W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 16, 2023 – 09:49 AM EDT

PDB ID	:	2A30
Title	:	Crystal structure of human deoxycytidine kinase in complex with deoxycytidine
Authors	:	Godsey, M.H.; Ort, S.; Sabini, E.; Konrad, M.; Lavie, A.
Deposited on	:	2005-06-23
Resolution	:	3.02 Å(reported)

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

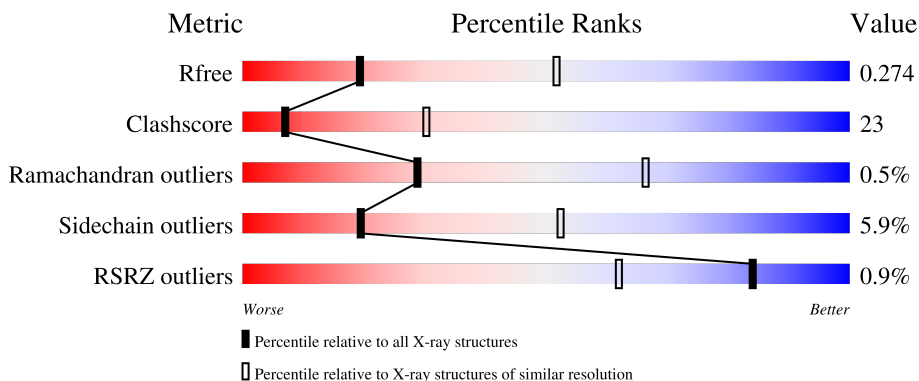|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.02 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	Percentile Ranks	Value
Rfree		0.274
Clashscore		23
Ramachandran outliers		0.5%
Sidechain outliers		5.9%
RSRZ outliers		0.9%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2399 (3.04-3.00)
Clashscore	141614	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)
RSRZ outliers	127900	2287 (3.04-3.00)

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 <=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	248	53% 33% • 11%
1	B	248	49% 33% • 15%
1	C	248	% 56% 31% • 11%
1	D	248	2% 52% 30% • 13%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 6944 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 Deoxycytidine kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	0	0
			1759	1130	296	325	8			
1	B	212	Total	C	N	O	S	0	0	0
			1673	1081	277	307	8			
1	C	221	Total	C	N	O	S	0	0	0
			1739	1117	293	321	8			
1	D	215	Total	C	N	O	S	0	0	0
			1681	1080	283	310	8			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	cloning artifact	UNP P27707
A	-1	SER	-	cloning artifact	UNP P27707
A	0	HIS	-	cloning artifact	UNP P27707
A	?	-	GLN	deletion	UNP P27707
A	?	-	ASP	deletion	UNP P27707
A	?	-	GLU	deletion	UNP P27707
A	?	-	PHE	deletion	UNP P27707
A	?	-	GLU	deletion	UNP P27707
A	?	-	GLU	deletion	UNP P27707
A	?	-	LEU	deletion	UNP P27707
A	?	-	THR	deletion	UNP P27707
A	?	-	MET	deletion	UNP P27707
A	?	-	SER	deletion	UNP P27707
A	?	-	GLN	deletion	UNP P27707
A	?	-	LYS	deletion	UNP P27707
A	?	-	ASN	deletion	UNP P27707
A	?	-	GLY	deletion	UNP P27707
A	?	-	GLY	deletion	UNP P27707
B	-2	GLY	-	cloning artifact	UNP P27707
B	-1	SER	-	cloning artifact	UNP P27707
B	0	HIS	-	cloning artifact	UNP P27707

