



Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 02:52 AM GMT

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 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>

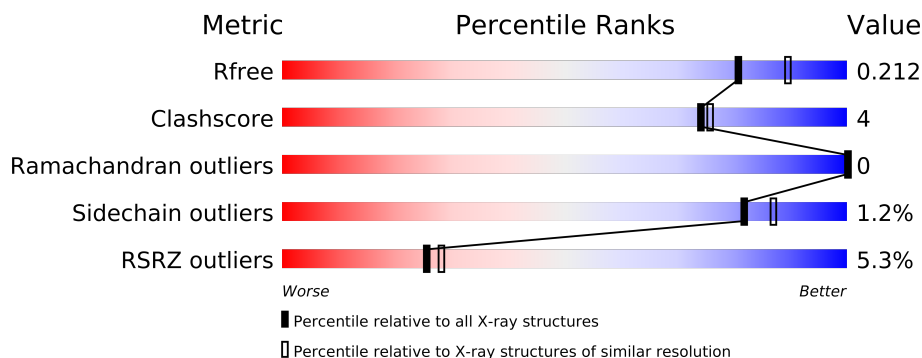
The following versions of software and data (see [references](#)) were used in the production of this report:

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 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 ≥ 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	466	
1	B	466	
1	C	466	
1	D	466	

2 Entry composition

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

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

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

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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

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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	B	1	Total Fe 1 1	0	0
2	A	1	Total Fe 1 1	0	0
2	D	1	Total Fe 1 1	0	0

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

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

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

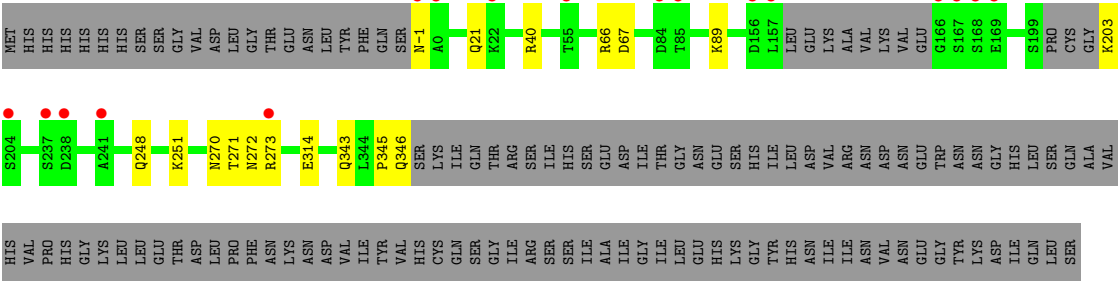
- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 5 is water.

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

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	3.37 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.156 , 0.197 0.177 , 0.212	Depositor DCC
R_{free} test set	4905 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	27.2	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 26.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 98323 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12459	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage'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.*

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: 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 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	2862	0	0	13	0
1	B	2810	0	0	8	0
1	C	2762	0	0	11	0
1	D	2779	0	0	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	B	1	0	0	0	0
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	9	0
5	B	305	0	0	5	0
5	C	295	0	0	4	0
5	D	303	0	0	8	0
All	All	12459	0	0	46	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 4.

All (46) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:273[B]:ARG:NH2	1:C:273[B]:ARG:CG	2.47	0.77
1:A:248:GLN:NE2	5:A:838:HOH:O	2.20	0.74
1:C:272[B]:ASN:ND2	1:C:314:GLU:O	2.22	0.72
1:D:21[B]:GLN:CA	5:D:1074[B]:HOH:O	2.40	0.68
1:C:60[B]:ASP:OD2	1:C:195:HIS:NE2	2.27	0.68
1:C:203:LYS:N	5:C:1166:HOH:O	2.29	0.66
1:B:93[A]:ASN:CA	5:B:1116[A]:HOH:O	2.44	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:A:273[A]:ARG:NE	5:A:588:HOH:O	2.32	0.63
1:C:66[B]:ARG:NH1	5:C:500:HOH:O	2.33	0.61
1:D:-1:ASN:O	1:D:21[B]:GLN:NE2	2.34	0.61
1:B:40[B]:ARG:NE	5:B:967:HOH:O	2.33	0.61
1:C:272[B]:ASN:OD1	1:C:273[B]:ARG:N	2.34	0.61
1:B:66[A]:ARG:NH2	5:B:544:HOH:O	2.35	0.60
1:D:343:GLN:NE2	5:D:567[B]:HOH:O	2.34	0.60
1:A:203[B]:LYS:N	1:A:203[B]:LYS:CE	2.66	0.59
1:A:326:LYS:NZ	5:A:993:HOH:O	2.35	0.58
1:D:271[B]:THR:O	1:D:272[B]:ASN:ND2	2.38	0.57
1:D:273[A]:ARG:NH1	1:D:314:GLU:OE1	2.38	0.56
1:B:75:ASN:ND2	5:B:549:HOH:O	2.42	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:270[A]:ASN:OD1	1:D:273[A]:ARG:NH2	2.44	0.51
1:B:101[B]:ASN:OD1	1:B:112:LYS:NZ	2.44	0.51
1:B:93[A]:ASN:O	1:B:94[A]:HIS:CB	2.58	0.50
1:B:21[B]:GLN:NE2	1:B:21[B]:GLN:CA	2.75	0.50
1:A:272[A]:ASN:ND2	5:A:1104:HOH:O	2.45	0.49
1:D:66[A]:ARG:NH2	5:D:549:HOH:O	2.45	0.49
1:C:289[B]:ILE:CG1	1:C:290[B]:GLU:N	2.76	0.48
1:C:148:PHE:CD2	1:C:205:LEU:CD2	2.97	0.48
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:A:210:THR:CG2	5:B:694:HOH:O	2.63	0.46
1:A:250:LYS:NZ	5:A:496:HOH:O	2.49	0.45
1:D:40[A]:ARG:NH2	5:D:1133:HOH:O	2.50	0.44
1:A:40[B]:ARG:NH2	5:A:842:HOH:O	2.51	0.43
1:C:65[A]:ILE:CG2	1:C:66[A]:ARG:N	2.82	0.43
1:B:249:MET:CE	1:B:334:ILE:CB	2.97	0.42
1:D:89:LYS:NZ	5:D:1135:HOH:O	2.52	0.42
1:D:345:PRO:O	1:D:346:GLN:CG	2.68	0.42
1:A:54:GLU:OE1	1:A:63:SER:OG	2.38	0.41
1:D:66[B]:ARG:NH2	5:D:1174:HOH:O	2.54	0.41
1:D:40[B]:ARG:NE	5:D:1205:HOH:O	2.53	0.41
1:A:110:LYS:NZ	5:A:693:HOH:O	2.54	0.40
1:C:99:GLN:NE2	5:C:1202:HOH:O	2.55	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	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1396/1864 (75%)	1352 (97%)	44 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	308/401 (77%)	302 (98%)	6 (2%)	69	73
1	B	303/401 (76%)	298 (98%)	5 (2%)	73	78
1	C	297/401 (74%)	293 (99%)	4 (1%)	80	85
1	D	299/401 (75%)	297 (99%)	2 (1%)	91	94
All	All	1207/1604 (75%)	1190 (99%)	17 (1%)	82	83

