



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2023 – 11:07 AM JST

PDB ID : 5C3P  
Title : Crystal structure of the full-length *Neurospora crassa* T7H in complex with alpha-KG  
Authors : Li, W.; Zhang, T.; Ding, J.  
Deposited on : 2015-06-17  
Resolution : 2.10 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](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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.36  
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) : 2.36

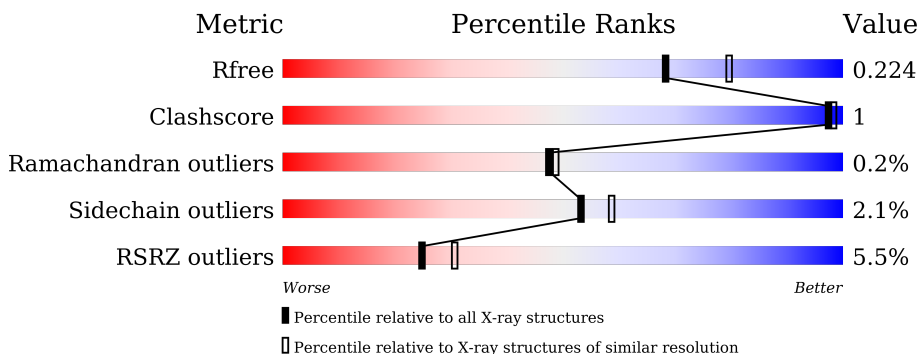
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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  $\geq 3$ , 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	343	
1	B	343	
1	C	343	
1	D	343	

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 10737 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
			Total	C	N	O	S			
1	A	329	Total 2604	C 1661	N 440	O 497	S 6	0	0	0
1	B	325	Total 2568	C 1637	N 438	O 487	S 6	0	0	0
1	C	325	Total 2566	C 1634	N 438	O 488	S 6	0	0	0
1	D	303	Total 2400	C 1535	N 410	O 449	S 6	0	1	0

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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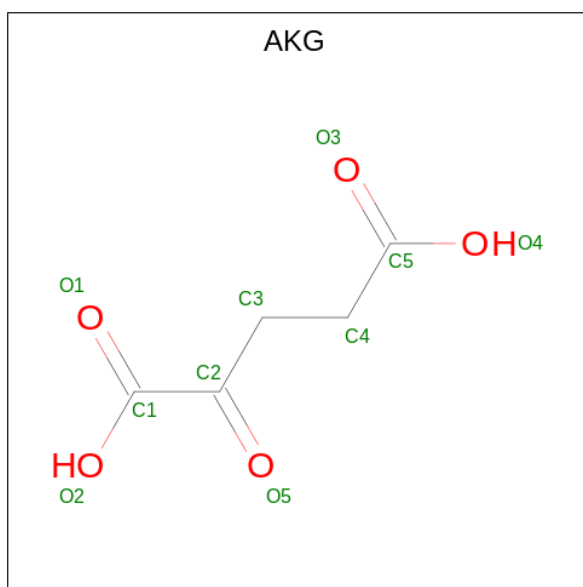
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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	SER	-	expression tag	UNP Q7RYZ9
C	334	LEU	-	expression tag	UNP Q7RYZ9
C	335	GLU	-	expression tag	UNP Q7RYZ9
C	336	HIS	-	expression tag	UNP Q7RYZ9
C	337	HIS	-	expression tag	UNP Q7RYZ9
C	338	HIS	-	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).

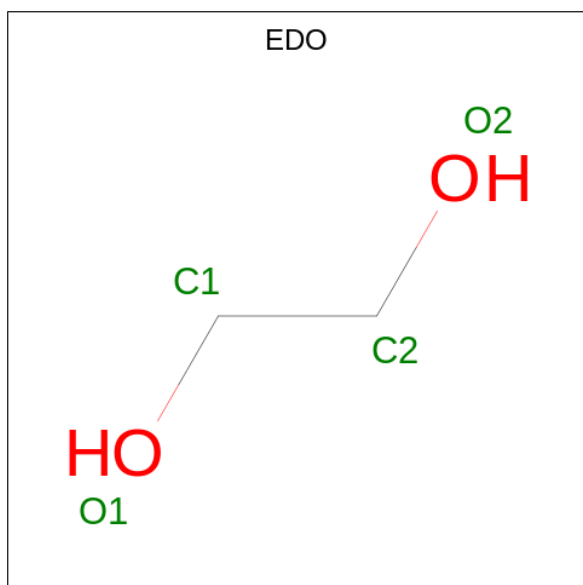
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ni 1 1	0	0
2	B	1	Total Ni 1 1	0	0
2	C	1	Total Ni 1 1	0	0
2	D	1	Total Ni 1 1	0	0

