



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 10:10 PM UTC

PDB ID : 4U4L / pdb_00004u4l
Title : Crystal structure of the metallo-beta-lactamase NDM-1 in complex with a bisthiazolidine inhibitor
Authors : Kosmopoulou, M.; Hinchliffe, P.; Spencer, J.
Deposited on : 2014-07-23
Resolution : 1.90 Å(reported)

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

We welcome your comments at 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

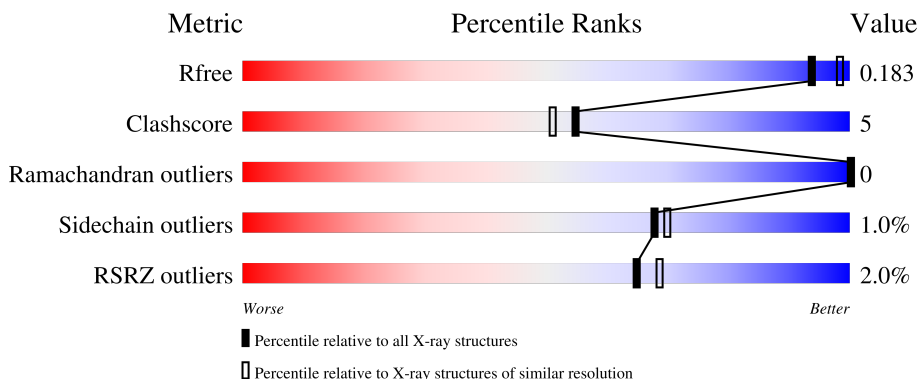
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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 ≥ 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	246	2% 83% 9% 7%
1	B	246	% 83% 10% 6%
1	C	246	% 80% 11% 9%
1	D	246	3% 80% 11% 9%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7515 atoms, of which 56 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 NDM-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	229	Total	C	N	O	S	0	0	0
			1703	1067	303	324	9			
1	B	231	Total	C	N	O	S	0	0	0
			1717	1078	305	326	8			
1	C	223	Total	C	N	O	S	0	1	0
			1670	1050	297	315	8			
1	D	224	Total	C	N	O	S	0	1	0
			1673	1051	298	317	7			

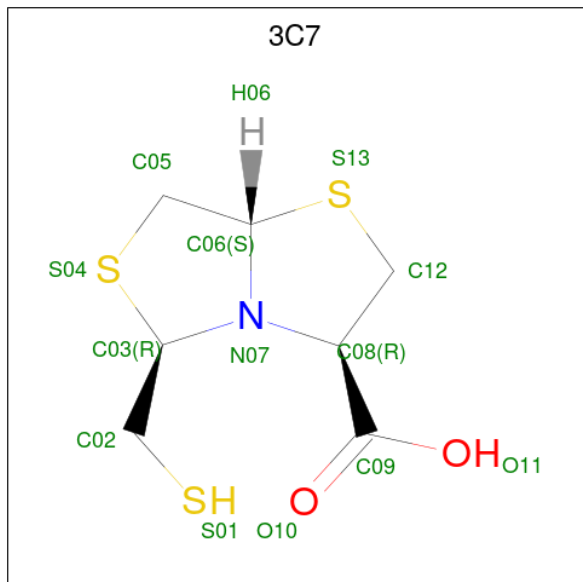
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	GLY	-	expression tag	UNP C7C422
A	26	PRO	-	expression tag	UNP C7C422
B	25	GLY	-	expression tag	UNP C7C422
B	26	PRO	-	expression tag	UNP C7C422
C	25	GLY	-	expression tag	UNP C7C422
C	26	PRO	-	expression tag	UNP C7C422
D	25	GLY	-	expression tag	UNP C7C422
D	26	PRO	-	expression tag	UNP C7C422

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is (3R,5R,7aS)-5-(sulfanylmethyl)tetrahydro[1,3]thiazolo[4,3-b][1,3]thiazole-3-carboxylic acid (CCD ID: 3C7) (formula: $C_7H_{11}NO_2S_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	S	0	0
			23	7	10	1	2	3		
3	B	1	Total	C	H	N	O	S	0	0
			23	7	10	1	2	3		
3	C	1	Total	C	H	N	O	S	0	0
			23	7	10	1	2	3		
3	D	1	Total	C	H	N	O	S	0	0
			23	7	10	1	2	3		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	H	O	0	0
			14	3	8	3		
4	D	1	Total	C	H	O	0	0
			14	3	8	3		

