



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 09:40 am BST

PDB ID : 1J79  
Title : Molecular Structure of Dihydroorotase: A Paradigm for Catalysis Through the Use of a Binuclear Metal Center  
Authors : Thoden, J.B.; Phillips Jr., G.N.; Neal, T.M.; Raushel, F.M.; Holden, H.M.  
Deposited on : 2001-05-16  
Resolution : 1.70 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](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

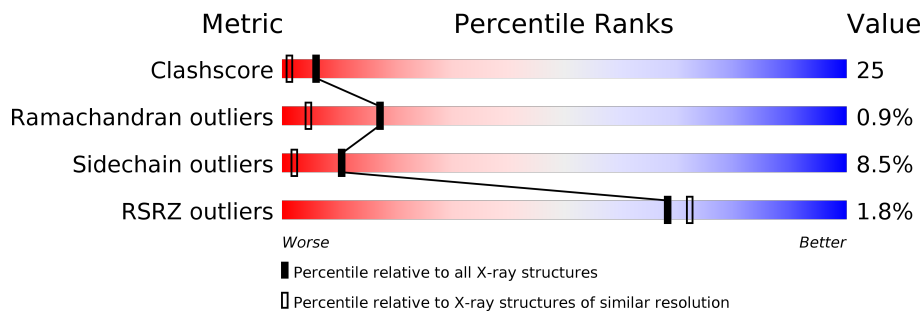
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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))
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	347	 3% 59% 30% 8% ..
1	B	347	 3% 52% 35% 9% ..

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 6212 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 dihydroorotase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	343	2751	1742	491	502	16	0	11	0
1	B	339	2691	1703	479	493	16	0	3	0

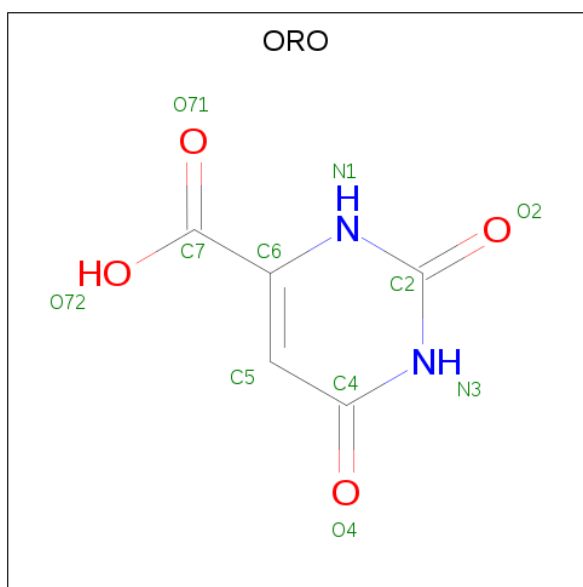
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	69	PRO	GLY	SEE REMARK 999	UNP P05020
A	102	KCX	LYS	MODIFIED RESIDUE	UNP P05020
A	119	VAL	ILE	SEE REMARK 999	UNP P05020
A	243	GLN	ASN	SEE REMARK 999	UNP P05020
B	69	PRO	GLY	SEE REMARK 999	UNP P05020
B	102	KCX	LYS	MODIFIED RESIDUE	UNP P05020
B	119	VAL	ILE	SEE REMARK 999	UNP P05020
B	243	GLN	ASN	SEE REMARK 999	UNP P05020