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	GLN	deletion	UNP P27707
B	?	-	ASP	deletion	UNP P27707
B	?	-	GLU	deletion	UNP P27707
B	?	-	PHE	deletion	UNP P27707
B	?	-	GLU	deletion	UNP P27707
B	?	-	GLU	deletion	UNP P27707
B	?	-	LEU	deletion	UNP P27707
B	?	-	THR	deletion	UNP P27707
B	?	-	MET	deletion	UNP P27707
B	?	-	SER	deletion	UNP P27707
B	?	-	GLN	deletion	UNP P27707
B	?	-	LYS	deletion	UNP P27707
B	?	-	ASN	deletion	UNP P27707
B	?	-	GLY	deletion	UNP P27707
B	?	-	GLY	deletion	UNP P27707
C	-2	GLY	-	cloning artifact	UNP P27707
C	-1	SER	-	cloning artifact	UNP P27707
C	0	HIS	-	cloning artifact	UNP P27707
C	?	-	GLN	deletion	UNP P27707
C	?	-	ASP	deletion	UNP P27707
C	?	-	GLU	deletion	UNP P27707
C	?	-	PHE	deletion	UNP P27707
C	?	-	GLU	deletion	UNP P27707
C	?	-	GLU	deletion	UNP P27707
C	?	-	LEU	deletion	UNP P27707
C	?	-	THR	deletion	UNP P27707
C	?	-	MET	deletion	UNP P27707
C	?	-	SER	deletion	UNP P27707
C	?	-	GLN	deletion	UNP P27707
C	?	-	LYS	deletion	UNP P27707
C	?	-	ASN	deletion	UNP P27707
C	?	-	GLY	deletion	UNP P27707
C	?	-	GLY	deletion	UNP P27707
D	-2	GLY	-	cloning artifact	UNP P27707
D	-1	SER	-	cloning artifact	UNP P27707
D	0	HIS	-	cloning artifact	UNP P27707
D	?	-	GLN	deletion	UNP P27707
D	?	-	ASP	deletion	UNP P27707
D	?	-	GLU	deletion	UNP P27707
D	?	-	PHE	deletion	UNP P27707
D	?	-	GLU	deletion	UNP P27707
D	?	-	GLU	deletion	UNP P27707

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	LEU	deletion	UNP P27707
D	?	-	THR	deletion	UNP P27707
D	?	-	MET	deletion	UNP P27707
D	?	-	SER	deletion	UNP P27707
D	?	-	GLN	deletion	UNP P27707
D	?	-	LYS	deletion	UNP P27707
D	?	-	ASN	deletion	UNP P27707
D	?	-	GLY	deletion	UNP P27707
D	?	-	GLY	deletion	UNP P27707

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is 2'-DEOXYCYTIDINE (three-letter code: DCZ) (formula: $C_9H_{13}N_3O_4$).
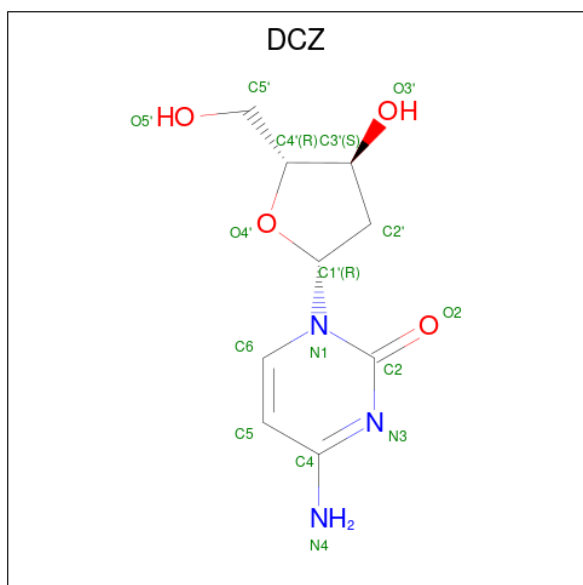
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 16	C 9	N 3	O 4	0	0
3	B	1	Total 16	C 9	N 3	O 4	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total 16	C 9	N 3	O 4	0	0
3	D	1	Total 16	C 9	N 3	O 4	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	9	Total 9	O 9	0	0
4	B	4	Total 4	O 4	0	0
4	C	12	Total 12	O 12	0	0
4	D	1	Total 1	O 1	0	0