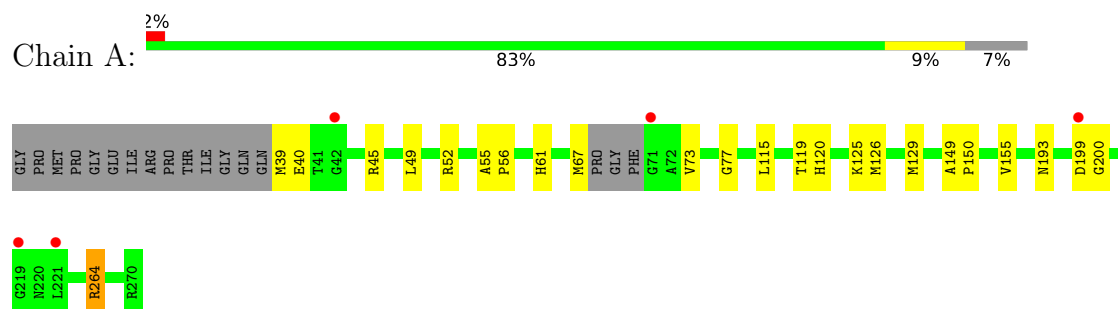
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	163	Total	O	0	0
			163	163		
5	B	165	Total	O	0	0
			165	165		
5	C	153	Total	O	0	0
			153	153		
5	D	143	Total	O	0	0
			143	143		

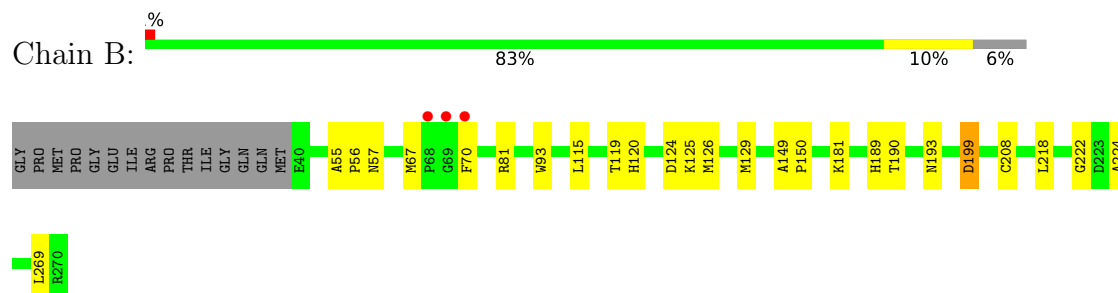
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 ($RSRZ > 2$). 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.