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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no

such sidechains identified.

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 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.

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	348/466 (74%)	-0.08	17 (4%) 28 31	15, 25, 56, 74	0
1	B	336/466 (72%)	0.01	21 (6%) 19 22	17, 27, 59, 78	0
1	C	338/466 (72%)	0.07	18 (5%) 25 28	16, 28, 63, 82	0
1	D	337/466 (72%)	-0.08	17 (5%) 28 30	17, 28, 52, 72	0
All	All	1359/1864 (72%)	-0.02	73 (5%) 25 27	15, 27, 58, 82	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	158	LEU	8.8
1	C	204	SER	6.7
1	B	238	ASP	5.6
1	D	238	ASP	5.4
1	A	201	CYS	5.3
1	B	157	LEU	5.1
1	A	165	GLU	5.1
1	D	167	SER	5.0
1	A	164[A]	VAL	4.9
1	C	168	SER	4.8
1	D	-1	ASN	4.7
1	A	202	GLY	4.7
1	C	238	ASP	4.6
1	C	157	LEU	4.4
1	D	157	LEU	4.4
1	C	-1	ASN	4.0
1	B	285	HIS	4.0
1	A	238	ASP	3.9
1	C	241	ALA	3.9
1	B	-3	GLN	3.9
1	C	167	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	239	GLN	3.7
1	A	0	ALA	3.6
1	A	167	SER	3.5
1	B	93[A]	ASN	3.5
1	C	203	LYS	3.4
1	D	166	GLY	3.4
1	A	161	ALA	3.4
1	A	-1	ASN	3.4
1	B	-1	ASN	3.3
1	A	200	PRO	3.3
1	B	-2	SER	3.2
1	D	0	ALA	3.1
1	C	166	GLY	3.0
1	A	94	HIS	3.0
1	D	156	ASP	2.9
1	C	346	GLN	2.8
1	B	156	ASP	2.7
1	B	290	GLU	2.7
1	C	169	GLU	2.6
1	A	166	GLY	2.6
1	A	158	LEU	2.5
1	A	160	LYS	2.5
1	C	237	SER	2.5
1	A	93	ASN	2.5
1	B	237	SER	2.5
1	D	22	LYS	2.5
1	B	199	SER	2.4
1	D	168	SER	2.4
1	D	169	GLU	2.4
1	D	241	ALA	2.4
1	C	21	GLN	2.4
1	B	94[A]	HIS	2.4
1	D	237	SER	2.4
1	B	346	GLN	2.3
1	C	285	HIS	2.3
1	B	236	ILE	2.3
1	B	142	PHE	2.3
1	D	84	ASP	2.2
1	C	205	LEU	2.2
1	B	141	LEU	2.2
1	B	22[A]	LYS	2.2
1	B	204	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	273[A]	ARG	2.1
1	B	239	GLN	2.1
1	D	85	THR	2.1
1	A	203[A]	LYS	2.1
1	B	307	TRP	2.1
1	D	204	SER	2.1
1	D	55	THR	2.1
1	C	22	LYS	2.1
1	B	168	SER	2.1
1	A	21	GLN	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(Å ²)	Q<0.9
3	MG	D	444	1/1	0.08	-1.29	47,47,47,47	0
2	FE	B	443	1/1	0.02	-1.62	49,49,49,49	0
2	FE	C	443	1/1	0.06	-1.80	54,54,54,54	0
2	FE	D	443	1/1	0.05	-2.43	53,53,53,53	0
3	MG	B	445	1/1	0.08	-2.59	57,57,57,57	0
3	MG	B	444	1/1	0.05	-2.66	41,41,41,41	0
3	MG	C	444	1/1	0.05	-2.93	49,49,49,49	0
2	FE	A	443	1/1	0.04	-3.33	52,52,52,52	0
4	CL	B	446	1/1	0.05	-3.72	38,38,38,38	0
3	MG	C	445	1/1	0.06	-5.51	59,59,59,59	0

6.5 Other polymers ⓘ

There are no such residues in this entry.