- Molecule 3 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula: C<sub>5</sub>H<sub>6</sub>O<sub>5</sub>).



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 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

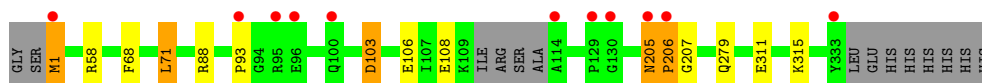
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	155	Total O 155 155	0	0
5	B	119	Total O 119 119	0	0
5	C	133	Total O 133 133	0	0
5	D	88	Total O 88 88	0	0

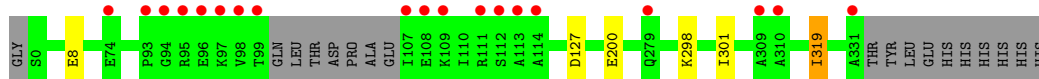
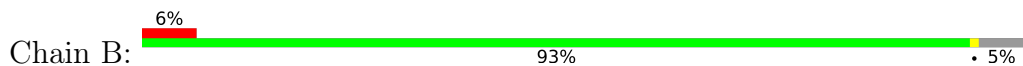
### 3 Residue-property plots [i](#)

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



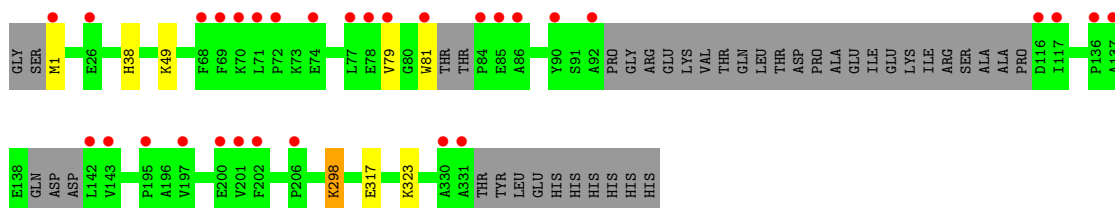
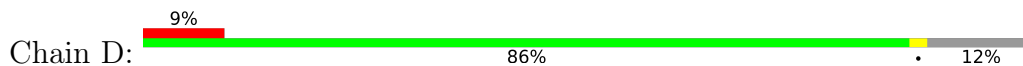
- Molecule 1: Thymine dioxygenase



- Molecule 1: Thymine dioxygenase



- Molecule 1: Thymine dioxygenase



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.19Å 154.73Å 75.43Å 90.00° 90.60° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 45.80 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.00-2.10) 99.0 (45.80-2.10)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.25 (at 2.10Å)	Xtrriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.185 , 0.222 0.189 , 0.224	Depositor DCC
$R_{free}$ test set	3731 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.6	Xtrriage
Anisotropy	0.341	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 52.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.047 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10737	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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: NI, EDO, AKG

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	0.38	0/2669	0.56	0/3621
1	B	0.33	0/2631	0.53	0/3566
1	C	0.35	0/2627	0.54	0/3559
1	D	0.32	0/2462	0.51	0/3332
All	All	0.35	0/10389	0.53	0/14078

