 2762	C 1759	N 464	O 531	S 8	0	11	0
1	D	337	Total 2779	C 1764	N 472	O 535	S 8	0	14	0

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	expression tag	UNP Q5HJV1
A	-22	HIS	-	expression tag	UNP Q5HJV1
A	-21	HIS	-	expression tag	UNP Q5HJV1
A	-20	HIS	-	expression tag	UNP Q5HJV1
A	-19	HIS	-	expression tag	UNP Q5HJV1
A	-18	HIS	-	expression tag	UNP Q5HJV1
A	-17	HIS	-	expression tag	UNP Q5HJV1
A	-16	SER	-	expression tag	UNP Q5HJV1
A	-15	SER	-	expression tag	UNP Q5HJV1
A	-14	GLY	-	expression tag	UNP Q5HJV1
A	-13	VAL	-	expression tag	UNP Q5HJV1
A	-12	ASP	-	expression tag	UNP Q5HJV1
A	-11	LEU	-	expression tag	UNP Q5HJV1
A	-10	GLY	-	expression tag	UNP Q5HJV1
A	-9	THR	-	expression tag	UNP Q5HJV1
A	-8	GLU	-	expression tag	UNP Q5HJV1
A	-7	ASN	-	expression tag	UNP Q5HJV1
A	-6	LEU	-	expression tag	UNP Q5HJV1
A	-5	TYR	-	expression tag	UNP Q5HJV1
A	-4	PHE	-	expression tag	UNP Q5HJV1
A	-3	GLN	-	expression tag	UNP Q5HJV1

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q5HJV1
A	-1	ASN	-	expression tag	UNP Q5HJV1
A	0	ALA	-	expression tag	UNP Q5HJV1
B	-23	MET	-	expression tag	UNP Q5HJV1
B	-22	HIS	-	expression tag	UNP Q5HJV1
B	-21	HIS	-	expression tag	UNP Q5HJV1
B	-20	HIS	-	expression tag	UNP Q5HJV1
B	-19	HIS	-	expression tag	UNP Q5HJV1
B	-18	HIS	-	expression tag	UNP Q5HJV1
B	-17	HIS	-	expression tag	UNP Q5HJV1
B	-16	SER	-	expression tag	UNP Q5HJV1
B	-15	SER	-	expression tag	UNP Q5HJV1
B	-14	GLY	-	expression tag	UNP Q5HJV1
B	-13	VAL	-	expression tag	UNP Q5HJV1
B	-12	ASP	-	expression tag	UNP Q5HJV1
B	-11	LEU	-	expression tag	UNP Q5HJV1
B	-10	GLY	-	expression tag	UNP Q5HJV1
B	-9	THR	-	expression tag	UNP Q5HJV1
B	-8	GLU	-	expression tag	UNP Q5HJV1
B	-7	ASN	-	expression tag	UNP Q5HJV1
B	-6	LEU	-	expression tag	UNP Q5HJV1
B	-5	TYR	-	expression tag	UNP Q5HJV1
B	-4	PHE	-	expression tag	UNP Q5HJV1
B	-3	GLN	-	expression tag	UNP Q5HJV1
B	-2	SER	-	expression tag	UNP Q5HJV1
B	-1	ASN	-	expression tag	UNP Q5HJV1
B	0	ALA	-	expression tag	UNP Q5HJV1
C	-23	MET	-	expression tag	UNP Q5HJV1
C	-22	HIS	-	expression tag	UNP Q5HJV1
C	-21	HIS	-	expression tag	UNP Q5HJV1
C	-20	HIS	-	expression tag	UNP Q5HJV1
C	-19	HIS	-	expression tag	UNP Q5HJV1
C	-18	HIS	-	expression tag	UNP Q5HJV1
C	-17	HIS	-	expression tag	UNP Q5HJV1
C	-16	SER	-	expression tag	UNP Q5HJV1
C	-15	SER	-	expression tag	UNP Q5HJV1
C	-14	GLY	-	expression tag	UNP Q5HJV1
C	-13	VAL	-	expression tag	UNP Q5HJV1
C	-12	ASP	-	expression tag	UNP Q5HJV1
C	-11	LEU	-	expression tag	UNP Q5HJV1
C	-10	GLY	-	expression tag	UNP Q5HJV1
C	-9	THR	-	expression tag	UNP Q5HJV1