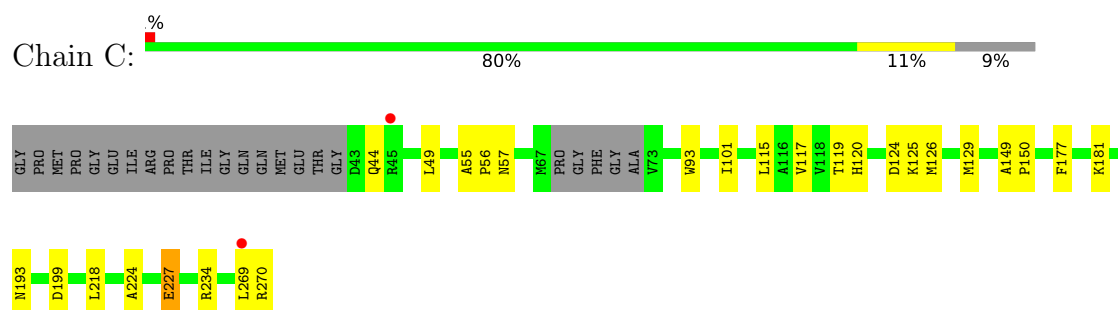
• Molecule 1: Beta-lactamase NDM-1



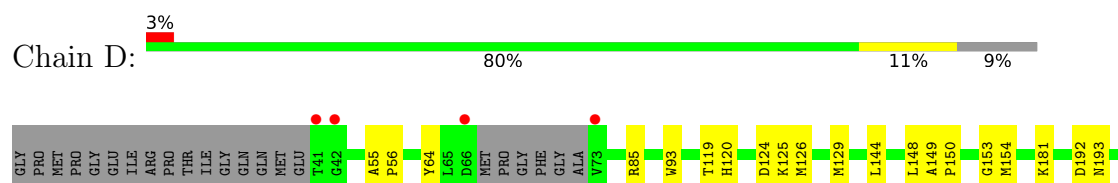
• Molecule 1: Beta-lactamase NDM-1

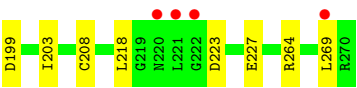


• Molecule 1: Beta-lactamase NDM-1



• Molecule 1: Beta-lactamase NDM-1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	46.57Å 69.02Å 69.65Å 87.39° 88.21° 76.75°	Depositor
Resolution (Å)	27.88 – 1.90 27.88 – 1.90	Depositor EDS
% Data completeness (in resolution range)	93.5 (27.88-1.90) 90.8 (27.88-1.90)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.29 (at 1.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.154 , 0.182 0.156 , 0.183	Depositor DCC
R_{free} test set	3168 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	17.1	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 54.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7515	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 3C7, ZN

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	0.56	1/1740 (0.1%)	0.75	0/2367
1	B	0.53	0/1757	0.80	1/2393 (0.0%)
1	C	0.53	1/1710 (0.1%)	0.75	0/2328
1	D	0.48	1/1713 (0.1%)	0.72	1/2333 (0.0%)
All	All	0.52	3/6920 (0.0%)	0.76	2/9421 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	264	ARG	C-O	-6.22	1.16	1.24
1	A	264	ARG	C-O	-5.87	1.17	1.24
1	C	227	GLU	C-O	-5.72	1.17	1.24

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	70	PHE	N-CA-C	6.53	118.40	111.28
1	D	203	ILE	N-CA-C	5.08	115.28	108.17

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	1703	0	1652	15	0
1	B	1717	0	1663	14	1
1	C	1670	0	1628	17	0
1	D	1673	0	1629	19	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	13	10	9	0	0
3	B	13	10	9	0	0
3	C	13	10	9	0	0
3	D	13	10	9	0	0
4	C	6	8	8	0	0
4	D	6	8	8	0	0
5	A	163	0	0	1	0
5	B	165	0	0	1	0
5	C	153	0	0	4	1
5	D	143	0	0	3	0
All	All	7459	56	6624	64	1

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.

The worst 5 of 64 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:C:44:GLN:NE2	5:C:523:HOH:O	1.84	0.94
1:C:218:LEU:HD12	1:C:269:LEU:HD11	1.68	0.74
1:C:224:ALA:O	5:C:401:HOH:O	2.05	0.74
1:B:222:GLY:O	5:B:401:HOH:O	2.09	0.70
1:A:40:GLU:HB2	1:A:52:ARG:HH22	1.55	0.70

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	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:ALA:O	5:C:401:HOH:O[1_545]	2.13	0.07

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	225/246 (92%)	221 (98%)	4 (2%)	0	100	100
1	B	229/246 (93%)	225 (98%)	4 (2%)	0	100	100
1	C	220/246 (89%)	216 (98%)	4 (2%)	0	100	100
1	D	221/246 (90%)	218 (99%)	3 (1%)	0	100	100
All	All	895/984 (91%)	880 (98%)	15 (2%)	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	172/185 (93%)	170 (99%)	2 (1%)	63	63
1	B	173/185 (94%)	170 (98%)	3 (2%)	53	52
1	C	170/185 (92%)	169 (99%)	1 (1%)	78	81
1	D	170/185 (92%)	169 (99%)	1 (1%)	78	81
All	All	685/740 (93%)	678 (99%)	7 (1%)	68	70

