



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:15 PM GMT

PDB ID : 1O68
Title : Crystal structure of 3-methyl-2-oxobutanoate hydroxymethyltransferase
Authors : Structural GenomiX
Deposited on : 2003-10-23
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
A user guide is available at
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

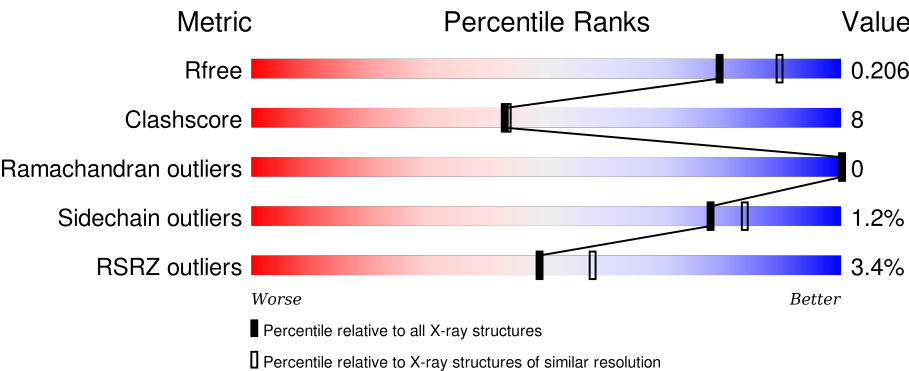
1 Overall quality at a glance ⓘ

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}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	275	<div> <div>80%</div> <div>11%</div> <div>9%</div> </div>
1	B	275	<div> <div>4%</div> <div>77%</div> <div>18%</div> <div>• 5%</div> </div>
1	C	275	<div> <div>73%</div> <div>16%</div> <div>• 11%</div> </div>
1	D	275	<div> <div>5%</div> <div>82%</div> <div>13%</div> <div>5%</div> </div>
1	E	275	<div> <div>4%</div> <div>73%</div> <div>17%</div> <div>9%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NA	B	274	-	-	-	X
2	NA	E	274	-	-	-	X
3	KIV	A	275	-	-	-	X
3	KIV	D	275	-	-	-	X
3	KIV	E	275	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9852 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 3-methyl-2-oxobutanoate hydroxymethyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	Se	0	2	0
			1813	1144	304	342	6	17			
1	B	262	Total	C	N	O	S	Se	0	2	0
			1896	1201	317	356	6	16			
1	C	246	Total	C	N	O	S	Se	0	6	0
			1807	1142	299	343	6	17			
1	D	262	Total	C	N	O	S	Se	0	3	0
			1909	1206	323	358	6	16			
1	E	249	Total	C	N	O	S	Se	0	1	0
			1808	1143	304	339	6	16			