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	GLU	-	expression tag	UNP Q5HJV1
C	-7	ASN	-	expression tag	UNP Q5HJV1
C	-6	LEU	-	expression tag	UNP Q5HJV1
C	-5	TYR	-	expression tag	UNP Q5HJV1
C	-4	PHE	-	expression tag	UNP Q5HJV1
C	-3	GLN	-	expression tag	UNP Q5HJV1
C	-2	SER	-	expression tag	UNP Q5HJV1
C	-1	ASN	-	expression tag	UNP Q5HJV1
C	0	ALA	-	expression tag	UNP Q5HJV1
D	-23	MET	-	expression tag	UNP Q5HJV1
D	-22	HIS	-	expression tag	UNP Q5HJV1
D	-21	HIS	-	expression tag	UNP Q5HJV1
D	-20	HIS	-	expression tag	UNP Q5HJV1
D	-19	HIS	-	expression tag	UNP Q5HJV1
D	-18	HIS	-	expression tag	UNP Q5HJV1
D	-17	HIS	-	expression tag	UNP Q5HJV1
D	-16	SER	-	expression tag	UNP Q5HJV1
D	-15	SER	-	expression tag	UNP Q5HJV1
D	-14	GLY	-	expression tag	UNP Q5HJV1
D	-13	VAL	-	expression tag	UNP Q5HJV1
D	-12	ASP	-	expression tag	UNP Q5HJV1
D	-11	LEU	-	expression tag	UNP Q5HJV1
D	-10	GLY	-	expression tag	UNP Q5HJV1
D	-9	THR	-	expression tag	UNP Q5HJV1
D	-8	GLU	-	expression tag	UNP Q5HJV1
D	-7	ASN	-	expression tag	UNP Q5HJV1
D	-6	LEU	-	expression tag	UNP Q5HJV1
D	-5	TYR	-	expression tag	UNP Q5HJV1
D	-4	PHE	-	expression tag	UNP Q5HJV1
D	-3	GLN	-	expression tag	UNP Q5HJV1
D	-2	SER	-	expression tag	UNP Q5HJV1
D	-1	ASN	-	expression tag	UNP Q5HJV1
D	0	ALA	-	expression tag	UNP Q5HJV1

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Fe 1 1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total Mg 2 2	0	0
3	C	2	Total Mg 2 2	0	0
3	D	1	Total Mg 1 1	0	0

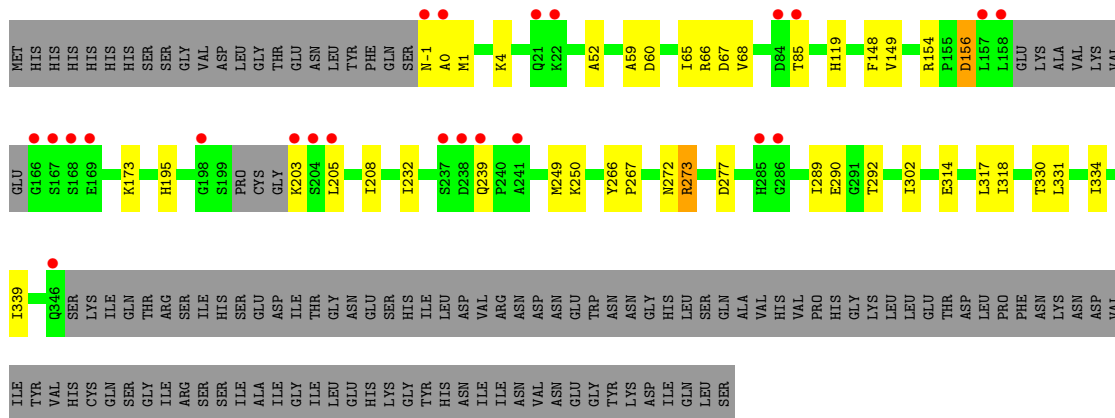
- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Cl 1 1	0	0