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3 Residue-property plots ⓘ

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.
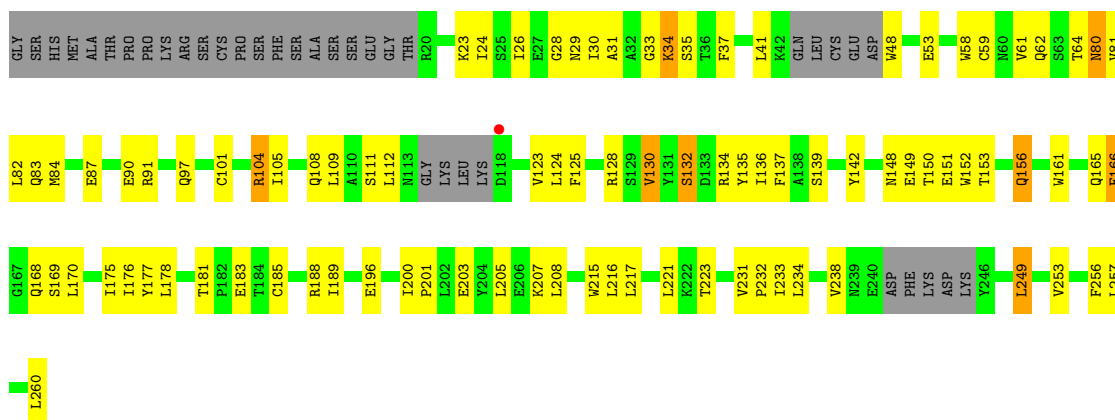
● Molecule 1: Deoxycytidine kinase

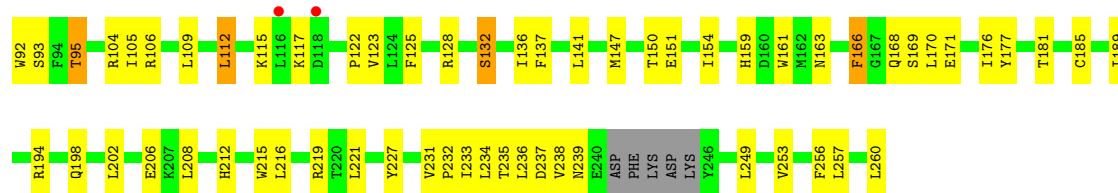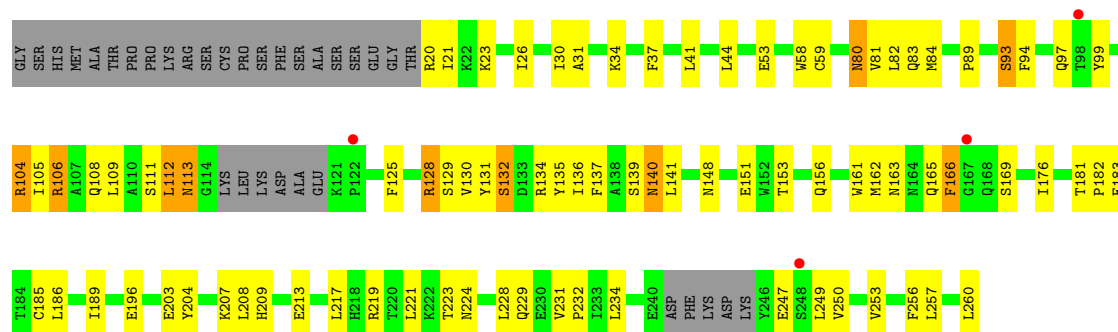Chain A:
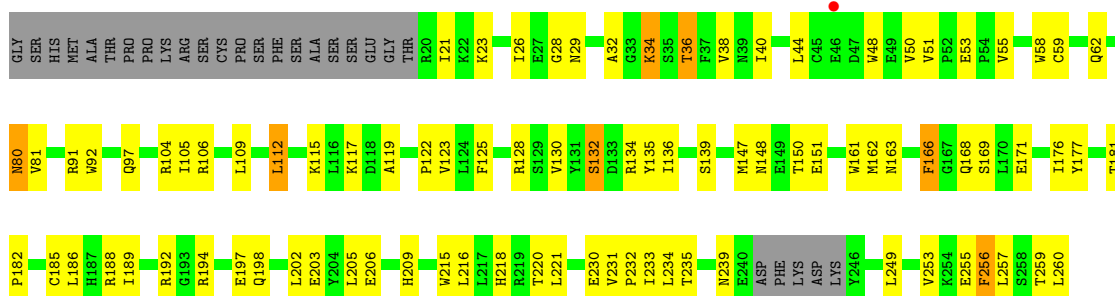
● Molecule 1: Deoxycytidine kinase

