



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 06:30 PM BST

PDB ID : 5C3Q
Title : Crystal structure of the full-length *Neurospora crassa* T7H in complex with alpha-KG and thymine (T)
Authors : Li, W.; Zhang, T.; Ding, J.
Deposited on : 2015-06-17
Resolution : 2.05 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 : 2.13.1
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) : 2.13.1

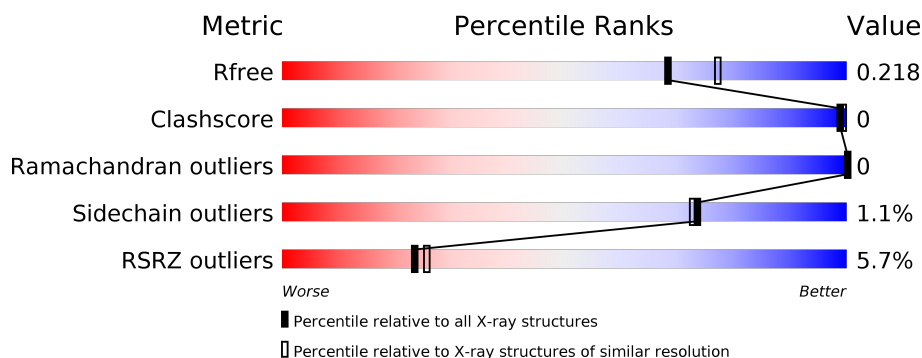
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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>3%</div> <div>96%</div> <div>• •</div> </div>
1	B	343	<div> <div>3%</div> <div>88%</div> <div>• 9%</div> </div>
1	C	343	<div> <div>4%</div> <div>90%</div> <div>• 9%</div> </div>
1	D	343	<div> <div>11%</div> <div>95%</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	TDR	A	403	-	X	-	-
4	TDR	B	403	-	X	-	-
4	TDR	C	403	-	X	-	-
4	TDR	D	403	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10920 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	335	Total	C	N	O	S	0	0	0
			2644	1684	449	505	6			
1	B	311	Total	C	N	O	S	0	0	0
			2461	1572	416	467	6			
1	C	311	Total	C	N	O	S	0	0	0
			2461	1572	416	467	6			
1	D	331	Total	C	N	O	S	0	0	0
			2617	1669	445	498	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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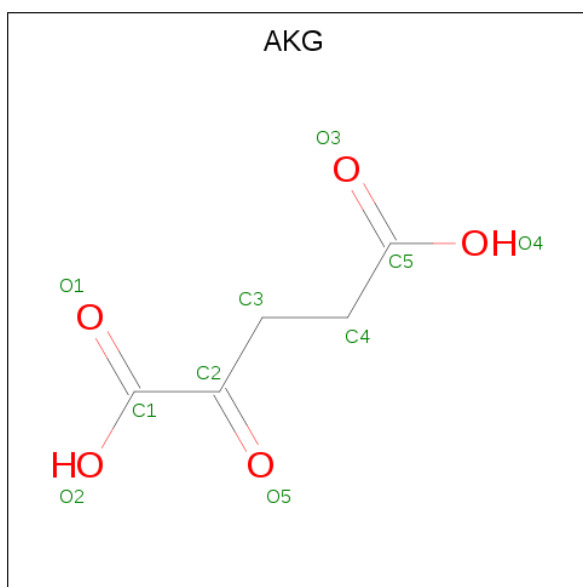
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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	SER	-	expression tag	UNP Q7RYZ9
C	334	LEU	-	expression tag	UNP Q7RYZ9
C	335	GLU	-	expression tag	UNP Q7RYZ9
C	336	HIS	-	expression tag	UNP Q7RYZ9
C	337	HIS	-	expression tag	UNP Q7RYZ9
C	338	HIS	-	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).