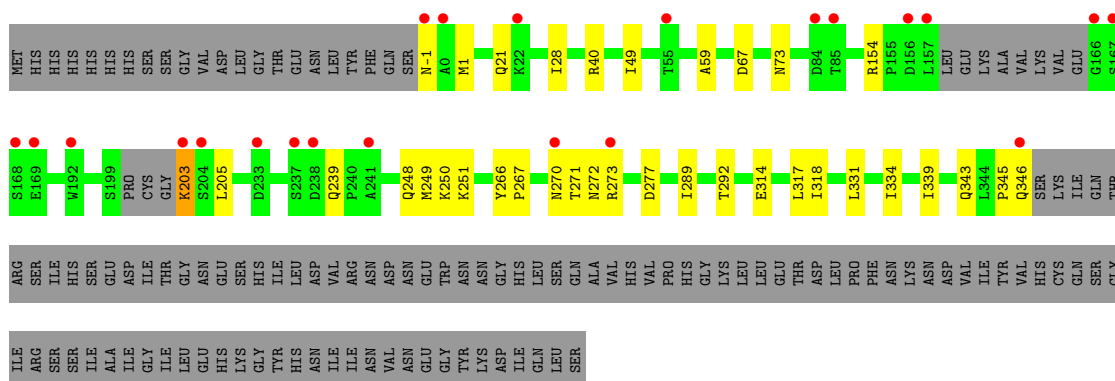
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	327	Total O 333 333	0	6
5	B	301	Total O 305 305	0	12
5	C	289	Total O 295 295	0	8
5	D	297	Total O 303 303	0	9





● Molecule 1: Metallo-beta-lactamase family protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.48Å 92.48Å 385.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.98 – 2.10 29.75 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.98-2.10) 99.9 (29.75-2.10)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.37 (at 2.10Å)	Xtrriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.156 , 0.197 0.169 , 0.207	Depositor DCC
$R_{free}$ test set	4909 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.2	Xtrriage
Anisotropy	0.233	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 45.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12459	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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: MG, FE, CL

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	0.55	0/2934	0.67	0/3978
1	B	0.54	0/2880	0.69	1/3907 (0.0%)
1	C	0.53	0/2831	0.68	0/3839
1	D	0.53	0/2848	0.68	0/3861
All	All	0.54	0/11493	0.68	1/15585 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	249	MET	CG-SD-CE	-6.02	90.57	100.20

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	2862	0	2749	26	0
1	B	2810	0	2672	29	0
1	C	2762	0	2648	40	0
1	D	2779	0	2661	26	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
4	B	1	0	0	0	0
5	A	333	0	0	8	0
5	B	305	0	0	6	0
5	C	295	0	0	5	0
5	D	303	0	0	6	0
All	All	12459	0	10730	119	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 5.

