



wwPDB X-ray Structure Validation Summary Report i

Feb 28, 2014 – 11:51 PM GMT

PDB ID : 2QRN
Title : Human Deoxycytidine kinase dCMP, UDP, Mg ion product complex
Authors : Ealick, S.E.; Soriano, E.V.
Deposited on : 2007-07-28
Resolution : 3.40 Å(reported)

This is a wwPDB validation summary 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>

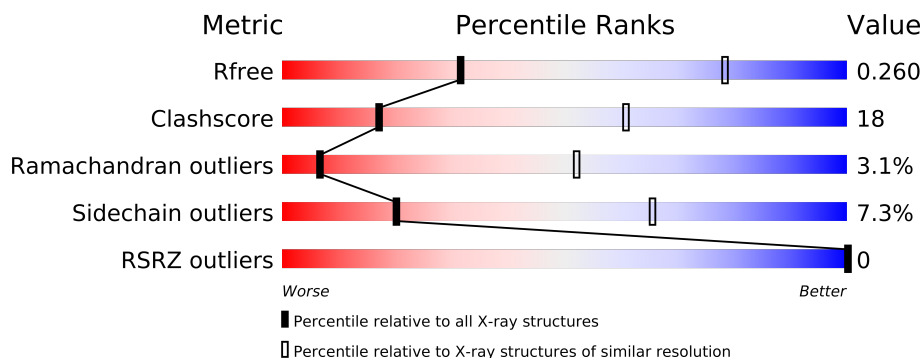
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.40 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	1017 (3.52-3.28)
Clashscore	79885	1214 (3.50-3.30)
Ramachandran outliers	78287	1177 (3.50-3.30)
Sidechain outliers	78261	1177 (3.50-3.30)
RSRZ outliers	66119	1017 (3.52-3.28)

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	280	<div><div></div><div></div><div></div><div></div><div></div></div>
1	B	280	<div><div></div><div></div><div></div><div></div><div></div></div>
1	C	280	<div><div></div><div></div><div></div><div></div><div></div></div>
1	D	280	<div><div></div><div></div><div></div><div></div><div></div></div>

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

Mol	Type	Chain	Res	Geometry	Electron density
2	MG	B	401	-	X
2	MG	C	401	-	X
2	MG	D	401	-	X
4	DCM	C	403	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7808 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 Deoxycytidine kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	S	0	0	0
			1906	1223	317	357	9			
1	B	228	Total	C	N	O	S	0	0	0
			1906	1223	317	357	9			
1	C	228	Total	C	N	O	S	0	0	0
			1906	1223	317	357	9			
1	D	228	Total	C	N	O	S	0	0	0
			1906	1223	317	357	9			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP P27707
A	-18	GLY	-	expression tag	UNP P27707
A	-17	SER	-	expression tag	UNP P27707
A	-16	SER	-	expression tag	UNP P27707
A	-15	HIS	-	expression tag	UNP P27707
A	-14	HIS	-	expression tag	UNP P27707
A	-13	HIS	-	expression tag	UNP P27707
A	-12	HIS	-	expression tag	UNP P27707
A	-11	HIS	-	expression tag	UNP P27707
A	-10	HIS	-	expression tag	UNP P27707
A	-9	SER	-	expression tag	UNP P27707
A	-8	SER	-	expression tag	UNP P27707
A	-7	GLY	-	expression tag	UNP P27707
A	-6	LEU	-	expression tag	UNP P27707
A	-5	VAL	-	expression tag	UNP P27707
A	-4	PRO	-	expression tag	UNP P27707
A	-3	ARG	-	expression tag	UNP P27707
A	-2	GLY	-	expression tag	UNP P27707
A	-1	SER	-	expression tag	UNP P27707
A	0	HIS	-	expression tag	UNP P27707
B	-19	MET	-	expression tag	UNP P27707

