



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 09:39 am BST

PDB ID : 5C3R
Title : Crystal structure of the full-length *Neurospora crassa* T7H in complex with alpha-KG and 5-hydroxymethyluracil (5hmU)
Authors : Li, W.; Zhang, T.; Ding, J.
Deposited on : 2015-06-17
Resolution : 2.35 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

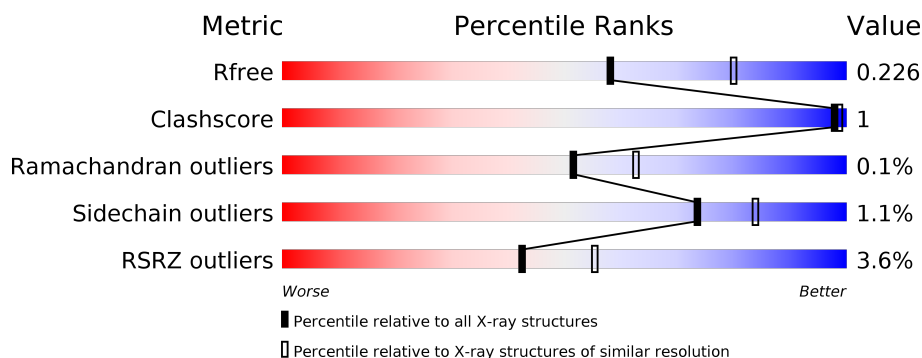
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 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	343	<div> <div>2%</div> <div>95%</div> <div>• •</div> </div>
1	B	343	<div> <div>3%</div> <div>88%</div> <div>• 10%</div> </div>
1	C	343	<div> <div>%</div> <div>86%</div> <div>• 10%</div> </div>
1	D	343	<div> <div>8%</div> <div>94%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	HMU	A	403	-	X	-	-
4	HMU	B	403	-	X	-	-
4	HMU	C	403	-	X	-	-
4	HMU	D	403	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10833 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 Thymine dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	0	0
			2634	1679	447	502	6			
1	B	310	Total	C	N	O	S	0	0	0
			2454	1567	415	466	6			
1	C	310	Total	C	N	O	S	0	0	0
			2454	1567	415	466	6			
1	D	329	Total	C	N	O	S	0	0	0
			2598	1656	443	494	5			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q7RYZ9
A	0	SER	-	expression tag	UNP Q7RYZ9
A	334	LEU	-	expression tag	UNP Q7RYZ9
A	335	GLU	-	expression tag	UNP Q7RYZ9
A	336	HIS	-	expression tag	UNP Q7RYZ9
A	337	HIS	-	expression tag	UNP Q7RYZ9
A	338	HIS	-	expression tag	UNP Q7RYZ9
A	339	HIS	-	expression tag	UNP Q7RYZ9
A	340	HIS	-	expression tag	UNP Q7RYZ9
A	341	HIS	-	expression tag	UNP Q7RYZ9
B	-1	GLY	-	expression tag	UNP Q7RYZ9
B	0	SER	-	expression tag	UNP Q7RYZ9
B	334	LEU	-	expression tag	UNP Q7RYZ9
B	335	GLU	-	expression tag	UNP Q7RYZ9
B	336	HIS	-	expression tag	UNP Q7RYZ9
B	337	HIS	-	expression tag	UNP Q7RYZ9
B	338	HIS	-	expression tag	UNP Q7RYZ9
B	339	HIS	-	expression tag	UNP Q7RYZ9
B	340	HIS	-	expression tag	UNP Q7RYZ9
B	341	HIS	-	expression tag	UNP Q7RYZ9
C	-1	GLY	-	expression tag	UNP Q7RYZ9