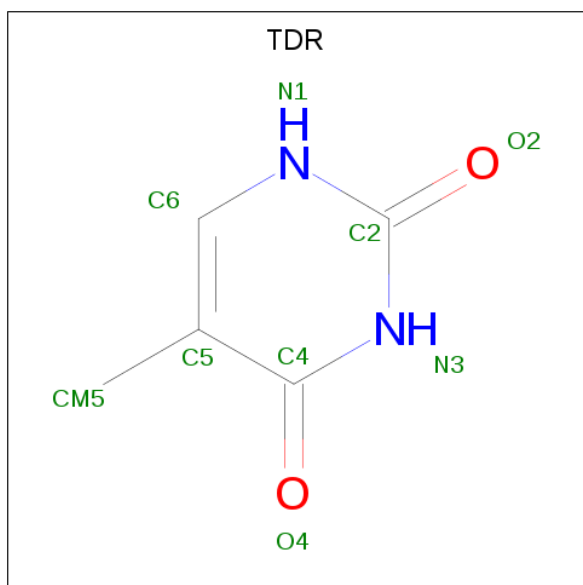
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Ni 1 1	0	0
2	A	1	Total Ni 1 1	0	0
2	D	1	Total Ni 1 1	0	0
2	C	1	Total Ni 1 1	0	0

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



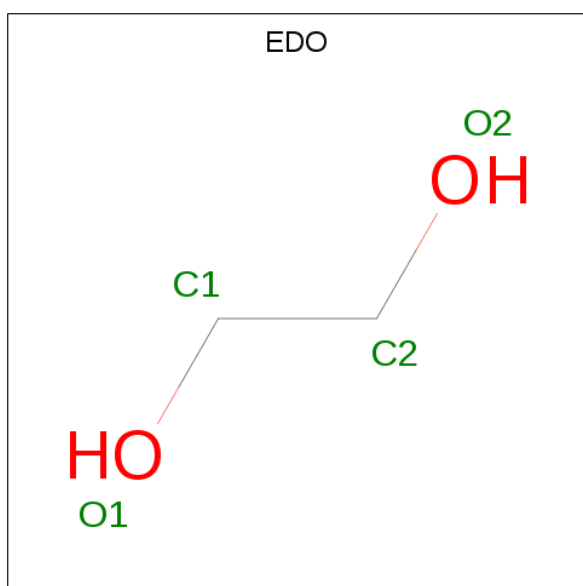
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	5	5		
3	B	1	Total	C	O	0	0
			10	5	5		
3	C	1	Total	C	O	0	0
			10	5	5		
3	D	1	Total	C	O	0	0
			10	5	5		

- Molecule 4 is THYMINE (three-letter code: TDR) (formula: $C_5H_6N_2O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 9 5 2 2	0	0
4	B	1	Total C N O 9 5 2 2	0	0
4	C	1	Total C N O 9 5 2 2	0	0
4	D	1	Total C N O 9 5 2 2	0	0

- 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 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0

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

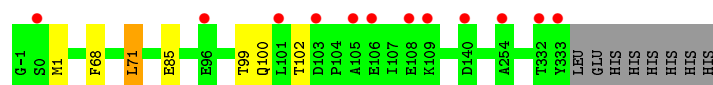
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	184	Total O 184 184	0	0
6	B	145	Total O 145 145	0	0
6	C	142	Total O 142 142	0	0
6	D	122	Total O 122 122	0	0

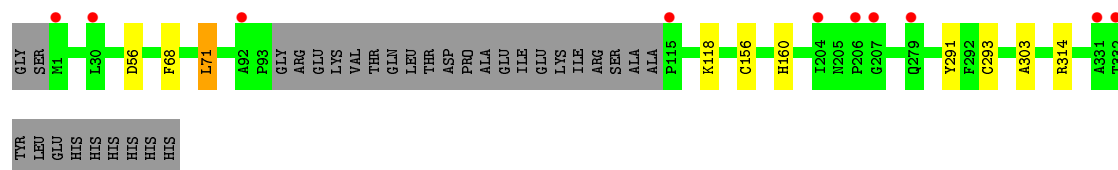
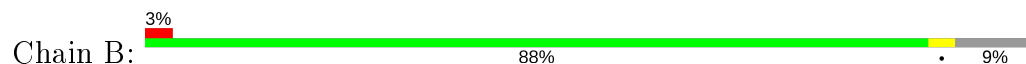
3 Residue-property plots [i](#)

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.