There are 140 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MSE	-	cloning artifact	UNP Q9JZW6
A	0	SER	-	cloning artifact	UNP Q9JZW6
A	1	LEU	-	cloning artifact	UNP Q9JZW6
A	10	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
A	19	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
A	31	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
A	38	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
A	47	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
A	63	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
A	78	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
A	103	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
A	109	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
A	118	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
A	127	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
A	178	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
A	213	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
A	216	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
A	232	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
A	264	GLU	-	cloning artifact	UNP Q9JZW6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	265	GLY	-	cloning artifact	UNP Q9JZW6
A	266	GLY	-	cloning artifact	UNP Q9JZW6
A	267	SER	-	cloning artifact	UNP Q9JZW6
A	268	HIS	-	cloning artifact	UNP Q9JZW6
A	269	HIS	-	cloning artifact	UNP Q9JZW6
A	270	HIS	-	cloning artifact	UNP Q9JZW6
A	271	HIS	-	cloning artifact	UNP Q9JZW6
A	272	HIS	-	cloning artifact	UNP Q9JZW6
A	273	HIS	-	cloning artifact	UNP Q9JZW6
B	-1	MSE	-	cloning artifact	UNP Q9JZW6
B	0	SER	-	cloning artifact	UNP Q9JZW6
B	1	LEU	-	cloning artifact	UNP Q9JZW6
B	10	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
B	19	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
B	31	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
B	38	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
B	47	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
B	63	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
B	78	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
B	103	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
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B	232	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
B	264	GLU	-	cloning artifact	UNP Q9JZW6
B	265	GLY	-	cloning artifact	UNP Q9JZW6
B	266	GLY	-	cloning artifact	UNP Q9JZW6
B	267	SER	-	cloning artifact	UNP Q9JZW6
B	268	HIS	-	cloning artifact	UNP Q9JZW6
B	269	HIS	-	cloning artifact	UNP Q9JZW6
B	270	HIS	-	cloning artifact	UNP Q9JZW6
B	271	HIS	-	cloning artifact	UNP Q9JZW6
B	272	HIS	-	cloning artifact	UNP Q9JZW6
B	273	HIS	-	cloning artifact	UNP Q9JZW6
C	-1	MSE	-	cloning artifact	UNP Q9JZW6
C	0	SER	-	cloning artifact	UNP Q9JZW6
C	1	LEU	-	cloning artifact	UNP Q9JZW6
C	10	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
C	19	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	31	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
C	38	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
C	47	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
C	63	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
C	78	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
C	103	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
C	109	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
C	118	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
C	127	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
C	178	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
C	213	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
C	216	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
C	232	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
C	264	GLU	-	cloning artifact	UNP Q9JZW6
C	265	GLY	-	cloning artifact	UNP Q9JZW6
C	266	GLY	-	cloning artifact	UNP Q9JZW6
C	267	SER	-	cloning artifact	UNP Q9JZW6
C	268	HIS	-	cloning artifact	UNP Q9JZW6
C	269	HIS	-	cloning artifact	UNP Q9JZW6
C	270	HIS	-	cloning artifact	UNP Q9JZW6
C	271	HIS	-	cloning artifact	UNP Q9JZW6
C	272	HIS	-	cloning artifact	UNP Q9JZW6
C	273	HIS	-	cloning artifact	UNP Q9JZW6
D	-1	MSE	-	cloning artifact	UNP Q9JZW6
D	0	SER	-	cloning artifact	UNP Q9JZW6
D	1	LEU	-	cloning artifact	UNP Q9JZW6
D	10	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
D	19	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
D	31	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
D	38	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
D	47	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
D	63	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
D	78	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
D	103	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
D	109	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
D	118	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
D	127	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
D	178	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
D	213	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
D	216	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
D	232	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
D	264	GLU	-	cloning artifact	UNP Q9JZW6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	265	GLY	-	cloning artifact	UNP Q9JZW6
D	266	GLY	-	cloning artifact	UNP Q9JZW6
D	267	SER	-	cloning artifact	UNP Q9JZW6
D	268	HIS	-	cloning artifact	UNP Q9JZW6
D	269	HIS	-	cloning artifact	UNP Q9JZW6
D	270	HIS	-	cloning artifact	UNP Q9JZW6
D	271	HIS	-	cloning artifact	UNP Q9JZW6
D	272	HIS	-	cloning artifact	UNP Q9JZW6
D	273	HIS	-	cloning artifact	UNP Q9JZW6
E	-1	MSE	-	cloning artifact	UNP Q9JZW6
E	0	SER	-	cloning artifact	UNP Q9JZW6
E	1	LEU	-	cloning artifact	UNP Q9JZW6
E	10	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
E	19	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
E	31	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
E	38	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
E	47	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
E	63	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
E	78	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
E	103	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
E	109	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
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E	264	GLU	-	cloning artifact	UNP Q9JZW6
E	265	GLY	-	cloning artifact	UNP Q9JZW6
E	266	GLY	-	cloning artifact	UNP Q9JZW6
E	267	SER	-	cloning artifact	UNP Q9JZW6
E	268	HIS	-	cloning artifact	UNP Q9JZW6
E	269	HIS	-	cloning artifact	UNP Q9JZW6
E	270	HIS	-	cloning artifact	UNP Q9JZW6
E	271	HIS	-	cloning artifact	UNP Q9JZW6
E	272	HIS	-	cloning artifact	UNP Q9JZW6
E	273	HIS	-	cloning artifact	UNP Q9JZW6