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	193	ASN
1	B	199	ASP
1	D	193	ASN

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Mol	Chain	Res	Type
1	C	193	ASN
1	B	67	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	220	ASN
1	C	44	GLN
1	D	97	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 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	3C7	A	303	2	11,14,14	1.88	2 (18%)	11,20,20	2.91	4 (36%)
3	3C7	B	303	2	11,14,14	1.90	2 (18%)	11,20,20	3.25	5 (45%)
3	3C7	C	304	2	11,14,14	2.27	6 (54%)	11,20,20	3.47	6 (54%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	D	303	-	5,5,5	0.40	0	5,5,5	0.57	0
4	GOL	C	303	-	5,5,5	0.38	0	5,5,5	0.43	0
3	3C7	D	304	2	11,14,14	1.88	2 (18%)	11,20,20	3.11	5 (45%)

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	3C7	A	303	2	-	1/4/28/28	0/2/2/2
3	3C7	B	303	2	-	0/4/28/28	0/2/2/2
3	3C7	C	304	2	-	2/4/28/28	0/2/2/2
4	GOL	D	303	-	-	2/4/4/4	-
4	GOL	C	303	-	-	0/4/4/4	-
3	3C7	D	304	2	-	0/4/28/28	0/2/2/2

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	303	3C7	C03-S04	-3.75	1.76	1.83
3	A	303	3C7	C03-S04	-3.62	1.76	1.83
3	D	304	3C7	C03-S04	-3.61	1.76	1.83
3	A	303	3C7	C06-S13	-3.58	1.76	1.83
3	D	304	3C7	C06-S13	-3.47	1.76	1.83

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	304	3C7	C06-C05-S04	8.32	107.42	103.59
3	B	303	3C7	C06-C05-S04	6.11	106.40	103.59
3	B	303	3C7	C05-S04-C03	5.61	100.25	90.61
3	D	304	3C7	C05-S04-C03	5.58	100.19	90.61
3	A	303	3C7	C05-S04-C03	5.48	100.02	90.61

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	303	GOL	O1-C1-C2-C3
4	D	303	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	A	303	3C7	C12-C08-C09-O10
3	C	304	3C7	C12-C08-C09-O11
3	C	304	3C7	C12-C08-C09-O10

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, 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	229/246 (93%)	-0.38	5 (2%) 62 66	8, 16, 37, 66	0
1	B	231/246 (93%)	-0.33	3 (1%) 75 78	9, 18, 34, 68	0
1	C	223/246 (90%)	-0.38	2 (0%) 81 83	8, 16, 31, 60	1 (0%)
1	D	224/246 (91%)	-0.19	8 (3%) 46 49	7, 18, 43, 95	1 (0%)
All	All	907/984 (92%)	-0.32	18 (1%) 65 69	7, 17, 37, 95	2 (0%)

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	70	PHE	6.2
1	B	69	GLY	4.9
1	D	220	ASN	4.8
1	D	221	LEU	4.3
1	D	41	THR	4.3

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 oligosaccharides 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, 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	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	3C7	A	303	13/13	0.88	0.13	27,43,54,56	0
3	3C7	B	303	13/13	0.94	0.10	21,36,43,43	0
3	3C7	C	304	13/13	0.94	0.09	25,33,40,41	0
3	3C7	D	304	13/13	0.94	0.10	27,45,54,54	0
4	GOL	D	303	6/6	0.94	0.08	22,26,32,37	0
4	GOL	C	303	6/6	0.95	0.06	13,19,26,31	0
2	ZN	A	302	1/1	0.99	0.05	21,21,21,21	0
2	ZN	C	301	1/1	0.99	0.06	20,20,20,20	0
2	ZN	B	301	1/1	1.00	0.06	18,18,18,18	0
2	ZN	B	302	1/1	1.00	0.04	18,18,18,18	0
2	ZN	A	301	1/1	1.00	0.05	19,19,19,19	0
2	ZN	C	302	1/1	1.00	0.05	18,18,18,18	0
2	ZN	D	301	1/1	1.00	0.07	25,25,25,25	0
2	ZN	D	302	1/1	1.00	0.08	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.