All (119) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93[A]:ASN:HA	5:B:1116[A]:HOH:O	1.47	1.10
1:D:21[B]:GLN:HA	5:D:1074[B]:HOH:O	1.60	1.02
1:C:273[B]:ARG:HH21	1:C:273[B]:ARG:CG	1.75	0.97
1:B:249:MET:HE2	1:B:334:ILE:HB	1.49	0.92
1:A:203[B]:LYS:H	1:A:203[B]:LYS:HE2	1.39	0.86
1:A:203[B]:LYS:H	1:A:203[B]:LYS:CE	1.88	0.85
1:A:166:GLY:O	1:A:170:ILE:HG23	1.77	0.84
1:C:273[B]:ARG:HH21	1:C:273[B]:ARG:HG3	1.44	0.81
1:A:203[B]:LYS:HE2	1:A:203[B]:LYS:N	1.97	0.79
1:A:170:ILE:HD11	5:A:1215:HOH:O	1.83	0.79
1:A:210:THR:HG21	5:B:694:HOH:O	1.84	0.78
1:A:164[A]:VAL:HG23	1:A:167:SER:HB3	1.67	0.76
1:C:273[B]:ARG:HH21	1:C:273[B]:ARG:HG2	1.50	0.73
1:C:272[B]:ASN:ND2	1:C:314:GLU:O	2.22	0.72
1:B:93[A]:ASN:O	1:B:94[A]:HIS:HB2	1.89	0.71
1:C:289[B]:ILE:HG12	1:C:290[B]:GLU:N	2.06	0.70
1:B:21[B]:GLN:NE2	1:B:21[B]:GLN:HA	2.07	0.69
1:D:345:PRO:O	1:D:346:GLN:HG3	1.91	0.69
1:C:60[B]:ASP:OD2	1:C:195:HIS:NE2	2.27	0.68
1:A:248:GLN:NE2	5:A:838:HOH:O	2.20	0.67
1:C:119:HIS:O	1:C:156:ASP:HB2	1.96	0.66
1:C:203:LYS:N	5:C:1166:HOH:O	2.29	0.66
1:C:273[B]:ARG:CG	1:C:273[B]:ARG:NH2	2.47	0.66

