



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 04:52 pm BST

PDB ID : 2WRS  
Title : Crystal Structure of the Mono-Zinc Metallo-beta-lactamase VIM-4 from *Pseudomonas aeruginosa*  
Authors : Lassaux, P.; Hamel, M.; Gulea, M.; Delbruck, H.; Traore, D.A.K.; Mercuri, P.S.; Horsfall, L.; Dehareng, D.; Gaumont, A.-C.; Frere, J.-M.; Ferrer, J.-L.; Hoffmann, K.; Galleni, M.; Bebrone, C.  
Deposited on : 2009-09-02  
Resolution : 2.79 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.

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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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

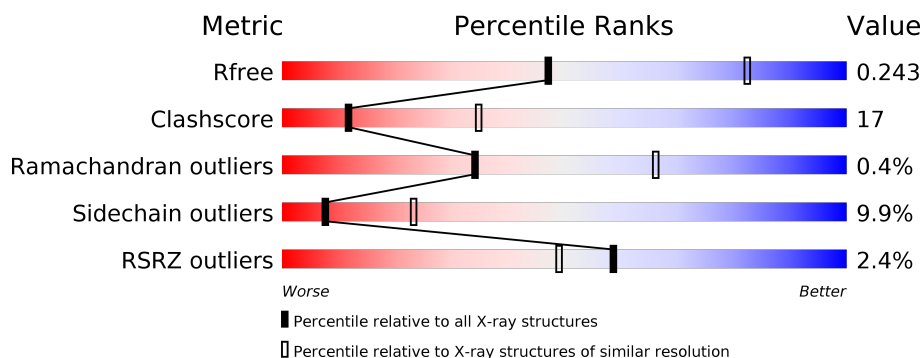
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.79 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 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	230	<div> <div>71%</div> <div>27%</div> <div>•</div> </div>
1	B	230	<div> <div>5%</div> <div>64%</div> <div>33%</div> <div>•</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FLC	A	1263	-	-	X	-
4	CIT	A	1264	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3546 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.

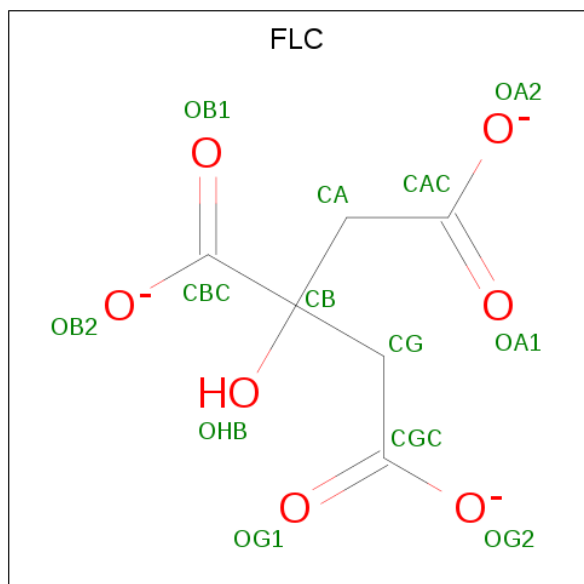
- Molecule 1 is a protein called BETA-LACTAMASE VIM-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	0	1	0
			1738	1091	306	340	1			
1	B	230	Total	C	N	O	S	0	0	0
			1727	1085	302	339	1			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

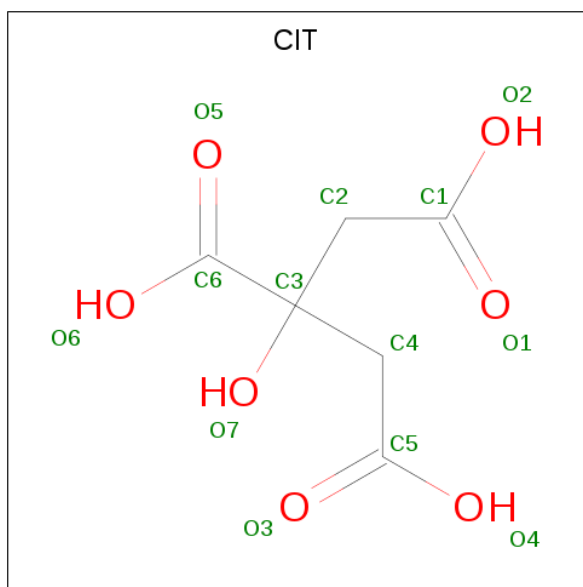
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is CITRATE ANION (three-letter code: FLC) (formula: C<sub>6</sub>H<sub>5</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is CITRIC ACID (three-letter code: CIT) (formula:  $C_6H_8O_7$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	6	7		
4	A	1	Total	C	O	0	0
			13	6	7		