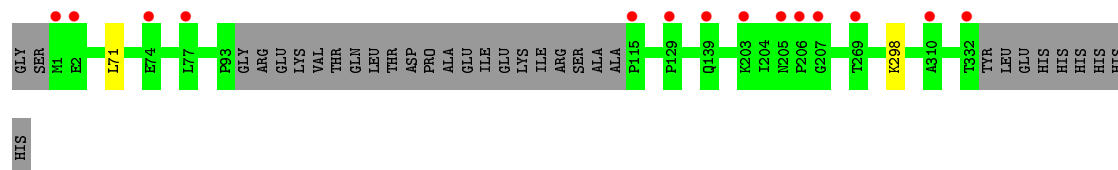
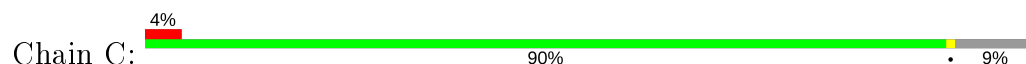
- Molecule 1: Thymine dioxygenase



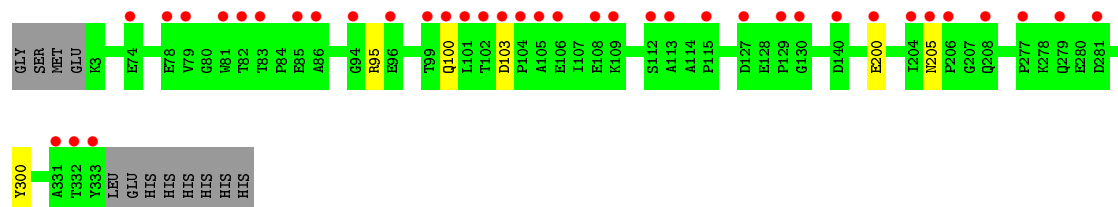
- Molecule 1: Thymine dioxygenase



- 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	56.90Å 156.32Å 76.03Å 90.00° 91.77° 90.00°	Depositor
Resolution (Å)	50.00 – 2.05 36.92 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.05) 99.8 (36.92-2.05)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.184 , 0.215 0.189 , 0.218	Depositor DCC
R_{free} test set	4130 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	28.5	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.032 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10920	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% 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, TDR

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	0.29	0/2710	0.51	0/3677
1	B	0.28	0/2524	0.49	0/3424
1	C	0.27	0/2524	0.48	0/3424
1	D	0.28	0/2683	0.48	0/3642
All	All	0.28	0/10441	0.49	0/14167

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	2644	0	2587	3	0
1	B	2461	0	2402	5	0
1	C	2461	0	2402	0	0
1	D	2617	0	2561	1	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	9	0	6	0	0
4	B	9	0	6	0	0
4	C	9	0	6	0	0
4	D	9	0	6	0	0
5	A	20	0	30	0	0
5	B	24	0	36	0	0
5	C	8	0	12	0	0
5	D	12	0	18	0	0
6	A	184	0	0	0	0
6	B	145	0	0	1	0
6	C	142	0	0	0	0
6	D	122	0	0	0	0
All	All	10920	0	10088	8	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 0.

All (8) 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:A:68:PHE:O	1:A:71:LEU:HB2	2.14	0.48
1:B:160:HIS:CE1	1:B:293:CYS:HB3	2.55	0.42
1:A:85:GLU:HG3	1:D:300:TYR:CD1	2.55	0.42
1:B:303:ALA:HB3	1:B:314:ARG:HE	1.85	0.41
1:B:68:PHE:O	1:B:71:LEU:HB2	2.19	0.41
1:B:118:LYS:NZ	6:B:504:HOH:O	2.55	0.40
1:B:156:CYS:HB3	1:B:291:TYR:CD2	2.56	0.40
1:A:99:THR:HG22	1:A:102:THR:HG23	2.03	0.40

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	333/343 (97%)	322 (97%)	11 (3%)	0	100	100
1	B	307/343 (90%)	297 (97%)	10 (3%)	0	100	100
1	C	307/343 (90%)	296 (96%)	11 (4%)	0	100	100
1	D	329/343 (96%)	313 (95%)	16 (5%)	0	100	100
All	All	1276/1372 (93%)	1228 (96%)	48 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	284/292 (97%)	281 (99%)	3 (1%)	73	73
1	B	265/292 (91%)	263 (99%)	2 (1%)	81	82
1	C	265/292 (91%)	263 (99%)	2 (1%)	81	82
1	D	281/292 (96%)	276 (98%)	5 (2%)	59	55
All	All	1095/1168 (94%)	1083 (99%)	12 (1%)	73	73