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:331:LEU:HD12	1:C:339:ILE:HD11	1.79	0.65
1:A:40[A]:ARG:NH2	5:A:474:HOH:O	2.31	0.64
1:C:1:MET:N	5:C:526:HOH:O	2.31	0.64
1:B:249:MET:CE	1:B:334:ILE:HB	2.25	0.64
1:D:59:ALA:HB2	1:D:250:LYS:HD3	1.81	0.62
1:D:-1:ASN:O	1:D:21[B]:GLN:NE2	2.34	0.61
1:B:21[B]:GLN:HA	1:B:21[B]:GLN:HE21	1.65	0.61
1:C:272[B]:ASN:OD1	1:C:273[B]:ARG:N	2.34	0.61
1:D:343:GLN:NE2	5:D:567[B]:HOH:O	2.34	0.60
1:B:248:GLN:HG2	1:B:311:TYR:CG	2.38	0.59
1:A:44[A]:GLU:HG3	5:A:576:HOH:O	2.03	0.59
1:B:343:GLN:HG2	5:B:574:HOH:O	2.03	0.58
1:B:289:ILE:HG22	5:B:1077:HOH:O	2.03	0.57
1:C:273[B]:ARG:HG3	1:C:273[B]:ARG:NH2	2.14	0.57
1:B:66[A]:ARG:NH2	5:B:544:HOH:O	2.35	0.57
1:D:271[B]:THR:O	1:D:272[B]:ASN:ND2	2.38	0.57
1:C:317:LEU:HD11	1:C:339:ILE:HD13	1.85	0.56
1:A:164[B]:VAL:HG12	5:A:984:HOH:O	2.05	0.56
1:D:273[A]:ARG:NH1	1:D:314:GLU:OE1	2.38	0.56
1:C:59:ALA:HB2	1:C:250:LYS:HD3	1.88	0.56
1:C:66[B]:ARG:NH1	5:C:500:HOH:O	2.33	0.55
1:B:289:ILE:HG23	1:B:292:THR:HG21	1.88	0.55
1:B:61:PHE:HA	1:B:249:MET:HE1	1.89	0.54
1:D:154:ARG:HG3	1:D:239:GLN:NE2	2.22	0.54
1:B:21[B]:GLN:HE21	1:B:21[B]:GLN:CA	2.20	0.54
1:D:331:LEU:HD12	1:D:339:ILE:HD11	1.88	0.54
1:C:148:PHE:CD2	1:C:205:LEU:HD21	2.43	0.53
1:C:173:LYS:HG2	1:C:232:ILE:HD11	1.90	0.53
1:C:277:ASP:HA	1:C:318[B]:ILE:HB	1.89	0.53
1:B:279:ARG:HD3	1:B:345:PRO:HG3	1.90	0.53
1:A:203[B]:LYS:H	1:A:203[B]:LYS:NZ	2.06	0.52
1:B:252[A]:ILE:HD12	1:B:252[A]:ILE:C	2.30	0.52
1:D:270[B]:ASN:ND2	5:D:768:HOH:O	2.42	0.52
1:D:248:GLN:OE1	1:D:251:LYS:NZ	2.44	0.51
1:B:315:ILE:CG1	1:B:339[B]:ILE:HD13	2.41	0.51
1:D:270[A]:ASN:OD1	1:D:273[A]:ARG:NH2	2.44	0.51
1:C:65[A]:ILE:HG23	1:C:66[A]:ARG:N	2.26	0.51
1:B:289:ILE:HG23	1:B:292:THR:CG2	2.41	0.51
1:B:315:ILE:HG12	1:B:339[B]:ILE:HD13	1.93	0.50
1:C:302:ILE:HD11	1:C:330:THR:HG22	1.92	0.50
1:B:93[A]:ASN:O	1:B:94[A]:HIS:CB	2.58	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:249:MET:HE1	1:D:334:ILE:O	2.12	0.50
1:B:315:ILE:HD11	1:B:339[B]:ILE:CD1	2.43	0.49
1:A:272[A]:ASN:ND2	5:A:1104:HOH:O	2.45	0.49
1:C:273[B]:ARG:HG2	1:C:273[B]:ARG:NH2	2.22	0.48
1:C:148:PHE:CD2	1:C:205:LEU:CD2	2.97	0.48
1:C:85:THR:HG23	5:C:953:HOH:O	2.13	0.48
1:B:44[A]:GLU:HG2	5:B:707:HOH:O	2.13	0.47
1:C:289[B]:ILE:CG1	1:C:290[B]:GLU:N	2.76	0.47
1:B:1:MET:HA	1:B:21[A]:GLN:HG3	1.96	0.47
1:C:52:ALA:HB2	1:C:68:VAL:HG11	1.95	0.47
1:A:66[B]:ARG:NH2	1:A:90:ASN:O	2.48	0.47
1:A:1:MET:N	5:A:485:HOH:O	2.48	0.46
1:B:52:ALA:HB2	1:B:68:VAL:HG11	1.96	0.46
1:D:203:LYS:O	1:D:203:LYS:HE2	2.15	0.46
1:C:292:THR:HG21	1:C:318[A]:ILE:CD1	2.45	0.46
1:D:317:LEU:HD11	1:D:339:ILE:HD13	1.97	0.46
1:C:4:LYS:HE2	5:C:797:HOH:O	2.15	0.45
1:D:205:LEU:N	1:D:205:LEU:HD23	2.31	0.45
1:A:248:GLN:HG2	1:A:311:TYR:CG	2.51	0.45
1:D:40[A]:ARG:NH2	5:D:1133:HOH:O	2.50	0.44
1:A:249:MET:HA	1:A:249:MET:CE	2.47	0.44
1:B:173:LYS:HG2	1:B:232:ILE:HD11	1.98	0.44
1:B:269:THR:HB	1:D:73:ASN:HD22	1.82	0.44
1:A:100:HIS:O	1:A:101:ASN:HB2	2.18	0.44
1:D:292:THR:HG21	1:D:318:ILE:CD1	2.48	0.44
1:A:248:GLN:HG2	1:A:311:TYR:CD1	2.53	0.44
1:D:28:ILE:HD11	1:D:49:ILE:HD13	2.00	0.43
1:A:40[B]:ARG:NH2	5:A:842:HOH:O	2.51	0.43
1:C:249:MET:HE1	1:C:334:ILE:O	2.18	0.43
1:C:266:TYR:HB3	1:C:267:PRO:HD2	2.00	0.43
1:C:317:LEU:CD1	1:C:339:ILE:HD13	2.48	0.43
1:D:266:TYR:HB3	1:D:267:PRO:HD2	2.00	0.43
1:A:9:LYS:HD2	1:B:44[B]:GLU:OE2	2.18	0.43
1:D:1:MET:HA	1:D:21[B]:GLN:HG2	2.00	0.43
1:D:277:ASP:HA	1:D:318:ILE:HB	2.00	0.43
1:A:156:ASP:OD2	1:A:250:LYS:HE2	2.19	0.43
1:C:65[A]:ILE:CG2	1:C:66[A]:ARG:N	2.82	0.43
1:C:-1:ASN:HA	1:C:0:ALA:HA	1.82	0.42
1:C:148:PHE:CB	1:C:205:LEU:HD22	2.49	0.42
1:A:148:PHE:CB	1:A:205:LEU:HD22	2.49	0.42
1:D:21[B]:GLN:CA	5:D:1074[B]:HOH:O	2.40	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:ILE:HG21	1:A:31:PRO:HB3	2.01	0.42
1:A:59:ALA:O	1:A:246:PHE:HA	2.20	0.42
1:C:277:ASP:HA	1:C:318[A]:ILE:HB	2.00	0.42
1:D:289:ILE:HG13	5:D:553:HOH:O	2.20	0.42
1:D:21[B]:GLN:H	1:D:21[B]:GLN:HG3	1.26	0.42
1:C:273[A]:ARG:HG3	1:C:273[A]:ARG:HH21	1.85	0.41
1:B:119:HIS:CD2	1:B:145:ASP:HB2	2.55	0.41
1:A:119:HIS:CD2	1:A:145:ASP:HB2	2.56	0.41
1:C:149:VAL:HG11	1:C:208:ILE:CG2	2.51	0.41
1:B:302:ILE:HD11	1:B:330:THR:HG22	2.03	0.41
1:C:148:PHE:CG	1:C:205:LEU:HD22	2.56	0.41
1:C:154:ARG:HG2	1:C:239:GLN:CD	2.41	0.41
1:C:273[A]:ARG:HG3	1:C:273[A]:ARG:NH2	2.37	0.40
1:B:328:THR:HG23	1:B:339[A]:ILE:HD12	2.04	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	360/466 (77%)	350 (97%)	10 (3%)	0	100	100
1	B	348/466 (75%)	339 (97%)	9 (3%)	0	100	100
1	C	343/466 (74%)	329 (96%)	14 (4%)	0	100	100
1	D	345/466 (74%)	334 (97%)	11 (3%)	0	100	100
All	All	1396/1864 (75%)	1352 (97%)	44 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	308/401 (77%)	302 (98%)	6 (2%)	57	63
1	B	303/401 (76%)	298 (98%)	5 (2%)	60	67
1	C	297/401 (74%)	293 (99%)	4 (1%)	69	75
1	D	299/401 (75%)	297 (99%)	2 (1%)	84	88
All	All	1207/1604 (75%)	1190 (99%)	17 (1%)	71	73