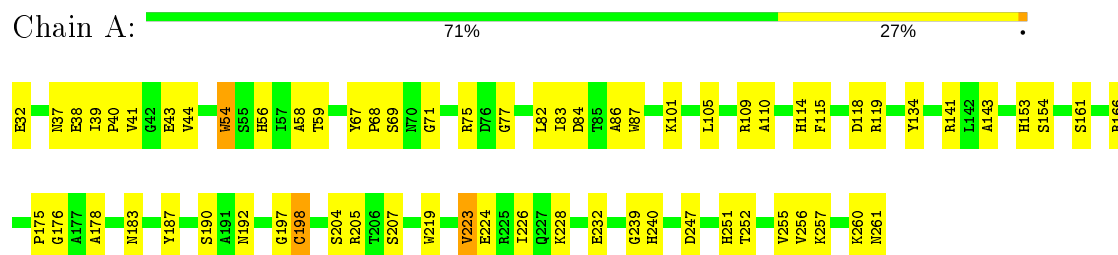
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	26	Total	O	0	0
			26	26		
5	B	1	Total	O	0	0
			1	1		

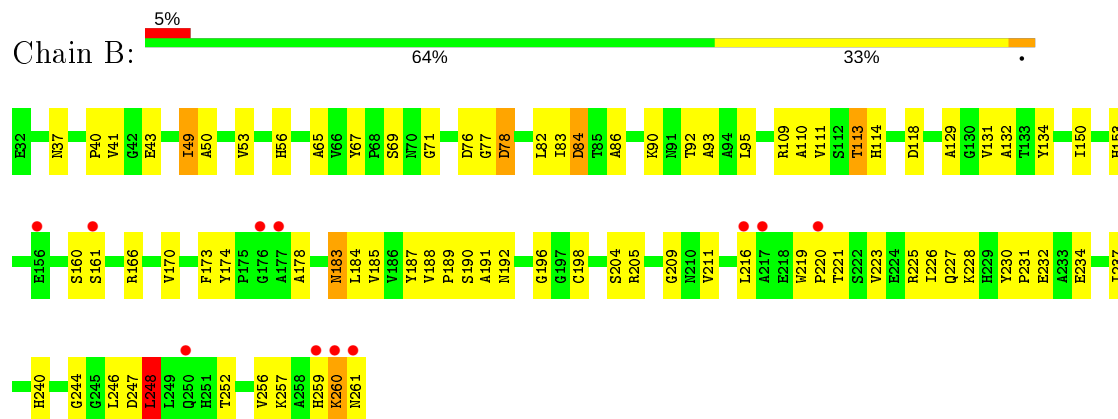
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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 ( $\text{RSRZ} > 2$ ). 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 VIM-4



- Molecule 1: BETA-LACTAMASE VIM-4



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	140.13Å 45.67Å 105.03Å 90.00° 105.41° 90.00°	Depositor
Resolution (Å)	43.27 – 2.79 43.26 – 2.79	Depositor EDS
% Data completeness (in resolution range)	100.0 (43.27-2.79) 98.9 (43.26-2.79)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.09 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.199 , 0.253 0.194 , 0.243	Depositor DCC
$R_{free}$ test set	806 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.5	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 42.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3546	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.43% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, FLC, CIT

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	0.99	0/1778	0.89	1/2431 (0.0%)
1	B	0.86	0/1767	0.84	3/2417 (0.1%)
All	All	0.93	0/3545	0.86	4/4848 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	78	ASP	N-CA-CB	-5.51	100.69	110.60
1	B	248	LEU	CA-CB-CG	5.45	127.84	115.30
1	A	141	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	B	78	ASP	CB-CG-OD1	-5.01	113.79	118.30

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	1738	0	1685	54	0
1	B	1727	0	1672	61	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	13	0	5	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	13	0	5	3	0
4	A	26	0	10	11	0
5	A	26	0	0	4	0
5	B	1	0	0	0	0
All	All	3546	0	3377	120	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 17.