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

Mol	Chain	Res	Type
1	A	1	MET
1	A	71	LEU
1	A	100	GLN
1	B	56	ASP
1	B	71	LEU
1	C	71	LEU
1	C	298	LYS
1	D	95	ARG
1	D	100	GLN
1	D	103	ASP

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Mol	Chain	Res	Type
1	D	200	GLU
1	D	205	ASN

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

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 28 ligands modelled in this entry, 4 are monoatomic - leaving 24 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	TDR	D	403	-	8,9,9	3.91	6 (75%)	6,12,12	5.59	4 (66%)
3	AKG	A	402	2	3,9,9	0.57	0	4,11,11	0.70	0
5	EDO	A	405	-	3,3,3	0.43	0	2,2,2	0.18	0
5	EDO	B	406	-	3,3,3	0.46	0	2,2,2	0.27	0
5	EDO	D	405	-	3,3,3	0.54	0	2,2,2	0.11	0
5	EDO	D	404	-	3,3,3	0.48	0	2,2,2	0.08	0
4	TDR	B	403	-	8,9,9	3.66	6 (75%)	6,12,12	5.53	4 (66%)
5	EDO	C	404	-	3,3,3	0.55	0	2,2,2	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	B	404	-	3,3,3	0.45	0	2,2,2	0.34	0
3	AKG	B	402	2	3,9,9	0.52	0	4,11,11	0.80	0
5	EDO	B	408	-	3,3,3	0.48	0	2,2,2	0.26	0
5	EDO	B	405	-	3,3,3	0.44	0	2,2,2	0.34	0
3	AKG	D	402	2	3,9,9	0.41	0	4,11,11	0.59	0
5	EDO	A	404	-	3,3,3	0.47	0	2,2,2	0.34	0
3	AKG	C	402	2	3,9,9	0.42	0	4,11,11	0.82	0
5	EDO	B	407	-	3,3,3	0.50	0	2,2,2	0.12	0
4	TDR	A	403	-	8,9,9	3.65	6 (75%)	6,12,12	5.68	4 (66%)
5	EDO	B	409	-	3,3,3	0.49	0	2,2,2	0.23	0
5	EDO	D	406	-	3,3,3	0.51	0	2,2,2	0.07	0
5	EDO	A	406	-	3,3,3	0.48	0	2,2,2	0.24	0
5	EDO	A	407	-	3,3,3	0.48	0	2,2,2	0.35	0
4	TDR	C	403	-	8,9,9	3.75	6 (75%)	6,12,12	5.55	4 (66%)
5	EDO	A	408	-	3,3,3	0.39	0	2,2,2	0.41	0
5	EDO	C	405	-	3,3,3	0.50	0	2,2,2	0.10	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	TDR	D	403	-	-	-	0/1/1/1
3	AKG	A	402	2	-	0/3/9/9	-
5	EDO	A	405	-	-	1/1/1/1	-
5	EDO	B	406	-	-	1/1/1/1	-
5	EDO	D	405	-	-	0/1/1/1	-
5	EDO	D	404	-	-	1/1/1/1	-
4	TDR	B	403	-	-	-	0/1/1/1
5	EDO	C	404	-	-	0/1/1/1	-
5	EDO	B	404	-	-	0/1/1/1	-
3	AKG	B	402	2	-	0/3/9/9	-
5	EDO	B	408	-	-	0/1/1/1	-
5	EDO	B	405	-	-	0/1/1/1	-
3	AKG	D	402	2	-	0/3/9/9	-
5	EDO	A	404	-	-	0/1/1/1	-
3	AKG	C	402	2	-	0/3/9/9	-
5	EDO	B	407	-	-	1/1/1/1	-
4	TDR	A	403	-	-	-	0/1/1/1
5	EDO	B	409	-	-	1/1/1/1	-
5	EDO	D	406	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	406	-	-	1/1/1/1	-
5	EDO	A	407	-	-	1/1/1/1	-
4	TDR	C	403	-	-	-	0/1/1/1
5	EDO	A	408	-	-	0/1/1/1	-
5	EDO	C	405	-	-	1/1/1/1	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	403	TDR	C4-N3	6.27	1.44	1.33
4	C	403	TDR	C4-N3	6.16	1.43	1.33
4	B	403	TDR	C4-N3	5.95	1.43	1.33
4	A	403	TDR	C4-N3	5.83	1.43	1.33
4	D	403	TDR	C6-C5	4.96	1.47	1.39
4	C	403	TDR	C6-C5	4.78	1.47	1.39
4	A	403	TDR	C6-C5	4.78	1.47	1.39
4	B	403	TDR	C6-C5	4.55	1.46	1.39
4	D	403	TDR	C6-N1	4.32	1.43	1.34
4	A	403	TDR	C6-N1	4.11	1.43	1.34
4	C	403	TDR	C6-N1	4.10	1.43	1.34
4	B	403	TDR	C6-N1	4.00	1.42	1.34
4	D	403	TDR	C2-N3	3.87	1.45	1.38
4	D	403	TDR	C2-N1	3.77	1.45	1.38
4	B	403	TDR	C2-N3	3.71	1.45	1.38
4	C	403	TDR	C2-N3	3.60	1.45	1.38
4	C	403	TDR	C2-N1	3.44	1.45	1.38
4	A	403	TDR	C2-N1	3.43	1.45	1.38
4	A	403	TDR	C2-N3	3.40	1.44	1.38
4	B	403	TDR	C2-N1	3.34	1.44	1.38
4	D	403	TDR	C4-C5	3.10	1.48	1.41
4	B	403	TDR	C4-C5	3.02	1.47	1.41
4	C	403	TDR	C4-C5	2.91	1.47	1.41
4	A	403	TDR	C4-C5	2.87	1.47	1.41