Chain B:

● Molecule 1: Deoxycytidine kinase

Chain C:

W92 S93 F94 T95 R104 I105 R106 L109 L112 K115 L116 K117 D118 P122 V123 L124 F125 R128 S132 I136 F137 L141 M147 T150 E151 I154 H159 D160 W161 M162 N163 F166 G167 Q168 S169 L170 E171 I176 Y177 T181 C185 I189

R194 Q198 L202 E206 K207 L208 H212 W215 L216 R219 T220 L221 Y227 V231 P232 I233 L234 T235 L236 D237 V238 N239 E240 ASP PHE LYS ASP LYS Y246 L249 V253 F256 L257 L260

• Molecule 1: Deoxycytidine kinase

Chain D:

2%

52% 30% • 13%

GLY SER HIS MET ALA THR PRO PRO LYS ARG SER CYS PRO SER PHE SER ALA SER SER GLU GLY THR R20 I21 K22 K23 I26 I30 A31 K34 F37 L41 L44 E53 W58 C59 N80 V81 L82 Q83 M84 P89 S93 F94 Q97 T98 Y99

R104 I105 R106 A107 Q108 L109 A110 S111 L112 N113 G114 LYS LEU LYS ASP ALA GLU K121 P122 F125 R128 S129 V130 Y131 S132 D133 R134 Y135 I136 F137 A138 S139 N140 L141 N148 E151 W152 T153 Q156 W161 M162 N163 N164 Q165 F166 G167 Q168 S169 I176 T181 P182 E183

T184 C185 L186 I189 E196 E203 Y204 K207 L208 H209 E213 L217 H218 R219 T220 L221 K222 T223 N224 L228 Q229 E230 V231 P232 I233 L234 E240 ASP PHE LYS ASP LYS Y246 E247 S248 L249 V250 V253 F256 L257 L260

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	79.34Å 64.94Å 108.60Å 90.00° 95.97° 90.00°	Depositor
Resolution (Å)	19.90 – 3.02 19.90 – 3.02	Depositor EDS
% Data completeness (in resolution range)	91.9 (19.90-3.02) 91.9 (19.90-3.02)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 3.04Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.235 , 0.285 0.222 , 0.274	Depositor DCC
R_{free} test set	2011 reflections (10.03%)	wwPDB-VP
Wilson B-factor (Å^2)	76.9	Xtriage
Anisotropy	0.585	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 58.1	EDS
L-test for twinning[2]	$< |L| > = 0.45, < L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6944	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.85% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: DCZ, CA

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	0.48	0/1803	0.62	0/2456
1	B	0.44	0/1714	0.60	0/2337
1	C	0.45	0/1783	0.62	0/2434
1	D	0.44	0/1722	0.62	0/2349
All	All	0.45	0/7022	0.61	0/9576

There are no bond length outliers.

There are no bond angle outliers.

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	1759	0	1635	77	0
1	B	1673	0	1552	84	0
1	C	1739	0	1594	75	0
1	D	1681	0	1543	86	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
3	A	16	0	13	1	0
3	B	16	0	13	1	0
3	C	16	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	16	0	13	1	0
4	A	9	0	0	0	0
4	B	4	0	0	0	0
4	C	12	0	0	0	0
4	D	1	0	0	0	0
All	All	6944	0	6376	305	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 23.

The worst 5 of 305 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:34:LYS:HD2	1:B:35:SER:H	0.98	1.15
1:A:234:LEU:HB2	1:A:256:PHE:CD2	1.97	0.99
1:D:97:GLN:HE22	3:D:602:DCZ:HN41	1.12	0.98
1:B:34:LYS:HD2	1:B:35:SER:N	1.79	0.96
1:D:106:ARG:HH11	1:D:106:ARG:CB	1.79	0.95

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	217/248 (88%)	194 (89%)	22 (10%)	1 (0%)	29	66
1	B	204/248 (82%)	187 (92%)	17 (8%)	0	100	100
1	C	217/248 (88%)	191 (88%)	25 (12%)	1 (0%)	29	66
1	D	209/248 (84%)	190 (91%)	17 (8%)	2 (1%)	15	50
All	All	847/992 (85%)	762 (90%)	81 (10%)	4 (0%)	29	66