All (120) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:PRO:HG2	1:A:43:GLU:OE2	1.51	1.08
1:A:198:CYS:SG	3:A:1263:FLC:OB1	2.13	1.06
1:B:49:ILE:HD12	1:B:237:ILE:HD11	1.44	0.99
4:A:1264:CIT:C6	4:A:1264:CIT:O4	2.13	0.96
1:A:109:ARG:HH12	4:A:1264:CIT:H41	1.28	0.95
1:A:109:ARG:HH12	4:A:1264:CIT:C4	1.79	0.95
1:B:240:HIS:NE2	3:B:1263:FLC:OG1	2.08	0.87
3:B:1263:FLC:HG2	3:B:1263:FLC:OA1	1.77	0.82
1:B:187:TYR:OH	1:B:192:ASN:HA	1.87	0.74
1:A:40:PRO:CG	1:A:43:GLU:OE2	2.34	0.70
1:A:118:ASP:OD2	3:A:1263:FLC:CBC	2.40	0.69
1:A:240:HIS:NE2	3:A:1263:FLC:OB1	2.19	0.68
1:A:240:HIS:NE2	3:A:1263:FLC:HG2	2.09	0.68
1:B:257:LYS:HD3	1:B:257:LYS:O	1.94	0.67
1:B:189:PRO:O	1:B:190:SER:C	2.29	0.67
1:B:244:GLY:HA3	1:B:248:LEU:HD21	1.76	0.67
1:A:198:CYS:SG	3:A:1263:FLC:CBC	2.85	0.65
1:A:109:ARG:HH12	4:A:1264:CIT:H42	1.61	0.65
4:A:1265:CIT:O4	4:A:1265:CIT:C6	2.44	0.65
1:B:40:PRO:HG2	1:B:43:GLU:OE2	1.96	0.64
1:B:83:ILE:O	1:B:84:ASP:HB2	1.97	0.64
4:A:1264:CIT:O5	4:A:1264:CIT:O4	2.16	0.63
1:A:109:ARG:NH1	4:A:1264:CIT:H41	2.10	0.63
1:A:251:HIS:O	1:A:255:VAL:HG23	2.00	0.62
1:B:118:ASP:OD2	3:B:1263:FLC:CGC	2.48	0.62
1:B:49:ILE:CD1	1:B:237:ILE:HD11	2.26	0.61
3:A:1263:FLC:HG1	5:A:2026:HOH:O	2.00	0.61
1:A:118:ASP:OD2	3:A:1263:FLC:OB1	2.19	0.60
1:A:240:HIS:HE2	3:A:1263:FLC:HG2	1.64	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:PRO:O	1:B:191:ALA:N	2.34	0.59
1:B:209:GLY:O	1:B:211:VAL:HG13	2.02	0.59
1:A:197:GLY:O	1:A:239:GLY:N	2.35	0.59
1:B:189:PRO:C	1:B:191:ALA:N	2.54	0.59
1:A:252:THR:O	1:A:256:VAL:HG23	2.04	0.57
1:A:187:TYR:CZ	1:A:192:ASN:HA	2.40	0.57
1:B:191:ALA:O	1:B:192:ASN:HB2	2.05	0.57
1:A:219:TRP:O	1:A:219:TRP:HD1	1.88	0.57
1:B:82:LEU:O	1:B:110:ALA:HA	2.05	0.57
1:B:84:ASP:OD1	1:B:113:THR:OG1	2.22	0.56
1:A:153:HIS:NE2	4:A:1265:CIT:O5	2.38	0.56
1:B:69:SER:HB3	1:B:240:HIS:CE1	2.41	0.56