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	403	TDR	N1-C2-N3	-10.82	119.83	128.43
4	A	403	TDR	N1-C2-N3	-10.73	119.90	128.43
4	C	403	TDR	N1-C2-N3	-10.57	120.03	128.43
4	B	403	TDR	N1-C2-N3	-10.53	120.06	128.43
4	A	403	TDR	C4-N3-C2	6.46	120.60	115.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	403	TDR	C4-N3-C2	6.27	120.44	115.14
4	D	403	TDR	C4-N3-C2	6.22	120.40	115.14
4	B	403	TDR	C4-N3-C2	6.19	120.36	115.14
4	A	403	TDR	C5-C6-N1	-5.03	120.04	125.16
4	B	403	TDR	C5-C6-N1	-4.77	120.30	125.16
4	C	403	TDR	C5-C6-N1	-4.73	120.35	125.16
4	D	403	TDR	C5-C6-N1	-4.60	120.48	125.16
4	A	403	TDR	C6-N1-C2	3.20	120.65	115.36
4	B	403	TDR	C6-N1-C2	3.13	120.52	115.36
4	D	403	TDR	C6-N1-C2	3.12	120.51	115.36
4	C	403	TDR	C6-N1-C2	3.10	120.48	115.36

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	409	EDO	O1-C1-C2-O2
5	D	406	EDO	O1-C1-C2-O2
5	A	407	EDO	O1-C1-C2-O2
5	A	406	EDO	O1-C1-C2-O2
5	A	405	EDO	O1-C1-C2-O2
5	B	407	EDO	O1-C1-C2-O2
5	C	405	EDO	O1-C1-C2-O2
5	D	404	EDO	O1-C1-C2-O2
5	B	406	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	335/343 (97%)	-0.00	12 (3%) 42 46	18, 28, 54, 70	0
1	B	311/343 (90%)	0.08	10 (3%) 47 52	20, 32, 50, 66	0
1	C	311/343 (90%)	0.14	14 (4%) 33 35	18, 35, 59, 76	0
1	D	331/343 (96%)	0.46	38 (11%) 4 4	20, 37, 77, 89	0
All	All	1288/1372 (93%)	0.17	74 (5%) 23 25	18, 32, 62, 89	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	204	ILE	9.0
1	D	333	TYR	6.8
1	A	101	LEU	6.1
1	D	106	GLU	5.6
1	D	332	THR	5.3
1	D	104	PRO	5.2
1	C	115	PRO	4.6
1	B	206	PRO	4.4
1	D	105	ALA	4.3
1	D	205	ASN	4.2
1	D	129	PRO	4.1
1	B	279	GLN	4.0
1	B	115	PRO	4.0
1	D	81	TRP	3.8
1	D	86	ALA	3.8
1	D	130	GLY	3.7
1	D	96	GLU	3.5
1	D	115	PRO	3.5
1	D	94	GLY	3.5
1	D	279	GLN	3.4
1	A	106	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	1	MET	3.4
1	A	0	SER	3.4
1	D	83	THR	3.3
1	C	205	ASN	3.2
1	A	103	ASP	3.2
1	A	333	TYR	3.2
1	A	105	ALA	3.2
1	D	99	THR	3.1
1	C	206	PRO	3.0
1	A	96	GLU	3.0
1	D	113	ALA	3.0
1	B	204	ILE	2.9
1	D	277	PRO	2.9
1	B	332	THR	2.9
1	D	281	ASP	2.9