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	44	LEU
1	A	44	LEU
1	D	113	ASN
1	C	55	VAL

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	180/228 (79%)	170 (94%)	10 (6%)	21	54
1	B	171/228 (75%)	158 (92%)	13 (8%)	13	41
1	C	175/228 (77%)	167 (95%)	8 (5%)	27	62
1	D	169/228 (74%)	159 (94%)	10 (6%)	19	52
All	All	695/912 (76%)	654 (94%)	41 (6%)	19	52

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	166	PHE
1	D	106	ARG
1	C	168	GLN
1	D	80	ASN
1	D	128	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	97	GLN
1	D	97	GLN
1	D	80	ASN
1	D	140	ASN
1	B	108	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\#|Z| > 2$
3	DCZ	C	502	-	17,17,17	1.69	3 (17%)	24,24,24	1.98	6 (25%)
3	DCZ	B	402	-	17,17,17	1.52	3 (17%)	24,24,24	1.91	5 (20%)
3	DCZ	A	302	-	17,17,17	1.76	4 (23%)	24,24,24	1.82	4 (16%)
3	DCZ	D	602	-	17,17,17	1.57	3 (17%)	24,24,24	1.92	4 (16%)

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	DCZ	C	502	-	-	2/6/18/18	0/2/2/2
3	DCZ	B	402	-	-	1/6/18/18	0/2/2/2
3	DCZ	A	302	-	-	2/6/18/18	0/2/2/2
3	DCZ	D	602	-	-	1/6/18/18	0/2/2/2

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	DCZ	C5-C4	-4.71	1.32	1.42
3	C	502	DCZ	C5-C4	-4.68	1.32	1.42
3	D	602	DCZ	C5-C4	-4.08	1.33	1.42
3	B	402	DCZ	C5-C4	-3.93	1.34	1.42
3	A	302	DCZ	O4'-C1'	2.47	1.47	1.42

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	602	DCZ	O2-C2-N3	-6.29	112.10	122.33
3	C	502	DCZ	O2-C2-N3	-6.15	112.32	122.33
3	B	402	DCZ	O2-C2-N3	-6.01	112.56	122.33
3	A	302	DCZ	O2-C2-N3	-5.60	113.22	122.33
3	D	602	DCZ	O2-C2-N1	3.52	126.17	118.89

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	DCZ	O4'-C4'-C5'-O5'
3	A	302	DCZ	C3'-C4'-C5'-O5'
3	D	602	DCZ	O4'-C4'-C5'-O5'
3	C	502	DCZ	C3'-C4'-C5'-O5'
3	B	402	DCZ	O4'-C4'-C5'-O5'

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	DCZ	1	0
3	A	302	DCZ	1	0
3	D	602	DCZ	1	0

5.7 Other polymers ⓘ

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 ⓘ

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	221/248 (89%)	-0.57	1 (0%)	91	75	40, 66, 100, 109	0
1	B	212/248 (85%)	-0.49	1 (0%)	91	75	48, 71, 96, 108	0
1	C	221/248 (89%)	-0.54	2 (0%)	84	62	38, 66, 101, 108	0
1	D	215/248 (86%)	-0.41	4 (1%)	66	37	47, 73, 101, 108	0
All	All	869/992 (87%)	-0.50	8 (0%)	84	62	38, 70, 101, 109	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	122	PRO	3.2
1	A	46	GLU	3.0
1	D	167	GLY	2.7
1	C	118	ASP	2.7
1	C	116	LEU	2.7

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 monosaccharides 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. 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(Å^2)	Q<0.9
2	CA	A	261	1/1	0.91	0.11	75,75,75,75	0
2	CA	C	261	1/1	0.93	0.09	76,76,76,76	0
3	DCZ	D	602	16/16	0.95	0.22	63,70,71,71	0
3	DCZ	C	502	16/16	0.96	0.17	40,42,47,49	0
3	DCZ	A	302	16/16	0.97	0.19	36,41,46,46	0
3	DCZ	B	402	16/16	0.97	0.17	45,51,54,55	0

6.5 Other polymers ⓘ

There are no such residues in this entry.