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP P27707
B	-17	SER	-	expression tag	UNP P27707
B	-16	SER	-	expression tag	UNP P27707
B	-15	HIS	-	expression tag	UNP P27707
B	-14	HIS	-	expression tag	UNP P27707
B	-13	HIS	-	expression tag	UNP P27707
B	-12	HIS	-	expression tag	UNP P27707
B	-11	HIS	-	expression tag	UNP P27707
B	-10	HIS	-	expression tag	UNP P27707
B	-9	SER	-	expression tag	UNP P27707
B	-8	SER	-	expression tag	UNP P27707
B	-7	GLY	-	expression tag	UNP P27707
B	-6	LEU	-	expression tag	UNP P27707
B	-5	VAL	-	expression tag	UNP P27707
B	-4	PRO	-	expression tag	UNP P27707
B	-3	ARG	-	expression tag	UNP P27707
B	-2	GLY	-	expression tag	UNP P27707
B	-1	SER	-	expression tag	UNP P27707
B	0	HIS	-	expression tag	UNP P27707
C	-19	MET	-	expression tag	UNP P27707
C	-18	GLY	-	expression tag	UNP P27707
C	-17	SER	-	expression tag	UNP P27707
C	-16	SER	-	expression tag	UNP P27707
C	-15	HIS	-	expression tag	UNP P27707
C	-14	HIS	-	expression tag	UNP P27707
C	-13	HIS	-	expression tag	UNP P27707
C	-12	HIS	-	expression tag	UNP P27707
C	-11	HIS	-	expression tag	UNP P27707
C	-10	HIS	-	expression tag	UNP P27707
C	-9	SER	-	expression tag	UNP P27707
C	-8	SER	-	expression tag	UNP P27707
C	-7	GLY	-	expression tag	UNP P27707
C	-6	LEU	-	expression tag	UNP P27707
C	-5	VAL	-	expression tag	UNP P27707
C	-4	PRO	-	expression tag	UNP P27707
C	-3	ARG	-	expression tag	UNP P27707
C	-2	GLY	-	expression tag	UNP P27707
C	-1	SER	-	expression tag	UNP P27707
C	0	HIS	-	expression tag	UNP P27707
D	-19	MET	-	expression tag	UNP P27707
D	-18	GLY	-	expression tag	UNP P27707
D	-17	SER	-	expression tag	UNP P27707

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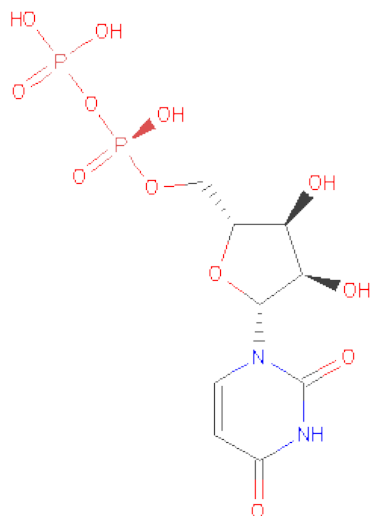
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP P27707
D	-15	HIS	-	expression tag	UNP P27707
D	-14	HIS	-	expression tag	UNP P27707
D	-13	HIS	-	expression tag	UNP P27707
D	-12	HIS	-	expression tag	UNP P27707
D	-11	HIS	-	expression tag	UNP P27707
D	-10	HIS	-	expression tag	UNP P27707
D	-9	SER	-	expression tag	UNP P27707
D	-8	SER	-	expression tag	UNP P27707
D	-7	GLY	-	expression tag	UNP P27707
D	-6	LEU	-	expression tag	UNP P27707
D	-5	VAL	-	expression tag	UNP P27707
D	-4	PRO	-	expression tag	UNP P27707
D	-3	ARG	-	expression tag	UNP P27707
D	-2	GLY	-	expression tag	UNP P27707
D	-1	SER	-	expression tag	UNP P27707
D	0	HIS	-	expression tag	UNP P27707

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

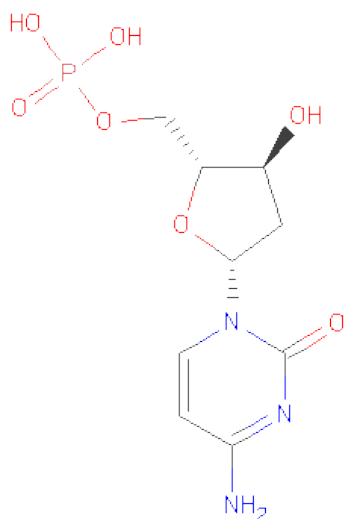
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0