1	D	140	ASP	2.9
1	D	103	ASP	2.8
1	D	200	GLU	2.8
1	C	1	MET	2.8
1	D	85	GLU	2.8
1	D	101	LEU	2.8
1	C	129	PRO	2.7
1	D	100	GLN	2.7
1	A	108	GLU	2.6
1	D	108	GLU	2.6
1	D	74	GLU	2.6
1	C	207	GLY	2.6
1	C	332	THR	2.5
1	A	332	THR	2.5
1	D	78	GLU	2.5
1	B	92	ALA	2.5
1	D	127	ASP	2.4
1	C	77	LEU	2.4
1	D	112	SER	2.4
1	C	2	GLU	2.3
1	D	331	ALA	2.3
1	B	207	GLY	2.3
1	D	82	THR	2.3
1	A	109	LYS	2.2
1	D	102	THR	2.2
1	D	109	LYS	2.2
1	A	254	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	74	GLU	2.1
1	A	140	ASP	2.1
1	B	331	ALA	2.1
1	C	139	GLN	2.1
1	C	269	THR	2.1
1	C	310	ALA	2.1
1	C	203	LYS	2.1
1	B	30	LEU	2.0
1	D	79	VAL	2.0
1	D	206	PRO	2.0
1	D	208	GLN	2.0

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 monosaccharides 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(Å ²)	Q<0.9
5	EDO	D	404	4/4	0.66	0.19	51,53,55,56	0
5	EDO	B	405	4/4	0.77	0.28	54,55,55,56	0
4	TDR	D	403	9/9	0.80	0.20	55,57,57,57	0
5	EDO	B	408	4/4	0.82	0.20	65,65,66,66	0
5	EDO	A	407	4/4	0.84	0.19	41,42,43,47	0
5	EDO	D	406	4/4	0.85	0.24	50,51,51,51	0
5	EDO	A	406	4/4	0.85	0.20	61,61,61,62	0
5	EDO	B	407	4/4	0.85	0.24	51,52,52,53	0
5	EDO	A	408	4/4	0.85	0.27	58,58,59,59	0
5	EDO	A	404	4/4	0.90	0.25	35,36,36,37	0
5	EDO	C	405	4/4	0.90	0.14	39,40,40,41	0
5	EDO	B	406	4/4	0.91	0.23	57,57,57,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	EDO	B	409	4/4	0.92	0.27	52,52,53,53	0
5	EDO	B	404	4/4	0.92	0.28	40,41,41,41	0
3	AKG	D	402	10/10	0.92	0.16	34,35,36,37	0
5	EDO	A	405	4/4	0.93	0.12	40,41,42,43	0
5	EDO	C	404	4/4	0.93	0.27	30,31,32,32	0
5	EDO	D	405	4/4	0.94	0.21	32,33,34,34	0
4	TDR	C	403	9/9	0.94	0.14	33,34,35,36	0
4	TDR	A	403	9/9	0.95	0.15	25,26,26,26	0
3	AKG	B	402	10/10	0.95	0.09	28,29,30,30	0
4	TDR	B	403	9/9	0.96	0.14	30,30,31,31	0
3	AKG	C	402	10/10	0.97	0.16	27,28,28,28	0
3	AKG	A	402	10/10	0.97	0.11	24,26,26,26	0
2	NI	C	401	1/1	0.98	0.16	26,26,26,26	0
2	NI	D	401	1/1	0.99	0.16	32,32,32,32	0
2	NI	B	401	1/1	0.99	0.16	27,27,27,27	0
2	NI	A	401	1/1	1.00	0.16	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.