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

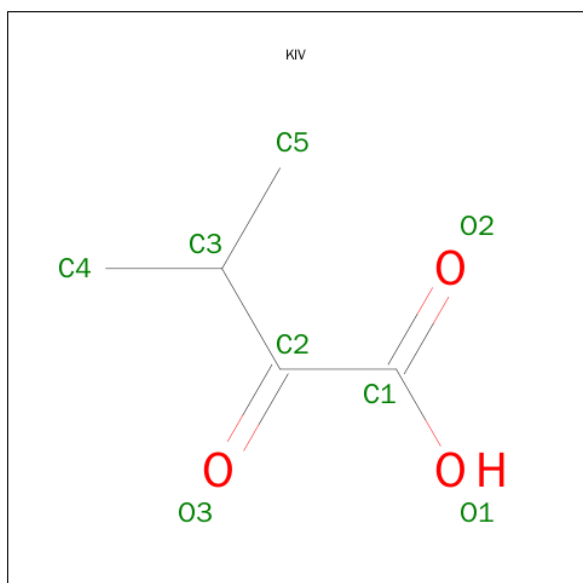
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Na 1 1	0	0
2	A	1	Total Na 1 1	0	0
2	D	1	Total Na 1 1	0	0
2	E	1	Total Na 1 1	0	0

- Molecule 3 is 3-METHYL-2-OXOBUTANOIC ACID (three-letter code: KIV) (formula: $C_5H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 8 5 3	0	0
3	D	1	Total C O 8 5 3	0	0
3	B	1	Total C O 8 5 3	0	0
3	E	1	Total C O 8 5 3	0	0

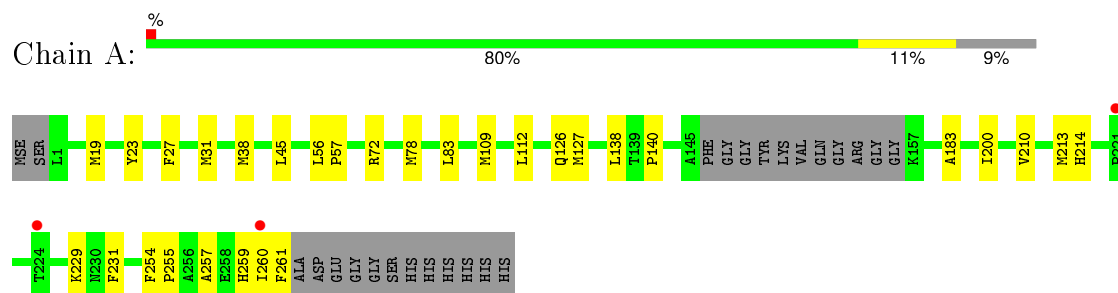
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	144	Total 144	O 144	0	0
4	B	114	Total 114	O 114	0	0
4	C	144	Total 144	O 144	0	0
4	D	102	Total 102	O 102	0	0
4	E	79	Total 79	O 79	0	0

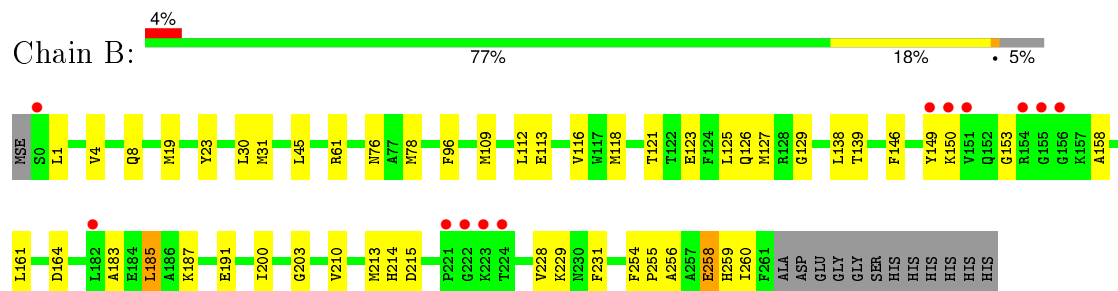
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