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

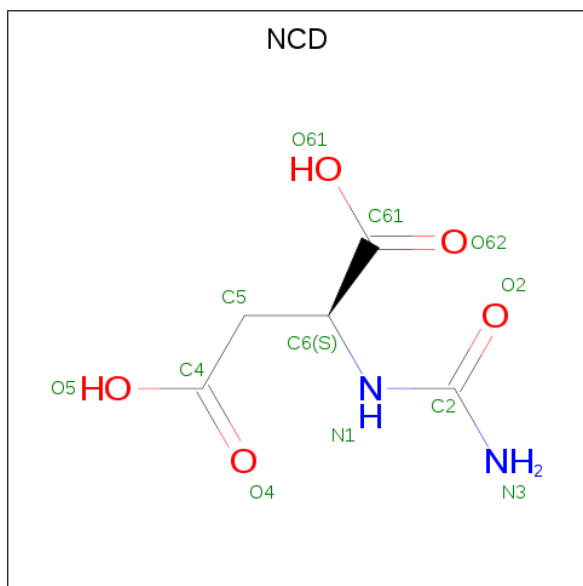
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is OROTIC ACID (three-letter code: ORO) (formula: C<sub>5</sub>H<sub>4</sub>N<sub>2</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	11	5	2	4	0	0

- Molecule 4 is N-CARBAMOYL-L-ASPARTATE (three-letter code: NCD) (formula:  $C_5H_8N_2O_5$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	12	5	2	5	0	0
4	B	1	12	5	2	5	0	0

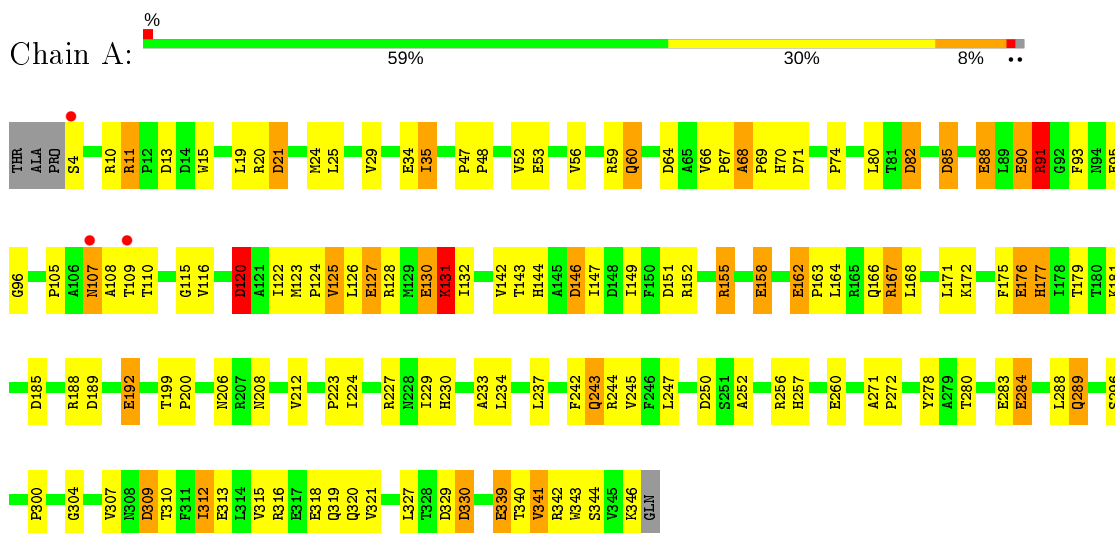
- Molecule 5 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
5	A	413	Total 413	O 413	0	0
5	B	318	Total 318	O 318	0	0