- Molecule 3 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: C₉H₁₄N₂O₁₂P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
3	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
3	C	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
3	D	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 4 is 2'-DEOXYCYTIDINE-5'-MONOPHOSPHATE (three-letter code: DCM) (formula: C₉H₁₄N₃O₇P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 20	C 9	N 3	O 7	P 1	0	0
4	B	1	Total 20	C 9	N 3	O 7	P 1	0	0
4	C	1	Total 20	C 9	N 3	O 7	P 1	0	0
4	D	1	Total 20	C 9	N 3	O 7	P 1	0	0

MET	GLY	SER	SER	HIS	HIS	HIS	HIS	HIS	SER	SER	GLY	LEU	VAL	PRO	ARG	CYS	PRO	SER	PHE	SER	ALA	ALA	THR	GLY	GLY	THR	R20	I21	I30	A31	K34	S35	F37	V38	K39	I40	L44	C45	E46	D47	W48	E49	V50								
V51	P52	E53	R57	W58	C59	N60	S63	THR	GLN	ASP	GLU	PHE	GLU	GLU	LEU	THR	MET	SER	GLN	LYS	G78	G79	N80	V81	L82	Q83	M84	M85	Y86	E87	K88	P89	E90	R91	W92	R104	I105	R106	A107	Q108	L109	L112	L116	A119	E120	K121	P122	E127	R128	S129	V130
Y131	S132	D133	I136	N148	W152	Q156	D157	W158	N163	N164	Q165	F166	G167	Q168	R192	G193	R194	N195	K211	H212	K222	T223	N224	F225	D226	Y227	L228	Q229	E230	V231	P232	V238	R243	F242	K243	D244	K245	Y246	L260												

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	94.56Å 94.56Å 335.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.12 – 3.40 48.11 – 3.20	Depositor EDS
% Data completeness (in resolution range)	89.9 (48.12-3.40) 82.9 (48.11-3.20)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 3.19Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.217 , 0.269 0.218 , 0.260	Depositor DCC
R_{free} test set	954 reflections (4.84%)	DCC
Wilson B-factor (Å ²)	65.6	Xtriage
Anisotropy	0.403	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 23589 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7808	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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, DCM, UDP

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	0.41	0/1952	0.62	0/2641
1	B	0.41	0/1952	0.61	0/2641
1	C	0.42	0/1952	0.61	0/2641
1	D	0.42	0/1952	0.61	0/2641
All	All	0.41	0/7808	0.61	0/10564

There are no bond length outliers.

There are no bond angle outliers.

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	1906	0	1854	71	0
1	B	1906	0	1855	70	0
1	C	1906	0	1855	80	0
1	D	1906	0	1855	70	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	25	0	11	5	0
3	B	25	0	11	6	0
3	C	25	0	11	4	0
3	D	25	0	11	4	0
4	A	20	0	12	1	0
4	B	20	0	12	1	0
4	C	20	0	12	1	0
4	D	20	0	12	1	0
All	All	7808	0	7511	269	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 18.

The worst 5 of 269 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:222:LYS:HE2	1:A:222:LYS:HA	1.54	0.88
1:D:222:LYS:HE2	1:D:222:LYS:HA	1.56	0.87
1:B:222:LYS:HE2	1:B:222:LYS:HA	1.56	0.84
1:C:222:LYS:HA	1:C:222:LYS:HE2	1.58	0.84
1:D:53:GLU:HG2	1:D:104:ARG:HH12	1.44	0.80

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	224/280 (80%)	184 (82%)	32 (14%)	8 (4%)	5 47
1	B	224/280 (80%)	185 (83%)	33 (15%)	6 (3%)	8 55
1	C	224/280 (80%)	188 (84%)	30 (13%)	6 (3%)	8 55
1	D	224/280 (80%)	187 (84%)	29 (13%)	8 (4%)	5 47
All	All	896/1120 (80%)	744 (83%)	124 (14%)	28 (3%)	7 52

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	194	ARG
1	A	243	LYS
1	B	194	ARG
1	B	243	LYS
1	C	194	ARG

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	210/256 (82%)	195 (93%)	15 (7%)	21	67
1	B	210/256 (82%)	196 (93%)	14 (7%)	23	70
1	C	210/256 (82%)	193 (92%)	17 (8%)	17	60
1	D	210/256 (82%)	195 (93%)	15 (7%)	21	67
All	All	840/1024 (82%)	779 (93%)	61 (7%)	20	65