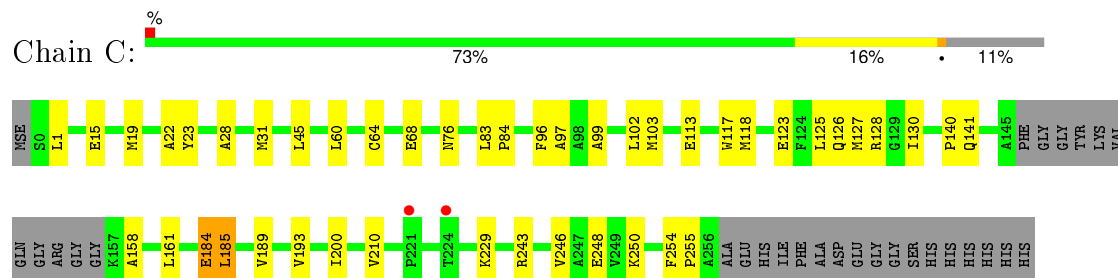
- Molecule 1: 3-methyl-2-oxobutanoate hydroxymethyltransferase



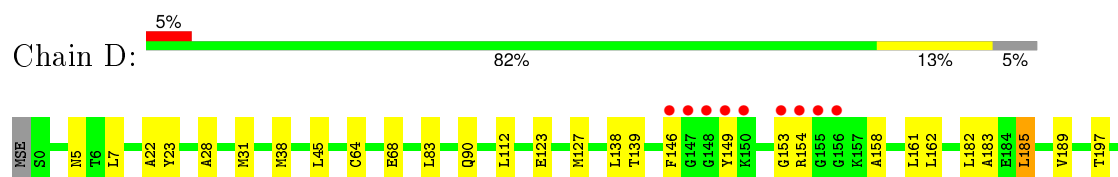
- Molecule 1: 3-methyl-2-oxobutanoate hydroxymethyltransferase

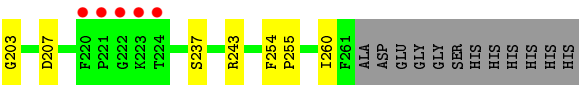


- Molecule 1: 3-methyl-2-oxobutanoate hydroxymethyltransferase

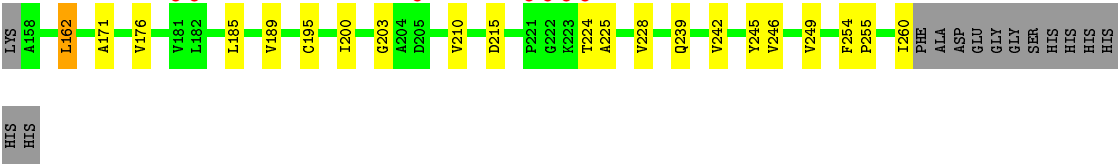
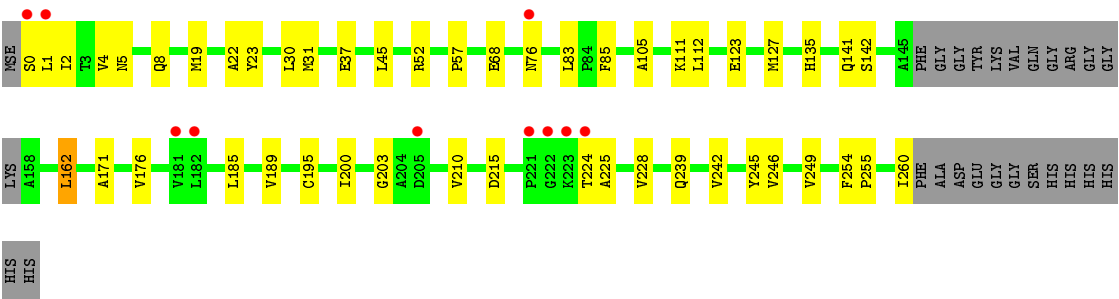