1:B:161:SER:OG	1:B:225:ARG:NH1	2.38	0.55
1:A:115:PHE:HB2	1:A:143:ALA:HB2	1.88	0.55
1:A:67:TYR:HH	1:B:67:TYR:HH	1.53	0.55
1:A:75:ARG:NH1	1:A:77:GLY:HA2	2.23	0.54
1:B:170:VAL:HG12	1:B:188:VAL:HG22	1.89	0.54
1:A:223:VAL:HA	1:A:226:ILE:HD12	1.91	0.53
1:A:109:ARG:NH1	4:A:1264:CIT:C4	2.61	0.53
1:A:161:SER:HB3	1:A:176:GLY:CA	2.39	0.53
1:B:134:TYR:CD2	1:B:153:HIS:HB2	2.44	0.53
1:A:114:HIS:CE1	1:A:119:ARG:HG3	2.45	0.52
1:B:114:HIS:HB3	1:B:183:ASN:HA	1.93	0.51
1:A:198:CYS:SG	5:A:2025:HOH:O	2.46	0.51
1:B:187:TYR:CZ	1:B:192:ASN:HA	2.46	0.51
1:B:132:ALA:HB1	1:B:134:TYR:CE1	2.46	0.50
1:A:178:ALA:HB1	1:A:219:TRP:CD1	2.46	0.50
1:B:83:ILE:HD12	1:B:111:VAL:HB	1.94	0.49
1:B:256:VAL:O	1:B:260:LYS:HD3	2.12	0.49
1:B:256:VAL:HG12	1:B:260:LYS:HZ3	1.77	0.49
1:B:223:VAL:O	1:B:226:ILE:HB	2.12	0.49
1:A:190:SER:HB3	5:A:2019:HOH:O	2.12	0.49
1:B:187:TYR:HB2	1:B:230:TYR:CE1	2.48	0.49
1:B:40:PRO:CG	1:B:43:GLU:OE2	2.60	0.49
1:B:76:ASP:O	1:B:78:ASP:N	2.45	0.49
1:B:114:HIS:HE1	1:B:198:CYS:HB2	1.77	0.49
1:B:65:ALA:HB3	1:B:67:TYR:CE1	2.48	0.48
1:A:197:GLY:O	1:A:239:GLY:CA	2.62	0.48
1:B:259:HIS:O	1:B:259:HIS:ND1	2.46	0.48
1:B:189:PRO:C	1:B:191:ALA:H	2.16	0.48
1:B:114:HIS:CE1	1:B:198:CYS:HB2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:ALA:HA	1:B:219:TRP:HA	1.96	0.48
1:A:109:ARG:NH1	4:A:1264:CIT:H42	2.26	0.48
1:A:68:PRO:O	1:A:240:HIS:ND1	2.46	0.48
1:A:83:ILE:O	1:A:84:ASP:HB2	2.13	0.48
1:B:50:ALA:HB3	1:B:53:VAL:HB	1.95	0.47
4:A:1265:CIT:O6	4:A:1265:CIT:O4	2.32	0.47
1:B:40:PRO:HD2	1:B:43:GLU:OE2	2.14	0.47
1:B:109:ARG:HG2	1:B:132:ALA:HB3	1.95	0.47
1:B:261:ASN:OXT	1:B:261:ASN:ND2	2.46	0.47
1:B:173:PHE:HB3	1:B:185:VAL:HG23	1.96	0.47
1:A:175:PRO:O	1:A:176:GLY:C	2.50	0.47
1:A:39:ILE:HA	1:A:40:PRO:HD2	1.83	0.47
1:A:118:ASP:OD1	1:A:119:ARG:HG2	2.14	0.46
1:B:84:ASP:OD2	1:B:113:THR:OG1	2.34	0.46