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	2604	0	2544	7	0
1	B	2568	0	2519	2	0
1	C	2566	0	2520	1	0
1	D	2400	0	2342	6	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	24	0	36	1	0
4	B	8	0	12	0	0
4	C	12	0	18	0	0
4	D	16	0	24	2	0
5	A	155	0	0	1	0
5	B	119	0	0	0	0
5	C	133	0	0	0	0
5	D	88	0	0	1	0
All	All	10737	0	10031	16	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 (16) 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:D:38:HIS:ND1	5:D:501:HOH:O	2.26	0.68
1:D:317:GLU:H	4:D:406:EDO:H12	1.65	0.62
1:A:206:PRO:HG2	1:A:207:GLY:H	1.68	0.57
1:A:206:PRO:CG	1:A:207:GLY:H	2.18	0.56
1:A:103:ASP:OD1	1:A:106:GLU:HG3	2.08	0.53
1:D:317:GLU:H	4:D:406:EDO:C1	2.22	0.53
1:A:205:ASN:N	1:A:205:ASN:OD1	2.44	0.51
1:D:298:LYS:CE	1:D:298:LYS:H	2.24	0.50
1:D:298:LYS:H	1:D:298:LYS:HE2	1.78	0.48
1:B:127:ASP:OD1	1:B:127:ASP:N	2.48	0.46
1:B:301:ILE:HB	1:B:319:ILE:HD12	1.98	0.45
1:A:58:ARG:HD2	4:A:408:EDO:H21	1.99	0.43
1:A:1:MET:HE3	5:A:560:HOH:O	2.18	0.43
1:D:298:LYS:HE2	1:D:298:LYS:N	2.35	0.41
1:C:68:PHE:O	1:C:71:LEU:HB2	2.21	0.41
1:A:68:PHE:O	1:A:71:LEU:HB2	2.21	0.41

There are no symmetry-related clashes.

## 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	325/343 (95%)	311 (96%)	13 (4%)	1 (0%)	41	41
1	B	321/343 (94%)	309 (96%)	12 (4%)	0	100	100
1	C	321/343 (94%)	305 (95%)	15 (5%)	1 (0%)	41	41
1	D	296/343 (86%)	285 (96%)	10 (3%)	1 (0%)	41	41
All	All	1263/1372 (92%)	1210 (96%)	50 (4%)	3 (0%)	47	49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	141	ASP
1	A	206	PRO
1	D	79	VAL

### 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	280/292 (96%)	270 (96%)	10 (4%)	35	36
1	B	276/292 (94%)	272 (99%)	4 (1%)	67	73
1	C	276/292 (94%)	272 (99%)	4 (1%)	67	73
1	D	255/292 (87%)	250 (98%)	5 (2%)	55	60
All	All	1087/1168 (93%)	1064 (98%)	23 (2%)	53	59

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	71	LEU
1	A	88	ARG
1	A	93	PRO
1	A	103	ASP
1	A	108	GLU
1	A	205	ASN
1	A	279	GLN
1	A	311	GLU
1	A	315	LYS
1	B	8	GLU
1	B	200	GLU
1	B	298	LYS
1	B	319	ILE
1	C	74	GLU
1	C	103	ASP
1	C	281	ASP
1	C	329	LEU
1	D	1	MET
1	D	49	LYS
1	D	81	TRP
1	D	298	LYS
1	D	323	LYS

Sometimes 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 monosaccharides in this entry.