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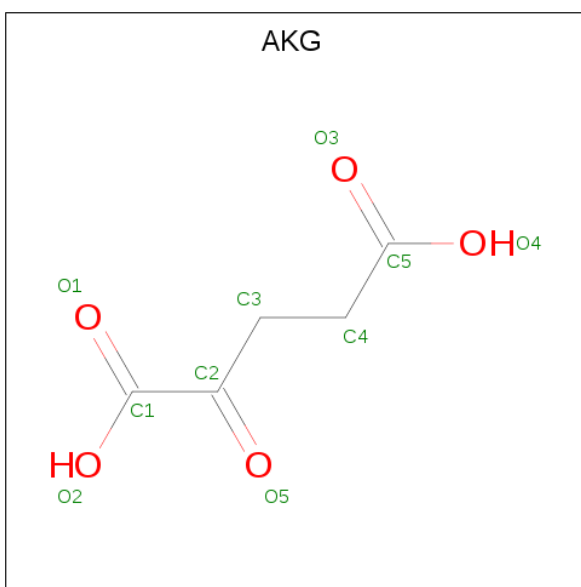
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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	SER	-	expression tag	UNP Q7RYZ9
C	334	LEU	-	expression tag	UNP Q7RYZ9
C	335	GLU	-	expression tag	UNP Q7RYZ9
C	336	HIS	-	expression tag	UNP Q7RYZ9
C	337	HIS	-	expression tag	UNP Q7RYZ9
C	338	HIS	-	expression tag	UNP Q7RYZ9
C	339	HIS	-	expression tag	UNP Q7RYZ9
C	340	HIS	-	expression tag	UNP Q7RYZ9
C	341	HIS	-	expression tag	UNP Q7RYZ9
D	-1	GLY	-	expression tag	UNP Q7RYZ9
D	0	SER	-	expression tag	UNP Q7RYZ9
D	334	LEU	-	expression tag	UNP Q7RYZ9
D	335	GLU	-	expression tag	UNP Q7RYZ9
D	336	HIS	-	expression tag	UNP Q7RYZ9
D	337	HIS	-	expression tag	UNP Q7RYZ9
D	338	HIS	-	expression tag	UNP Q7RYZ9
D	339	HIS	-	expression tag	UNP Q7RYZ9
D	340	HIS	-	expression tag	UNP Q7RYZ9
D	341	HIS	-	expression tag	UNP Q7RYZ9

- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

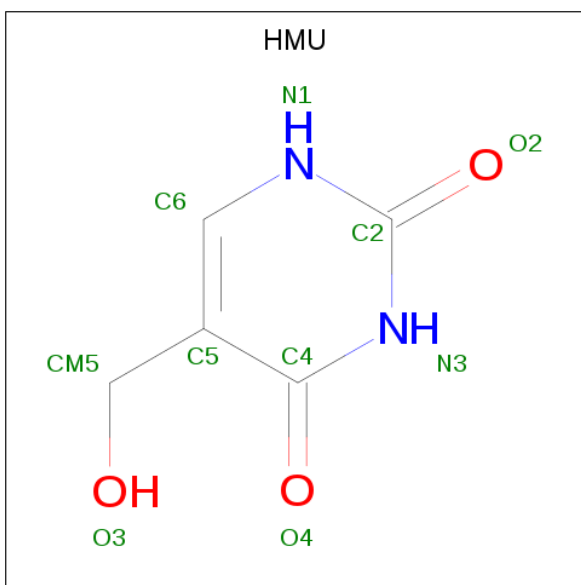
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Ni 1 1	0	0
2	A	1	Total Ni 1 1	0	0
2	D	1	Total Ni 1 1	0	0
2	C	1	Total Ni 1 1	0	0

- Molecule 3 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula: C₅H₆O₅).