1:B:56:HIS:CE1	1:B:71:GLY:HA3	2.50	0.46
1:B:221:THR:HG22	1:B:225:ARG:HH21	1.79	0.46
1:A:41:VAL:HG22	1:A:59:THR:OG1	2.16	0.46
1:A:240:HIS:CD2	5:A:2025:HOH:O	2.68	0.45
1:B:256:VAL:HG12	1:B:260:LYS:NZ	2.31	0.45
1:B:86:ALA:HB2	1:B:95:LEU:HD22	1.98	0.45
1:B:228:LYS:O	1:B:231:PRO:HG3	2.16	0.45
1:A:161:SER:HB3	1:A:176:GLY:HA2	1.97	0.45
1:A:187:TYR:OH	1:A:192:ASN:HA	2.16	0.45
1:A:75:ARG:HH12	1:A:77:GLY:HA2	1.80	0.45
1:A:228:LYS:HB3	1:A:228:LYS:HE2	1.81	0.45
1:B:84:ASP:CG	1:B:113:THR:OG1	2.55	0.45
1:B:187:TYR:CB	1:B:230:TYR:CE1	3.00	0.45
1:A:205:ARG:HD3	1:A:207:SER:O	2.17	0.44
1:B:219:TRP:N	1:B:220:PRO:HD2	2.31	0.44
1:B:185:VAL:HG12	1:B:196:GLY:O	2.18	0.44
1:B:161:SER:HA	1:B:174:TYR:CD2	2.53	0.44
1:B:252:THR:O	1:B:256:VAL:HG23	2.18	0.43
1:B:173:PHE:HB2	1:B:230:TYR:OH	2.17	0.43
1:B:257:LYS:HA	1:B:260:LYS:HE2	2.01	0.43
1:A:257:LYS:O	1:A:260:LYS:HB2	2.18	0.42
1:B:69:SER:HB3	1:B:240:HIS:ND1	2.34	0.42
1:B:174:TYR:HB2	1:B:184:LEU:CD2	2.50	0.42
1:B:56:HIS:NE2	1:B:71:GLY:HA3	2.35	0.41
1:A:114:HIS:ND1	1:A:119:ARG:HG3	2.34	0.41
1:B:92:THR:O	1:B:93:ALA:C	2.58	0.41
1:A:44:VAL:HG22	1:A:58:ALA:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:TYR:CD2	1:A:153:HIS:HB2	2.56	0.41
1:A:54:TRP:CE3	1:A:54:TRP:N	2.89	0.41
1:A:114:HIS:CE1	1:A:198:CYS:HB2	2.55	0.41
1:B:129:ALA:O	1:B:131:VAL:HG23	2.21	0.41
1:A:82:LEU:O	1:A:110:ALA:HA	2.21	0.41
1:A:86:ALA:O	1:A:87:TRP:CB	2.67	0.40
1:A:59:THR:HA	1:A:67:TYR:O	2.22	0.40
1:A:219:TRP:CD1	1:A:219:TRP:O	2.72	0.40
1:A:56:HIS:CE1	1:A:71:GLY:HA3	2.57	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	229/230 (100%)	212 (93%)	17 (7%)	0	100	100
1	B	228/230 (99%)	196 (86%)	30 (13%)	2 (1%)	17	46
All	All	457/460 (99%)	408 (89%)	47 (10%)	2 (0%)	34	66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	77	GLY
1	B	84	ASP