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	241	ASP
1	C	63	SER
1	D	222	LYS
1	B	246	TYR
1	C	34	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	163	ASN
1	B	224	ASN
1	D	43	GLN
1	B	43	GLN
1	B	77	ASN

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 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	UDP	A	402	-	26,26,26	1.24	4 (15%)	36,40,40	2.03	6 (16%)
4	DCM	A	403	-	21,21,21	1.29	4 (19%)	28,31,31	1.53	3 (10%)
3	UDP	B	402	-	26,26,26	1.46	4 (15%)	36,40,40	2.01	6 (16%)
4	DCM	B	403	-	21,21,21	1.24	3 (14%)	28,31,31	1.51	3 (10%)
3	UDP	C	402	2	26,26,26	1.29	3 (11%)	36,40,40	2.03	6 (16%)
4	DCM	C	403	-	21,21,21	1.33	3 (14%)	28,31,31	1.53	3 (10%)
3	UDP	D	402	-	26,26,26	1.45	5 (19%)	36,40,40	2.01	6 (16%)
4	DCM	D	403	-	21,21,21	1.38	4 (19%)	28,31,31	1.51	3 (10%)

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	UDP	A	402	-	-	0/14/32/32	0/2/2/2
4	DCM	A	403	-	-	0/7/22/22	0/2/2/2
3	UDP	B	402	-	-	0/14/32/32	0/2/2/2
4	DCM	B	403	-	-	0/7/22/22	0/2/2/2
3	UDP	C	402	2	-	0/14/32/32	0/2/2/2
4	DCM	C	403	-	-	0/7/22/22	0/2/2/2
3	UDP	D	402	-	-	0/14/32/32	0/2/2/2
4	DCM	D	403	-	-	0/7/22/22	0/2/2/2

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	UDP	PB-O3A	3.54	1.66	1.60
4	D	403	DCM	P-O3P	3.22	1.66	1.54
3	D	402	UDP	PA-O3A	3.00	1.65	1.59
3	B	402	UDP	C6-N1	2.99	1.40	1.35
4	C	403	DCM	P-O3P	2.95	1.65	1.54

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	UDP	PA-O3A-PB	-8.38	107.11	131.68
3	B	402	UDP	PA-O3A-PB	-8.37	107.13	131.68
3	C	402	UDP	PA-O3A-PB	-8.32	107.29	131.68
3	D	402	UDP	PA-O3A-PB	-8.29	107.36	131.68
3	C	402	UDP	N3-C2-N1	5.85	120.86	115.97

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	228/280 (81%)	-0.01	0 100 100	23, 63, 132, 173	0
1	B	228/280 (81%)	-0.09	0 100 100	26, 63, 135, 190	0
1	C	228/280 (81%)	-0.19	0 100 100	24, 59, 134, 161	0
1	D	228/280 (81%)	-0.13	0 100 100	26, 62, 128, 193	0
All	All	912/1120 (81%)	-0.11	0 100 100	23, 62, 134, 193	0

There are no RSRZ outliers to report.

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
2	MG	C	401	1/1	0.38	7.82	56,56,56,56	0
4	DCM	C	403	20/20	0.28	4.07	51,80,89,89	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	MG	D	401	1/1	0.33	3.91	56,56,56,56	0
2	MG	B	401	1/1	0.28	2.06	56,56,56,56	0
3	UDP	C	402	25/25	0.25	0.95	66,82,87,88	0
4	DCM	A	403	20/20	0.26	0.77	51,80,89,89	0
4	DCM	D	403	20/20	0.22	0.48	51,80,89,89	0
3	UDP	D	402	25/25	0.23	0.21	66,82,87,88	0
4	DCM	B	403	20/20	0.22	0.06	51,80,89,89	0
3	UDP	B	402	25/25	0.21	-0.13	66,82,87,88	0
3	UDP	A	402	25/25	0.20	-0.62	66,82,87,88	0
2	MG	A	401	1/1	0.14	-1.70	56,56,56,56	0

6.5 Other polymers ⓘ

There are no such residues in this entry.