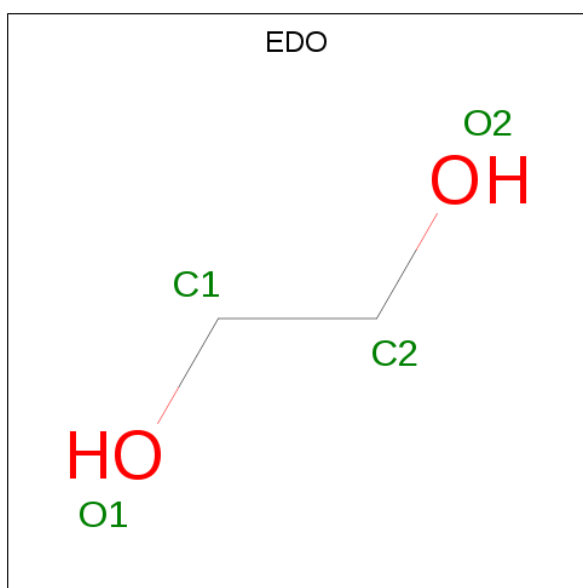
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	5	5		
3	B	1	Total	C	O	0	0
			10	5	5		
3	C	1	Total	C	O	0	0
			10	5	5		
3	D	1	Total	C	O	0	0
			10	5	5		

- Molecule 4 is 5-HYDROXYMETHYL URACIL (three-letter code: HMU) (formula: $C_5H_6N_2O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			10	5	2	3		
4	B	1	Total	C	N	O	0	0
			10	5	2	3		
4	C	1	Total	C	N	O	0	0
			10	5	2	3		
4	D	1	Total	C	N	O	0	0
			10	5	2	3		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0

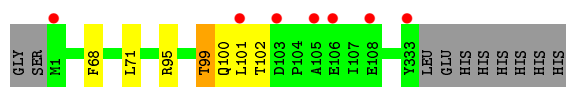
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	172	Total 172	O 172	0	0
6	B	134	Total 134	O 134	0	0
6	C	134	Total 134	O 134	0	0
6	D	117	Total 117	O 117	0	0

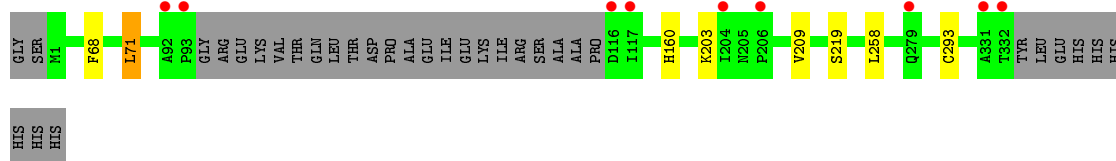
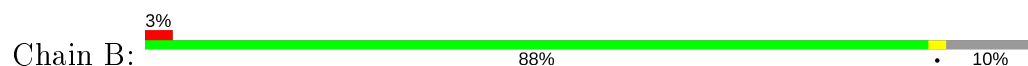
3 Residue-property plots [i](#)

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.

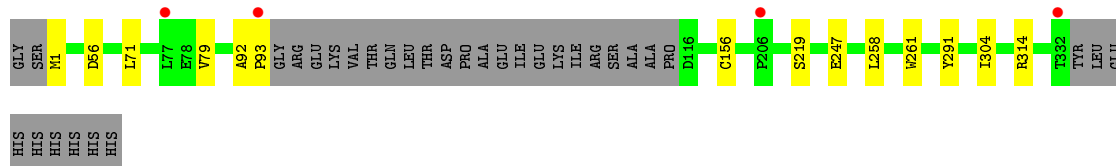
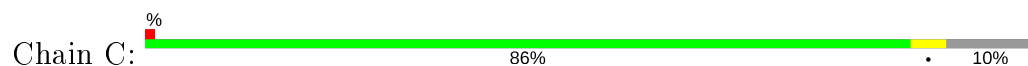
- Molecule 1: Thymine dioxygenase