### 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	182/181 (101%)	165 (91%)	17 (9%)	9	26
1	B	181/181 (100%)	162 (90%)	19 (10%)	7	20
All	All	363/362 (100%)	327 (90%)	36 (10%)	8	23

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

Mol	Chain	Res	Type
1	A	32	GLU
1	A	37	ASN
1	A	38	GLU
1	A	54	TRP
1	A	69	SER
1	A	101	LYS
1	A	105	LEU
1	A	154	SER
1	A	166	ARG
1	A	183	ASN
1	A	198	CYS
1	A	204	SER
1	A	223	VAL
1	A	224	GLU
1	A	232	GLU
1	A	247	ASP
1	A	261	ASN
1	B	37	ASN
1	B	41	VAL
1	B	49	ILE
1	B	90	LYS
1	B	113	THR
1	B	150	ILE
1	B	160	SER
1	B	166	ARG
1	B	183	ASN
1	B	204	SER
1	B	205	ARG
1	B	216	LEU
1	B	227	GLN
1	B	232	GLU
1	B	234	GLU
1	B	246	LEU

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Mol	Chain	Res	Type
1	B	247	ASP
1	B	248	LEU
1	B	260	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	201	HIS
1	A	250	GLN
1	A	254	ASN
1	B	114	HIS
1	B	254	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\# Z  > 2$
4	CIT	A	1265	-	3,12,12	3.00	1 (33%)	3,17,17	2.97	2 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	FLC	A	1263	2	3,12,12	0.97	0	3,17,17	1.12	0
3	FLC	B	1263	2	3,12,12	1.43	1 (33%)	3,17,17	2.74	2 (66%)
4	CIT	A	1264	-	3,12,12	1.94	1 (33%)	3,17,17	0.32	0

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
4	CIT	A	1265	-	-	6/6/16/16	-
3	FLC	A	1263	2	-	3/6/16/16	-
3	FLC	B	1263	2	-	6/6/16/16	-
4	CIT	A	1264	-	-	6/6/16/16	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1265	CIT	O7-C3	4.79	1.50	1.43
4	A	1264	CIT	O7-C3	2.86	1.47	1.43
3	B	1263	FLC	CG-CB	-2.23	1.51	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1265	CIT	C3-C4-C5	-3.99	108.60	114.98
3	B	1263	FLC	CB-CA-CAC	3.60	120.75	114.98
4	A	1265	CIT	C3-C2-C1	-3.19	109.87	114.98
3	B	1263	FLC	CB-CG-CGC	-2.99	110.20	114.98

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1263	FLC	CA-CB-CG-CGC
3	A	1263	FLC	CBC-CB-CG-CGC
3	A	1263	FLC	OHB-CB-CG-CGC
4	A	1264	CIT	C1-C2-C3-C6
4	A	1264	CIT	C6-C3-C4-C5
4	A	1265	CIT	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
4	A	1265	CIT	C6-C3-C4-C5
3	B	1263	FLC	CAC-CA-CB-CBC
3	B	1263	FLC	CAC-CA-CB-CG
3	B	1263	FLC	CAC-CA-CB-OHB
3	B	1263	FLC	CA-CB-CG-CGC
3	B	1263	FLC	CBC-CB-CG-CGC
3	B	1263	FLC	OHB-CB-CG-CGC
4	A	1264	CIT	O7-C3-C4-C5
4	A	1264	CIT	C1-C2-C3-O7
4	A	1264	CIT	C1-C2-C3-C4
4	A	1264	CIT	C2-C3-C4-C5
4	A	1265	CIT	C1-C2-C3-O7
4	A	1265	CIT	C2-C3-C4-C5
4	A	1265	CIT	C1-C2-C3-C6
4	A	1265	CIT	O7-C3-C4-C5

There are no ring outliers.

4 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1265	CIT	3	0
3	A	1263	FLC	8	0
3	B	1263	FLC	3	0
4	A	1264	CIT	8	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data [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	230/230 (100%)	-0.41	0 <span>100</span> <span>100</span>	5, 22, 49, 76	0
1	B	230/230 (100%)	0.16	11 (4%) <span>30</span> <span>21</span>	16, 47, 86, 104	0
All	All	460/460 (100%)	-0.13	11 (2%) <span>59</span> <span>49</span>	5, 33, 82, 104	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	261	ASN	5.2
1	B	156	GLU	3.5
1	B	260	LYS	3.3
1	B	176	GLY	3.1
1	B	217	ALA	3.1
1	B	220	PRO	2.7
1	B	259	HIS	2.7
1	B	216	LEU	2.4
1	B	161	SER	2.3
1	B	177	ALA	2.3
1	B	250	GLN	2.2

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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( $\text{\AA}^2$ )	Q<0.9
4	CIT	A	1264	13/13	0.87	0.46	22,24,28,32	0
4	CIT	A	1265	13/13	0.87	0.39	22,25,31,31	0
3	FLC	B	1263	13/13	0.89	0.18	69,70,71,71	0
3	FLC	A	1263	13/13	0.94	0.13	55,62,63,64	0
2	ZN	B	1262	1/1	0.98	0.03	58,58,58,58	0
2	ZN	A	1262	1/1	0.99	0.08	38,38,38,38	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.