- Molecule 1: 3-methyl-2-oxobutanoate hydroxymethyltransferase





● Molecule 1: 3-methyl-2-oxobutanoate hydroxymethyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	164.42Å 111.24Å 98.81Å 90.00° 122.93° 90.00°	Depositor
Resolution (Å)	69.00 – 2.10 69.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (69.00-2.10) 94.3 (69.00-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.20 (at 2.10Å)	Xtriage
Refinement program	REFMAC 4	Depositor
R, R_{free}	0.186 , 0.224 0.171 , 0.206	Depositor DCC
R_{free} test set	8258 reflections (11.20%)	DCC
Wilson B-factor (Å ²)	22.1	Xtriage
Anisotropy	0.574	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 60.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 81973 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9852	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, KIV

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	0.51	0/1841	0.87	1/2466 (0.0%)
1	B	0.49	0/1921	0.87	0/2571
1	C	0.52	0/1853	0.89	2/2479 (0.1%)
1	D	0.51	0/1940	0.90	3/2596 (0.1%)
1	E	0.45	0/1825	0.81	0/2442
All	All	0.50	0/9380	0.87	6/12554 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	243	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	C	243	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	D	243	ARG	CD-NE-CZ	5.36	131.11	123.60
1	A	72	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	D	237	SER	N-CA-CB	5.04	118.05	110.50
1	C	243	ARG	CD-NE-CZ	5.03	130.64	123.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	200	ILE	Mainchain
1	C	200	ILE	Mainchain

5.2 Too-close contacts

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	1813	0	1788	22	0
1	B	1896	0	1870	41	0
1	C	1807	0	1798	39	0
1	D	1909	0	1898	24	0
1	E	1808	0	1808	29	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
3	A	8	0	7	0	0
3	B	8	0	7	0	0
3	D	8	0	7	0	0
3	E	8	0	7	2	0
4	A	144	0	0	1	0
4	B	114	0	0	0	0
4	C	144	0	0	2	0
4	D	102	0	0	0	0
4	E	79	0	0	0	0
All	All	9852	0	9190	152	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 8.