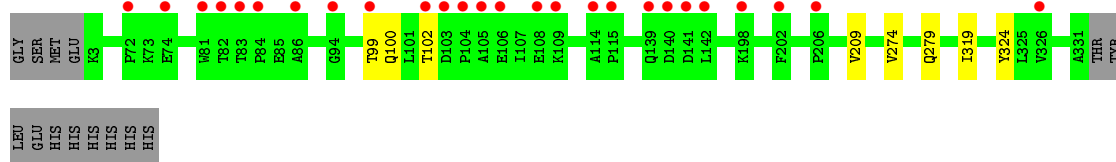
- Molecule 1: Thymine dioxygenase



- Molecule 1: Thymine dioxygenase



- Molecule 1: Thymine dioxygenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.82Å 155.78Å 75.99Å 90.00° 91.65° 90.00°	Depositor
Resolution (Å)	50.00 – 2.35 44.87 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.2 (50.00-2.35) 98.2 (44.87-2.35)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.54 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.180 , 0.225 0.185 , 0.226	Depositor DCC
R_{free} test set	2689 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	25.2	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10833	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.20% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NI, AKG, EDO, HMU

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	0.30	0/2700	0.52	0/3664
1	B	0.30	0/2516	0.50	0/3413
1	C	0.30	0/2516	0.49	0/3413
1	D	0.29	0/2663	0.49	0/3614
All	All	0.30	0/10395	0.50	0/14104

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	2634	0	2579	3	0
1	B	2454	0	2394	3	0
1	C	2454	0	2394	5	0
1	D	2598	0	2545	3	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
3	A	10	0	4	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	10	0	4	0	0
3	C	10	0	4	0	0
3	D	10	0	4	0	0
4	A	10	0	6	0	0
4	B	10	0	6	0	0
4	C	10	0	6	0	0
4	D	10	0	6	0	0
5	A	24	0	36	0	0
5	B	8	0	12	0	0
5	C	8	0	12	0	0
5	D	12	0	18	0	0
6	A	172	0	0	0	0
6	B	134	0	0	0	0
6	C	134	0	0	1	0
6	D	117	0	0	0	0
All	All	10833	0	10030	14	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 1.

All (14) 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:92:ALA:HB1	1:C:93:PRO:HD2	1.82	0.61
1:B:68:PHE:O	1:B:71:LEU:HB2	2.07	0.54
1:A:99:THR:HG22	1:A:102:THR:HG23	1.92	0.52
1:D:319:ILE:HD12	1:D:324:TYR:HB2	1.92	0.51
1:D:209:VAL:HG22	1:D:274:VAL:HG12	1.92	0.50
1:A:68:PHE:O	1:A:71:LEU:HB2	2.12	0.50
1:B:160:HIS:CE1	1:B:293:CYS:HB3	2.47	0.49
1:A:99:THR:HG23	1:A:101:LEU:H	1.78	0.49
1:C:261:TRP:CD1	1:C:304:ILE:HG13	2.50	0.46
1:C:219:SER:HA	1:C:258:LEU:HB2	2.00	0.43
1:C:156:CYS:HB3	1:C:291:TYR:CD2	2.55	0.42
1:B:219:SER:HA	1:B:258:LEU:HB2	2.02	0.41
1:C:314:ARG:HD3	6:C:580:HOH:O	2.20	0.41
1:D:99:THR:HG22	1:D:102:THR:HG23	2.03	0.41

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	331/343 (96%)	318 (96%)	13 (4%)	0	100	100
1	B	306/343 (89%)	295 (96%)	11 (4%)	0	100	100
1	C	306/343 (89%)	295 (96%)	10 (3%)	1 (0%)	41	47
1	D	327/343 (95%)	311 (95%)	16 (5%)	0	100	100
All	All	1270/1372 (93%)	1219 (96%)	50 (4%)	1 (0%)	51	63

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	79	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	283/292 (97%)	280 (99%)	3 (1%)	73	84
1	B	264/292 (90%)	261 (99%)	3 (1%)	73	84
1	C	264/292 (90%)	260 (98%)	4 (2%)	65	76
1	D	279/292 (96%)	277 (99%)	2 (1%)	84	91
All	All	1090/1168 (93%)	1078 (99%)	12 (1%)	73	84