## 5.6 Ligand geometry

Of 23 ligands modelled in this entry, 4 are monoatomic - leaving 19 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	EDO	D	403	-	3,3,3	0.48	0	2,2,2	0.17	0
4	EDO	D	404	-	3,3,3	0.44	0	2,2,2	0.35	0
4	EDO	D	406	-	3,3,3	0.54	0	2,2,2	0.13	0
4	EDO	B	404	-	3,3,3	0.59	0	2,2,2	0.12	0
4	EDO	C	403	-	3,3,3	0.41	0	2,2,2	0.27	0
4	EDO	A	407	-	3,3,3	0.46	0	2,2,2	0.24	0
3	AKG	D	402	2	9,9,9	1.84	1 (11%)	11,11,11	1.35	1 (9%)
4	EDO	A	405	-	3,3,3	0.49	0	2,2,2	0.27	0
3	AKG	A	402	2	9,9,9	1.72	1 (11%)	11,11,11	1.50	3 (27%)
4	EDO	A	408	-	3,3,3	0.37	0	2,2,2	0.36	0
4	EDO	D	405	-	3,3,3	0.57	0	2,2,2	0.06	0
4	EDO	A	403	-	3,3,3	0.51	0	2,2,2	0.14	0
3	AKG	B	402	2	9,9,9	1.75	1 (11%)	11,11,11	1.35	2 (18%)
4	EDO	C	404	-	3,3,3	0.49	0	2,2,2	0.14	0
4	EDO	B	403	-	3,3,3	0.46	0	2,2,2	0.29	0
4	EDO	A	406	-	3,3,3	0.44	0	2,2,2	0.29	0
4	EDO	C	405	-	3,3,3	0.45	0	2,2,2	0.19	0
3	AKG	C	402	2	9,9,9	1.66	1 (11%)	11,11,11	1.28	1 (9%)
4	EDO	A	404	-	3,3,3	0.74	0	2,2,2	0.58	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	D	403	-	-	0/1/1/1	-
4	EDO	D	404	-	-	1/1/1/1	-
4	EDO	D	406	-	-	1/1/1/1	-
4	EDO	B	404	-	-	0/1/1/1	-
4	EDO	C	403	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	407	-	-	0/1/1/1	-
3	AKG	D	402	2	-	0/9/9/9	-
4	EDO	A	405	-	-	0/1/1/1	-
3	AKG	A	402	2	-	1/9/9/9	-
4	EDO	A	408	-	-	0/1/1/1	-
4	EDO	D	405	-	-	0/1/1/1	-
4	EDO	A	403	-	-	1/1/1/1	-
3	AKG	B	402	2	-	0/9/9/9	-
4	EDO	C	404	-	-	1/1/1/1	-
4	EDO	B	403	-	-	1/1/1/1	-
4	EDO	A	406	-	-	0/1/1/1	-
4	EDO	C	405	-	-	1/1/1/1	-
3	AKG	C	402	2	-	0/9/9/9	-
4	EDO	A	404	-	-	1/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	402	AKG	C2-C1	-4.63	1.47	1.53
3	A	402	AKG	C2-C1	-4.33	1.47	1.53
3	B	402	AKG	C2-C1	-4.22	1.47	1.53
3	C	402	AKG	C2-C1	-4.05	1.48	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	AKG	O1-C1-C2	-2.51	118.36	121.72
3	C	402	AKG	O2-C1-C2	2.49	120.79	113.97
3	B	402	AKG	O2-C1-C2	2.46	120.70	113.97
3	B	402	AKG	O1-C1-C2	-2.39	118.53	121.72
3	A	402	AKG	O2-C1-C2	2.36	120.43	113.97
3	D	402	AKG	O4-C5-C4	2.14	120.89	114.03
3	A	402	AKG	O4-C5-C4	2.01	120.47	114.03

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	403	EDO	O1-C1-C2-O2
4	C	404	EDO	O1-C1-C2-O2
4	C	405	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	D	406	EDO	O1-C1-C2-O2
4	A	404	EDO	O1-C1-C2-O2
4	D	404	EDO	O1-C1-C2-O2
4	A	403	EDO	O1-C1-C2-O2
3	A	402	AKG	C3-C4-C5-O4

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	406	EDO	2	0
4	A	408	EDO	1	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