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	ASP
1	A	164[A]	VAL
1	A	164[B]	VAL
1	A	170	ILE
1	A	249	MET
1	A	343	GLN
1	B	21[A]	GLN
1	B	21[B]	GLN
1	B	67	ASP
1	B	157	LEU
1	B	338	ASP
1	C	67	ASP
1	C	156	ASP
1	C	273[A]	ARG
1	C	273[B]	ARG
1	D	67	ASP
1	D	203	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	174	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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	348/466 (74%)	-0.07	22 (6%) 20 24	15, 25, 56, 74	0
1	B	336/466 (72%)	0.01	25 (7%) 14 18	17, 27, 59, 78	0
1	C	338/466 (72%)	0.08	23 (6%) 17 21	16, 28, 63, 82	0
1	D	337/466 (72%)	-0.09	22 (6%) 18 23	17, 28, 52, 72	0
All	All	1359/1864 (72%)	-0.02	92 (6%) 17 21	15, 27, 58, 82	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	158	LEU	9.0
1	C	204	SER	7.4
1	B	157	LEU	6.5
1	D	238	ASP	6.4
1	B	238	ASP	6.3
1	A	164[A]	VAL	6.1
1	A	201	CYS	5.5
1	D	167	SER	5.4
1	D	-1	ASN	5.3
1	C	168	SER	5.1
1	A	165	GLU	5.0
1	A	202	GLY	5.0
1	C	238	ASP	4.8
1	D	157	LEU	4.7
1	A	238	ASP	4.6
1	B	-3	GLN	4.5
1	C	-1	ASN	4.3
1	C	203	LYS	4.2
1	A	200	PRO	4.1
1	A	-1	ASN	4.0
1	A	0	ALA	4.0