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	ARG
1	A	99	THR
1	A	100	GLN
1	B	71	LEU
1	B	203	LYS
1	B	209	VAL
1	C	1	MET
1	C	56	ASP
1	C	71	LEU
1	C	247	GLU
1	D	100	GLN
1	D	279	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 25 ligands modelled in this entry, 4 are monoatomic - leaving 21 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	HMU	A	403	-	9,10,10	3.45	6 (66%)	9,13,13	4.64	5 (55%)
3	AKG	D	402	2	3,9,9	0.27	0	4,11,11	0.72	0
5	EDO	A	406	-	3,3,3	0.54	0	2,2,2	0.08	0
5	EDO	A	408	-	3,3,3	0.37	0	2,2,2	0.43	0
4	HMU	D	403	-	9,10,10	3.66	6 (66%)	9,13,13	4.79	5 (55%)
5	EDO	D	406	-	3,3,3	0.52	0	2,2,2	0.16	0
5	EDO	A	405	-	3,3,3	0.46	0	2,2,2	0.25	0
5	EDO	C	405	-	3,3,3	0.51	0	2,2,2	0.19	0
4	HMU	B	403	-	9,10,10	3.55	6 (66%)	9,13,13	4.77	5 (55%)
3	AKG	B	402	2	3,9,9	0.48	0	4,11,11	0.76	0
3	AKG	C	402	2	3,9,9	0.31	0	4,11,11	0.62	0
3	AKG	A	402	2	3,9,9	0.86	0	4,11,11	0.60	0
5	EDO	C	404	-	3,3,3	0.53	0	2,2,2	0.21	0
5	EDO	B	404	-	3,3,3	0.46	0	2,2,2	0.22	0
5	EDO	A	404	-	3,3,3	0.45	0	2,2,2	0.22	0
5	EDO	A	409	-	3,3,3	0.44	0	2,2,2	0.35	0
5	EDO	B	405	-	3,3,3	0.49	0	2,2,2	0.27	0
5	EDO	A	407	-	3,3,3	0.53	0	2,2,2	0.02	0
5	EDO	D	404	-	3,3,3	0.53	0	2,2,2	0.13	0
4	HMU	C	403	-	9,10,10	3.60	6 (66%)	9,13,13	4.68	5 (55%)
5	EDO	D	405	-	3,3,3	0.44	0	2,2,2	0.25	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	HMU	A	403	-	-	1/2/2/2	0/1/1/1
3	AKG	D	402	2	-	0/3/9/9	-
5	EDO	A	406	-	-	1/1/1/1	-
5	EDO	A	408	-	-	1/1/1/1	-
4	HMU	D	403	-	-	1/2/2/2	0/1/1/1
5	EDO	D	406	-	-	1/1/1/1	-
5	EDO	A	405	-	-	0/1/1/1	-
5	EDO	C	405	-	-	0/1/1/1	-
4	HMU	B	403	-	-	1/2/2/2	0/1/1/1
3	AKG	B	402	2	-	0/3/9/9	-
3	AKG	C	402	2	-	0/3/9/9	-
3	AKG	A	402	2	-	0/3/9/9	-
5	EDO	C	404	-	-	0/1/1/1	-
5	EDO	B	404	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	404	-	-	0/1/1/1	-
5	EDO	A	409	-	-	0/1/1/1	-
5	EDO	B	405	-	-	1/1/1/1	-
5	EDO	A	407	-	-	1/1/1/1	-
5	EDO	D	404	-	-	0/1/1/1	-
4	HMU	C	403	-	-	1/2/2/2	0/1/1/1
5	EDO	D	405	-	-	0/1/1/1	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	403	HMU	C4-N3	5.90	1.43	1.33
4	C	403	HMU	C4-N3	5.84	1.43	1.33
4	B	403	HMU	C4-N3	5.84	1.43	1.33
4	A	403	HMU	C4-N3	5.58	1.42	1.33
4	D	403	HMU	C2-N3	5.04	1.48	1.38
4	C	403	HMU	C2-N3	4.96	1.48	1.38
4	B	403	HMU	C2-N3	4.96	1.48	1.38
4	D	403	HMU	C2-N1	4.73	1.47	1.38
4	C	403	HMU	C2-N1	4.72	1.47	1.38
4	A	403	HMU	C2-N3	4.65	1.47	1.38
4	A	403	HMU	C2-N1	4.54	1.47	1.38
4	B	403	HMU	C2-N1	4.50	1.47	1.38
4	C	403	HMU	C6-C5	4.14	1.46	1.37
4	B	403	HMU	C6-C5	4.00	1.46	1.37
4	D	403	HMU	C6-C5	3.96	1.46	1.37
4	A	403	HMU	C6-C5	3.90	1.45	1.37
4	D	403	HMU	C6-N1	3.73	1.42	1.34
4	C	403	HMU	C6-N1	3.36	1.41	1.34
4	B	403	HMU	C6-N1	3.34	1.41	1.34
4	A	403	HMU	C6-N1	3.17	1.41	1.34
4	A	403	HMU	C4-C5	2.51	1.46	1.41
4	D	403	HMU	C4-C5	2.48	1.46	1.41
4	B	403	HMU	C4-C5	2.41	1.46	1.41
4	C	403	HMU	C4-C5	2.40	1.46	1.41