All (152) 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:127[B]:MSE:SE	1:A:127[B]:MSE:CE	1.29	1.47
1:A:127[B]:MSE:HE2	1:A:127[B]:MSE:SE	1.86	1.17
1:A:127[B]:MSE:SE	1:A:127[B]:MSE:HE3	1.86	1.11
1:A:127[B]:MSE:HE1	1:A:127[B]:MSE:SE	1.86	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:GLU:O	1:B:127[D]:MSE:HG3	1.66	0.93
1:C:96:PHE:HA	1:C:125[A]:LEU:HD11	1.53	0.90
1:B:127[D]:MSE:SE	1:B:127[D]:MSE:CG	2.71	0.88
1:C:123:GLU:O	1:C:127[B]:MSE:HG3	1.74	0.86
1:E:111:LYS:HE3	1:E:135:HIS:ND1	1.92	0.85
1:C:127[A]:MSE:HE3	1:C:128:ARG:HH12	1.47	0.78
1:B:256:ALA:H	1:B:259:HIS:HD2	1.32	0.78
1:C:22:ALA:HB2	1:C:31:MSE:HE1	1.71	0.73
1:A:127[B]:MSE:CG	1:A:127[B]:MSE:CE	2.67	0.72
1:D:138:LEU:HD11	1:D:149:TYR:HA	1.74	0.70
1:C:117[B]:TRP:CZ3	1:C:118:MSE:HE3	2.26	0.69
1:B:203:GLY:HA2	1:B:260:ILE:HG12	1.73	0.69
1:C:22:ALA:CB	1:C:31:MSE:HE1	2.24	0.68
1:B:138:LEU:HD21	1:B:149:TYR:HA	1.78	0.66
1:C:127[B]:MSE:HE2	1:C:127[B]:MSE:HB3	1.79	0.65
1:B:112:LEU:HD13	1:B:118:MSE:HE2	1.79	0.65
1:B:127[D]:MSE:CB	1:B:127[D]:MSE:SE	2.95	0.64
1:D:22:ALA:HB2	1:D:31:MSE:HE1	1.79	0.64
1:A:183:ALA:HB2	1:A:260:ILE:CG2	2.30	0.61
1:D:22:ALA:CB	1:D:31:MSE:HE1	2.30	0.60
1:E:200:ILE:HD13	3:E:275:KIV:HC41	1.83	0.60
1:A:140:PRO:HB2	4:A:389:HOH:O	2.02	0.60
1:D:154:ARG:HB3	1:D:182:LEU:HD11	1.84	0.60
1:C:158:ALA:HA	1:C:185:LEU:HD11	1.85	0.59
1:D:83:LEU:HD12	1:D:112:LEU:HB3	1.84	0.59
1:C:1:LEU:HD23	1:C:76:ASN:HD22	1.68	0.59
1:C:184:GLU:HG3	1:C:185:LEU:N	2.17	0.58
1:C:96:PHE:HD1	1:C:125[A]:LEU:HD13	1.70	0.57
1:A:27:PHE:HB3	1:A:31:MSE:HE2	1.86	0.56
1:B:19:MSE:HG2	1:B:210:VAL:HG23	1.89	0.55
1:B:161:LEU:HD23	1:B:185:LEU:HD13	1.88	0.55
1:E:5:ASN:HA	1:E:8:GLN:HE21	1.70	0.55
1:C:254:PHE:CD1	1:C:255:PRO:HA	2.41	0.55
1:E:225:ALA:HB3	1:E:228:VAL:HG23	1.89	0.55
1:E:4:VAL:O	1:E:8:GLN:HG3	2.07	0.54
1:C:15[B]:GLU:HG3	4:C:402:HOH:O	2.08	0.54
1:D:203:GLY:HA2	1:D:260:ILE:HG12	1.89	0.54
1:C:246:VAL:O	1:C:250:LYS:HG2	2.07	0.54
1:E:215:ASP:HB3	1:E:228:VAL:HG11	1.90	0.54
1:D:139:THR:H	1:D:146:PHE:HE1	1.56	0.54
1:C:117[B]:TRP:CE3	1:C:118:MSE:HE3	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:LYS:NZ	1:D:5:ASN:OD1	2.24	0.53
1:C:140:PRO:HB2	4:C:349:HOH:O	2.08	0.53
1:C:28:ALA:HA	1:C:31:MSE:HE3	1.92	0.52
1:D:153:GLY:HA3	1:D:185:LEU:HD12	1.91	0.52
1:A:183:ALA:HB2	1:A:260:ILE:HG21	1.92	0.52
1:E:23:TYR:CD2	1:E:45:LEU:HB3	2.45	0.52
1:C:125[A]:LEU:HD12	1:C:130:ILE:HD12	1.93	0.51
1:D:161:LEU:HD23	1:D:185:LEU:HD13	1.93	0.51
1:B:229:LYS:HD3	1:B:231:PHE:CZ	2.45	0.51