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	241	ALA	4.0
1	B	285	HIS	3.9
1	B	-2	SER	3.9
1	A	161	ALA	3.9
1	C	167	SER	3.8
1	D	166	GLY	3.8
1	D	0	ALA	3.8
1	C	157	LEU	3.8
1	A	167	SER	3.7
1	A	94	HIS	3.7
1	C	239	GLN	3.7
1	B	93[A]	ASN	3.5
1	C	166	GLY	3.5
1	B	-1	ASN	3.4
1	B	156	ASP	3.3
1	A	160	LYS	3.3
1	D	156	ASP	3.2
1	C	169	GLU	3.1
1	B	199	SER	3.0
1	D	203	LYS	3.0
1	C	346	GLN	3.0
1	D	22	LYS	3.0
1	D	204	SER	2.8
1	C	198	GLY	2.7
1	B	290	GLU	2.7
1	B	237	SER	2.7
1	A	158	LEU	2.7
1	C	22	LYS	2.7
1	C	285	HIS	2.6
1	C	21	GLN	2.6
1	C	237	SER	2.6
1	B	142	PHE	2.6
1	A	166	GLY	2.6
1	D	168	SER	2.6
1	B	84	ASP	2.6
1	D	237	SER	2.6
1	B	22[A]	LYS	2.5
1	A	93	ASN	2.5
1	B	94[A]	HIS	2.5
1	B	236	ILE	2.5
1	D	273[A]	ARG	2.4
1	B	141	LEU	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	239	GLN	2.3
1	B	242	PRO	2.3
1	A	240	PRO	2.3
1	D	55	THR	2.3
1	D	346	GLN	2.3
1	B	307	TRP	2.2
1	A	203[A]	LYS	2.2
1	C	0	ALA	2.2
1	C	205	LEU	2.2
1	D	169	GLU	2.2
1	D	241	ALA	2.2
1	A	204	SER	2.2
1	B	204	SER	2.2
1	C	85	THR	2.2
1	D	84	ASP	2.1
1	B	198	GLY	2.1
1	B	168	SER	2.1
1	A	22	LYS	2.1
1	C	84	ASP	2.1
1	B	291	GLY	2.1
1	D	270[A]	ASN	2.1
1	A	21	GLN	2.1
1	A	168	SER	2.1
1	B	346	GLN	2.0
1	D	192	TRP	2.0
1	D	233[A]	ASP	2.0
1	C	286	GLY	2.0
1	A	346	GLN	2.0
1	D	85	THR	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	MG	B	445	1/1	0.58	0.10	57,57,57,57	0
3	MG	D	444	1/1	0.85	0.08	47,47,47,47	0
3	MG	B	444	1/1	0.89	0.04	41,41,41,41	0
3	MG	C	444	1/1	0.92	0.07	49,49,49,49	0
3	MG	C	445	1/1	0.94	0.06	59,59,59,59	0
2	FE	C	443	1/1	0.96	0.06	54,54,54,54	0
2	FE	A	443	1/1	0.97	0.04	52,52,52,52	0
2	FE	B	443	1/1	0.97	0.03	49,49,49,49	0
2	FE	D	443	1/1	0.98	0.06	53,53,53,53	0
4	CL	B	446	1/1	0.98	0.05	38,38,38,38	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.