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	403	HMU	N1-C2-N3	-12.04	118.86	128.43
4	B	403	HMU	N1-C2-N3	-11.65	119.17	128.43
4	A	403	HMU	N1-C2-N3	-11.51	119.28	128.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	403	HMU	N1-C2-N3	-11.35	119.41	128.43
4	D	403	HMU	C4-N3-C2	6.01	120.22	115.14
4	C	403	HMU	C4-N3-C2	5.95	120.17	115.14
4	B	403	HMU	C4-N3-C2	5.88	120.11	115.14
4	A	403	HMU	C4-N3-C2	5.40	119.70	115.14
4	C	403	HMU	C5-C4-N3	-3.77	119.73	125.25
4	B	403	HMU	C5-C4-N3	-3.70	119.83	125.25
4	A	403	HMU	C5-C4-N3	-3.33	120.37	125.25
4	D	403	HMU	C5-C4-N3	-3.24	120.50	125.25
4	A	403	HMU	C6-N1-C2	3.13	120.52	115.36
4	B	403	HMU	C6-N1-C2	2.96	120.24	115.36
4	D	403	HMU	C6-N1-C2	2.77	119.94	115.36
4	C	403	HMU	C6-C5-C4	2.68	119.87	115.73
4	C	403	HMU	C6-N1-C2	2.68	119.78	115.36
4	B	403	HMU	C6-C5-C4	2.66	119.83	115.73
4	A	403	HMU	C6-C5-C4	2.47	119.55	115.73
4	D	403	HMU	C6-C5-C4	2.07	118.92	115.73