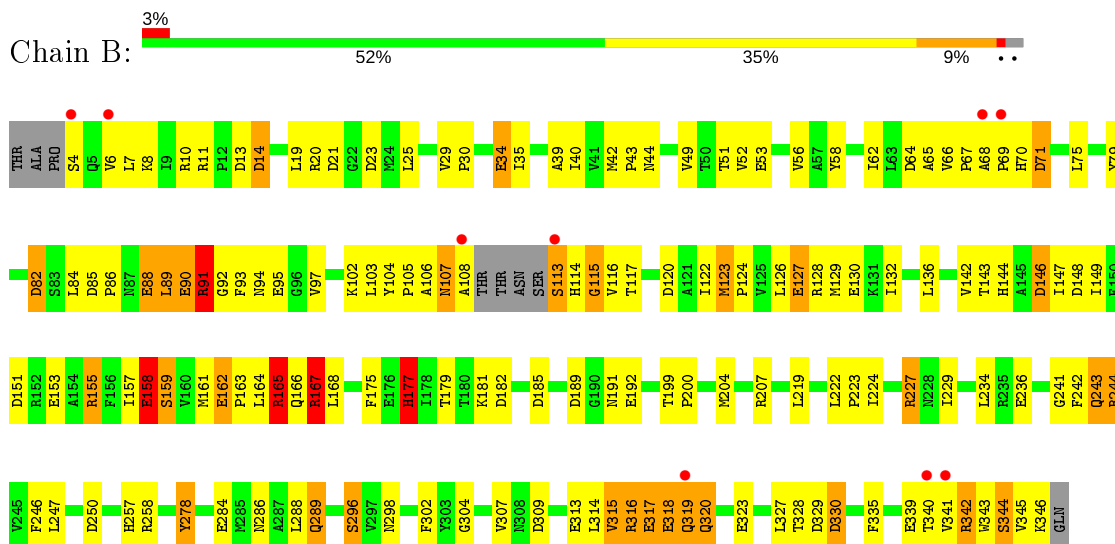
### 3 Residue-property plots [i](#)

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 ( $RSRZ > 2$ ). 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: dihydroorotase



- Molecule 1: dihydroorotase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.60Å 78.80Å 180.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.70 29.58 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.0 (30.00-1.70) 95.8 (29.58-1.50)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.80 (at 1.50Å)	Xtrriage
Refinement program	TNT	Depositor
R, $R_{free}$	0.191 , 0.258 0.203 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.8	Xtrriage
Anisotropy	0.271	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 110.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6212	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% 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: ORO, ZN, NCD, KCX

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	0.92	14/2845 (0.5%)	1.31	38/3869 (1.0%)
1	B	0.93	14/2752 (0.5%)	1.33	46/3740 (1.2%)
All	All	0.93	28/5597 (0.5%)	1.32	84/7609 (1.1%)

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	176	GLU	CD-OE2	7.46	1.33	1.25
1	A	260	GLU	CD-OE2	6.88	1.33	1.25
1	A	158	GLU	CD-OE2	6.83	1.33	1.25
1	B	153	GLU	CD-OE2	6.65	1.32	1.25
1	B	158	GLU	CD-OE2	6.60	1.32	1.25

The worst 5 of 84 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	148	ASP	CB-CG-OD2	-8.73	110.44	118.30
1	A	256[A]	ARG	NE-CZ-NH1	8.63	124.62	120.30
1	A	256[B]	ARG	NE-CZ-NH1	8.63	124.62	120.30
1	B	71	ASP	CB-CG-OD1	8.23	125.71	118.30
1	B	167	ARG	NE-CZ-NH1	8.16	124.38	120.30

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	2751	0	2725	121	0
1	B	2691	0	2658	146	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	11	0	3	0	0
4	A	12	0	6	5	0
4	B	12	0	6	2	0
5	A	413	0	0	12	1
5	B	318	0	0	19	0
All	All	6212	0	5398	270	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 25.

The worst 5 of 270 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:243:GLN:H	1:B:243:GLN:NE2	1.50	1.10
1:B:29:VAL:HG23	1:B:30:PRO:HD3	1.33	1.04
1:B:6:VAL:HG12	1:B:315:VAL:HG13	1.49	0.95
1:B:319:GLN:HG2	1:B:320:GLN:H	1.38	0.88
1:B:123:MET:HE3	1:B:167:ARG:HD2	1.55	0.88

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)
5:A:1316:HOH:O	5:A:1687:HOH:O[1_455]	2.19	0.01

## 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	351/347 (101%)	333 (95%)	16 (5%)	2 (1%)	25	11
1	B	337/347 (97%)	309 (92%)	23 (7%)	5 (2%)	10	2
All	All	688/694 (99%)	642 (93%)	39 (6%)	7 (1%)	17	4

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	318	GLU
1	A	177	HIS
1	B	115	GLY
1	B	177	HIS
1	B	91[A]	ARG