1:C:127[B]:MSE:CE	1:C:127[B]:MSE:HB3	2.40	0.51
1:B:215:ASP:HB3	1:B:228:VAL:HG11	1.93	0.50
1:D:28:ALA:HA	1:D:31:MSE:HE3	1.94	0.50
1:B:31:MSE:HE2	1:B:213:MSE:SE	2.62	0.50
1:A:78:MSE:SE	1:A:109:MSE:HE3	2.62	0.50
1:C:23:TYR:CD2	1:C:45:LEU:HB3	2.47	0.49
1:B:126:GLN:NE2	1:B:127[D]:MSE:HG2	2.27	0.49
1:E:245:TYR:O	1:E:249:VAL:HG23	2.12	0.49
1:E:22:ALA:HB2	1:E:31:MSE:HE1	1.94	0.49
1:C:97:ALA:HB2	1:D:90:GLN:NE2	2.27	0.49
1:B:4:VAL:O	1:B:8:GLN:HG3	2.12	0.49
1:E:22:ALA:CB	1:E:31:MSE:HE1	2.43	0.49
1:C:189:VAL:O	1:C:193:VAL:HG22	2.12	0.49
1:E:254:PHE:CD1	1:E:255:PRO:HA	2.48	0.48
1:A:213:MSE:HE2	1:A:214:HIS:CE1	2.48	0.48
1:B:126:GLN:CD	1:B:127[D]:MSE:HG2	2.33	0.48
1:D:162:LEU:HD23	1:D:189:VAL:HG22	1.96	0.48
1:E:176:VAL:HG23	1:E:195:CYS:SG	2.54	0.48
1:C:123:GLU:O	1:C:127[B]:MSE:CG	2.55	0.47
1:B:19:MSE:O	1:B:210:VAL:HA	2.13	0.47
1:B:112:LEU:HD13	1:B:118:MSE:CE	2.45	0.47
1:B:116:VAL:HG23	1:B:164:ASP:OD1	2.14	0.47
1:E:162:LEU:HD22	1:E:189:VAL:HG22	1.96	0.47
1:D:254:PHE:CD1	1:D:255:PRO:HA	2.49	0.47
1:B:213:MSE:HE2	1:B:214:HIS:CE1	2.49	0.47
1:D:123:GLU:O	1:D:127[A]:MSE:HG3	2.14	0.47
1:A:56:LEU:N	1:A:57:PRO:CD	2.78	0.46
1:A:200:ILE:HB	1:A:210:VAL:HG13	1.98	0.46
1:B:187:LYS:HE2	1:B:191:GLU:OE1	2.16	0.46
1:C:83:LEU:HD23	1:C:102:LEU:HD12	1.98	0.45
1:E:68:GLU:HG3	1:E:105:ALA:HB1	1.98	0.45
1:E:0:SER:OG	1:E:1:LEU:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:GLY:HA3	1:B:185:LEU:HD12	1.98	0.45
1:E:123:GLU:HB2	1:E:171:ALA:HB1	1.99	0.45
1:E:162:LEU:HD23	1:E:185:LEU:HD11	1.98	0.45
1:B:78:MSE:SE	1:B:109:MSE:HE3	2.67	0.45
1:A:229:LYS:HD3	1:A:231:PHE:CZ	2.52	0.45
1:D:153:GLY:O	1:D:158:ALA:HB2	2.16	0.44
1:D:7:LEU:HD11	1:D:38:MSE:HE3	2.00	0.44
1:D:162:LEU:HD23	1:D:189:VAL:CG2	2.47	0.44
1:C:22:ALA:HB2	1:C:31:MSE:CE	2.44	0.44
1:C:19:MSE:HG2	1:C:210:VAL:HG23	1.99	0.44
1:C:161:LEU:HD22	1:C:185:LEU:HD13	1.99	0.44
1:B:113:GLU:OE2	1:B:139:THR:HB	2.18	0.44
1:A:254:PHE:CD1	1:A:255:PRO:HA	2.52	0.44
1:D:197:THR:H	1:D:207:ASP:HB2	1.83	0.44
1:E:85:PHE:HB2	1:E:141:GLN:HG2	2.00	0.44
1:E:0:SER:HB2	1:E:76:ASN:OD1	2.18	0.44
1:D:183:ALA:HB2	1:D:260:ILE:CG2	2.48	0.43
1:E:242:VAL:O	1:E:246:VAL:HG23	2.18	0.43
1:E:52:ARG:HD3	1:E:57:PRO:HG2	2.00	0.43
1:A:19:MSE:HE3	1:A:38:MSE:SE	2.69	0.43
1:E:30:LEU:C	1:E:30:LEU:HD23	2.39	0.43
1:C:161:LEU:CD2	1:C:185:LEU:HD13	2.48	0.43
1:E:111:LYS:NZ	3:E:275:KIV:O3	2.51	0.43
1:A:138:LEU:O	1:A:140:PRO:HD3	2.18	0.43
1:B:161:LEU:CD2	1:B:185:LEU:HD13	2.48	0.43
1:B:183:ALA:HB2	1:B:260:ILE:HG23	2.00	0.43
1:A:83:LEU:HD12	1:A:112:LEU:HB3	2.01	0.43