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	403	HMU	C6-C5-CM5-O3
4	C	403	HMU	C6-C5-CM5-O3
4	D	403	HMU	C6-C5-CM5-O3
5	D	406	EDO	O1-C1-C2-O2
5	A	406	EDO	O1-C1-C2-O2
5	B	405	EDO	O1-C1-C2-O2
4	B	403	HMU	C6-C5-CM5-O3
5	A	408	EDO	O1-C1-C2-O2
5	A	407	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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	333/343 (97%)	-0.12	7 (2%) 63 74	11, 23, 49, 66	0
1	B	310/343 (90%)	-0.08	9 (2%) 51 62	14, 28, 50, 61	0
1	C	310/343 (90%)	-0.07	4 (1%) 77 84	11, 29, 57, 78	0
1	D	329/343 (95%)	0.14	26 (7%) 12 19	13, 31, 70, 77	0
All	All	1282/1372 (93%)	-0.03	46 (3%) 42 55	11, 27, 60, 78	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	332	THR	5.9
1	D	86	ALA	5.8
1	D	206	PRO	5.1
1	B	206	PRO	4.0
1	A	101	LEU	3.9
1	D	104	PRO	3.8
1	D	72	PRO	3.7
1	D	114	ALA	3.5
1	D	106	GLU	3.4
1	A	333	TYR	3.4
1	D	84	PRO	3.3
1	D	103	ASP	3.2
1	B	93	PRO	3.2
1	A	103	ASP	3.2
1	C	206	PRO	3.1
1	A	108	GLU	3.1
1	C	332	THR	3.0
1	D	81	TRP	2.9
1	A	105	ALA	2.9
1	D	105	ALA	2.7
1	A	1	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	99	THR	2.7
1	D	115	PRO	2.7
1	B	117	ILE	2.6
1	B	204	ILE	2.6
1	D	140	ASP	2.6
1	C	93	PRO	2.6
1	D	141	ASP	2.6
1	D	109	LYS	2.5
1	B	331	ALA	2.5
1	D	83	THR	2.5
1	D	139	GLN	2.4
1	A	106	GLU	2.4
1	D	202	PHE	2.4
1	C	77	LEU	2.4
1	B	92	ALA	2.4
1	D	142	LEU	2.3
1	D	108	GLU	2.3
1	B	279	GLN	2.3
1	D	102	THR	2.2
1	D	94	GLY	2.2
1	B	116	ASP	2.2
1	D	326	VAL	2.1
1	D	74	GLU	2.1
1	D	82	THR	2.1
1	D	198	LYS	2.0

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. 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(\AA^2)	Q<0.9
5	EDO	A	406	4/4	0.56	0.31	63,63,63,63	0
4	HMU	D	403	10/10	0.70	0.32	50,54,56,57	0
5	EDO	B	405	4/4	0.70	0.29	54,56,57,60	0
5	EDO	D	406	4/4	0.73	0.23	45,47,48,49	0
5	EDO	A	407	4/4	0.78	0.29	35,36,36,36	0
5	EDO	D	405	4/4	0.81	0.44	49,50,50,51	0
5	EDO	C	405	4/4	0.82	0.18	43,44,45,47	0
5	EDO	A	408	4/4	0.86	0.26	52,53,53,54	0
5	EDO	A	405	4/4	0.89	0.24	40,41,42,43	0
5	EDO	A	409	4/4	0.90	0.23	34,34,35,36	0
4	HMU	B	403	10/10	0.92	0.16	38,38,39,39	0
5	EDO	C	404	4/4	0.94	0.19	22,22,23,23	0
4	HMU	C	403	10/10	0.94	0.18	35,37,38,39	0
5	EDO	D	404	4/4	0.94	0.21	24,24,24,25	0
5	EDO	A	404	4/4	0.96	0.16	27,28,28,29	0
3	AKG	D	402	10/10	0.96	0.13	31,32,35,35	0
5	EDO	B	404	4/4	0.98	0.12	31,31,31,31	0
3	AKG	B	402	10/10	0.98	0.11	27,28,29,30	0
3	AKG	A	402	10/10	0.98	0.11	18,19,19,20	0
4	HMU	A	403	10/10	0.98	0.13	27,27,28,28	0
2	NI	D	401	1/1	0.98	0.15	26,26,26,26	0
2	NI	A	401	1/1	0.99	0.17	18,18,18,18	0
3	AKG	C	402	10/10	0.99	0.10	22,22,23,23	0
2	NI	C	401	1/1	1.00	0.13	20,20,20,20	0
2	NI	B	401	1/1	1.00	0.13	23,23,23,23	0

6.5 Other polymers ⓘ

There are no such residues in this entry.