### 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, 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	329/343 (95%)	-0.06	11 (3%) 46 53	26, 37, 70, 98	0
1	B	325/343 (94%)	0.11	19 (5%) 23 28	30, 44, 76, 100	0
1	C	325/343 (94%)	0.01	10 (3%) 49 55	27, 41, 69, 82	0
1	D	303/343 (88%)	0.36	31 (10%) 6 8	30, 50, 81, 107	0
All	All	1282/1372 (93%)	0.10	71 (5%) 25 31	26, 43, 76, 107	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	95	ARG	6.1
1	B	108	GLU	6.0
1	B	107	ILE	5.9
1	D	86	ALA	5.8
1	D	331	ALA	5.8
1	B	95	ARG	5.1
1	D	71	LEU	4.8
1	B	113	ALA	4.8
1	B	309	ALA	4.7
1	B	99	THR	4.6
1	D	206	PRO	4.5
1	C	206	PRO	4.3
1	D	116	ASP	4.3
1	D	70	LYS	4.3
1	B	112	SER	4.2
1	D	74	GLU	4.2
1	D	137	ALA	4.1
1	D	117	ILE	3.9
1	D	85	GLU	3.9
1	D	197	VAL	3.7
1	D	69	PHE	3.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	96	GLU	3.4
1	A	114	ALA	3.3
1	D	195	PRO	3.3
1	D	330	ALA	3.3
1	B	114	ALA	3.0
1	B	98	VAL	3.0
1	A	96	GLU	3.0
1	B	97	LYS	3.0
1	D	84	PRO	3.0
1	B	310	ALA	3.0
1	D	1	MET	2.9
1	D	77	LEU	2.9
1	D	78	GLU	2.9
1	C	77	LEU	2.9
1	A	100	GLN	2.9
1	B	109	LYS	2.8
1	D	136	PRO	2.8
1	B	93	PRO	2.8
1	A	130	GLY	2.8
1	D	143	VAL	2.7
1	A	333	TYR	2.7
1	B	94	GLY	2.7
1	C	141	ASP	2.7
1	C	96	GLU	2.7
1	D	90	TYR	2.6
1	B	111	ARG	2.6
1	D	92	ALA	2.6
1	A	129	PRO	2.6
1	A	93	PRO	2.6
1	D	142	LEU	2.5
1	D	68	PHE	2.5
1	A	1	MET	2.5
1	C	282	VAL	2.4
1	D	200	GLU	2.4
1	A	206	PRO	2.4
1	A	205	ASN	2.4
1	D	81	TRP	2.3
1	D	202	PHE	2.3
1	C	87	ASN	2.3
1	C	140	ASP	2.2
1	C	116	ASP	2.2
1	D	201	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	113	ALA	2.2
1	B	74	GLU	2.1
1	D	72	PRO	2.1
1	B	279	GLN	2.1
1	D	26	GLU	2.1
1	C	74	GLU	2.0
1	B	331	ALA	2.0
1	D	79	VAL	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, 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	EDO	A	406	4/4	0.71	0.15	82,86,86,87	0
4	EDO	A	403	4/4	0.73	0.22	66,71,71,72	0
4	EDO	D	406	4/4	0.75	0.18	63,65,66,68	0
4	EDO	A	408	4/4	0.79	0.36	70,71,72,75	0
4	EDO	D	403	4/4	0.81	0.26	62,69,71,75	0
4	EDO	A	405	4/4	0.87	0.18	59,63,64,65	0
4	EDO	C	405	4/4	0.88	0.17	58,63,65,71	0
4	EDO	A	404	4/4	0.88	0.24	44,45,46,46	0
4	EDO	C	404	4/4	0.88	0.26	59,61,63,67	0
4	EDO	B	403	4/4	0.91	0.30	76,77,78,80	0
4	EDO	B	404	4/4	0.91	0.19	45,49,49,49	0
4	EDO	A	407	4/4	0.91	0.17	64,66,67,68	0
4	EDO	D	404	4/4	0.93	0.12	67,68,68,69	0
3	AKG	B	402	10/10	0.94	0.14	41,48,51,52	0
4	EDO	D	405	4/4	0.95	0.17	44,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	AKG	D	402	10/10	0.95	0.15	55,59,61,61	0
3	AKG	A	402	10/10	0.96	0.15	39,42,43,44	0
3	AKG	C	402	10/10	0.97	0.12	44,46,48,48	0
4	EDO	C	403	4/4	0.98	0.18	46,50,52,54	0
2	NI	D	401	1/1	0.99	0.19	47,47,47,47	0
2	NI	C	401	1/1	0.99	0.20	42,42,42,42	0
2	NI	B	401	1/1	1.00	0.21	43,43,43,43	0
2	NI	A	401	1/1	1.00	0.21	39,39,39,39	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.