### 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	302/295 (102%)	275 (91%)	27 (9%)	9	2
1	B	291/295 (99%)	264 (91%)	27 (9%)	9	2
All	All	593/590 (100%)	539 (91%)	54 (9%)	10	2

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	312	ILE
1	B	91[A]	ARG
1	B	289	GLN
1	A	341	VAL
1	B	4	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	5	GLN
1	B	107	ASN
1	B	257	HIS
1	A	320	GLN
1	B	243	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](#)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z  > 2$
1	KCX	B	102	1,2	7,11,12	0.62	0	4,12,14	5.14	1 (25%)
1	KCX	A	102	1,2	7,11,12	0.69	0	4,12,14	4.87	1 (25%)

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
1	KCX	B	102	1,2	-	1/7/10/12	-
1	KCX	A	102	1,2	-	1/7/10/12	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	102	KCX	CE-NZ-CX	-10.22	105.64	122.95
1	A	102	KCX	CE-NZ-CX	-9.74	106.45	122.95

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	102	KCX	CG-CD-CE-NZ
1	A	102	KCX	CG-CD-CE-NZ

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	102	KCX	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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	NCD	A	950	-	5,11,11	1.34	1 (20%)	5,14,14	1.96	2 (40%)
4	NCD	B	411	2	5,11,11	0.95	0	5,14,14	2.13	3 (60%)
3	ORO	A	410	-	6,11,11	5.38	4 (66%)	3,15,15	8.21	3 (100%)

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	NCD	A	950	-	-	3/6/12/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NCD	B	411	2	-	3/6/12/12	-
3	ORO	A	410	-	-	0/0/4/4	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	410	ORO	C6-N1	11.13	1.51	1.34
3	A	410	ORO	C2-N1	4.98	1.48	1.38
3	A	410	ORO	C4-N3	4.39	1.40	1.33
4	A	950	NCD	C5-C6	-2.53	1.50	1.53
3	A	410	ORO	C5-C6	2.24	1.46	1.40

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	410	ORO	C5-C6-N1	-12.51	107.48	122.35
3	A	410	ORO	C5-C4-N3	-5.50	117.66	124.08
3	A	410	ORO	C4-C5-C6	3.93	119.27	116.73
4	B	411	NCD	O2-C2-N3	-3.23	117.67	123.22
4	A	950	NCD	O2-C2-N3	-3.14	117.82	123.22

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	411	NCD	C61-C6-N1-C2
4	A	950	NCD	C61-C6-N1-C2
4	B	411	NCD	O2-C2-N1-C6
4	B	411	NCD	N3-C2-N1-C6
4	A	950	NCD	O2-C2-N1-C6

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	950	NCD	5	0
4	B	411	NCD	2	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	342/347 (98%)	-0.32	3 (0%) 84 87	13, 25, 51, 78	0
1	B	338/347 (97%)	-0.01	9 (2%) 54 58	16, 31, 62, 92	0
All	All	680/694 (97%)	-0.16	12 (1%) 68 72	13, 28, 58, 92	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	108	ALA	3.7
1	B	113	SER	3.2
1	B	319	GLN	2.7
1	B	4	SER	2.7
1	B	68	ALA	2.6

### 6.2 Non-standard residues in protein, DNA, RNA chains [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(Å <sup>2</sup> )	Q<0.9
1	KCX	B	102	12/13	0.89	0.13	20,27,32,52	0
1	KCX	A	102	12/13	0.95	0.11	16,19,27,30	0

### 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(Å <sup>2</sup> )	Q<0.9
4	NCD	A	950	12/12	0.78	0.28	37,45,71,77	0
4	NCD	B	411	12/12	0.91	0.09	24,30,40,48	0
3	ORO	A	410	11/11	0.97	0.09	17,21,39,100	0
2	ZN	B	401	1/1	0.97	0.06	35,35,35,35	0
2	ZN	B	400	1/1	0.98	0.06	30,30,30,30	0
2	ZN	A	400	1/1	0.99	0.05	22,22,22,22	0
2	ZN	A	401	1/1	1.00	0.04	29,29,29,29	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.