1:B:30:LEU:HD23	1:B:30:LEU:C	2.40	0.43
1:C:229:LYS:NZ	1:C:248:GLU:OE1	2.45	0.42
1:A:23:TYR:CD2	1:A:45:LEU:HB3	2.54	0.42
1:B:138:LEU:HD21	1:B:149:TYR:CA	2.46	0.42
1:A:260:ILE:HG22	1:A:261:PHE:N	2.34	0.42
1:B:229:LYS:HB3	1:B:231:PHE:CE1	2.54	0.42
1:B:23:TYR:CD2	1:B:45:LEU:HB3	2.54	0.42
1:E:19:MSE:O	1:E:210:VAL:HA	2.19	0.42
1:C:76:ASN:HD22	1:C:76:ASN:HA	1.68	0.42
1:C:64:CYS:O	1:C:68:GLU:HG3	2.19	0.42
1:B:254:PHE:CD1	1:B:255:PRO:HA	2.54	0.42
1:A:257:ALA:HA	1:A:260:ILE:HD12	2.02	0.42
1:A:255:PRO:HB2	1:A:259:HIS:HB2	2.01	0.42
1:B:158:ALA:HA	1:B:185:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127[B]:MSE:SE	1:C:127[B]:MSE:HB3	2.70	0.41
1:B:255:PRO:HB2	1:B:259:HIS:HB2	2.02	0.41
1:E:203:GLY:HA2	1:E:260:ILE:HG12	2.01	0.41
1:C:99:ALA:O	1:C:103:MSE:HG2	2.20	0.41
1:C:113:GLU:OE2	1:C:141:GLN:HB2	2.20	0.41
1:B:118:MSE:HE1	1:B:121:THR:HG21	2.01	0.41
1:B:146:PHE:O	1:B:150:LYS:NZ	2.48	0.41
1:B:129:GLY:HA3	1:E:142:SER:HB3	2.03	0.41
1:D:64:CYS:O	1:D:68:GLU:HG3	2.20	0.41
1:E:123:GLU:O	1:E:127[B]:MSE:HG3	2.21	0.41
1:E:2:ILE:HD13	1:E:37:GLU:HB3	2.02	0.41
1:B:96:PHE:HA	1:B:125:LEU:HD11	2.03	0.41
1:E:83:LEU:HD12	1:E:112:LEU:HB3	2.03	0.41
1:B:258:GLU:H	1:B:258:GLU:HG3	1.51	0.41
1:B:127[D]:MSE:SE	1:B:127[D]:MSE:HB3	2.69	0.40
1:D:23:TYR:CD2	1:D:45:LEU:HB3	2.55	0.40
1:C:96:PHE:CD1	1:C:125[A]:LEU:HD13	2.54	0.40
1:B:45:LEU:C	1:B:45:LEU:HD12	2.42	0.40
1:C:60:LEU:HA	1:C:84:PRO:HG3	2.02	0.40
1:D:22:ALA:HB2	1:D:31:MSE:CE	2.50	0.40
1:D:161:LEU:CD2	1:D:185:LEU:HD13	2.51	0.40
1:B:1:LEU:HD23	1:B:76:ASN:HA	2.03	0.40

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	249/275 (90%)	245 (98%)	4 (2%)	0	100	100
1	B	262/275 (95%)	258 (98%)	4 (2%)	0	100	100
1	C	249/275 (90%)	244 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	263/275 (96%)	258 (98%)	5 (2%)	0	100	100
1	E	246/275 (90%)	239 (97%)	7 (3%)	0	100	100
All	All	1269/1375 (92%)	1244 (98%)	25 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	181/189 (96%)	180 (99%)	1 (1%)	90	94
1	B	186/189 (98%)	183 (98%)	3 (2%)	70	76
1	C	185/189 (98%)	182 (98%)	3 (2%)	70	76
1	D	191/189 (101%)	190 (100%)	1 (0%)	92	95
1	E	181/189 (96%)	178 (98%)	3 (2%)	68	74
All	All	924/945 (98%)	913 (99%)	11 (1%)	78	84

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	126	GLN
1	B	61	ARG
1	B	185	LEU
1	B	258	GLU
1	C	126	GLN
1	C	184	GLU
1	C	185	LEU
1	D	185	LEU
1	E	162	LEU
1	E	224	THR
1	E	239	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such

sidechains are listed below:

Mol	Chain	Res	Type
1	B	233	GLN
1	B	259	HIS
1	C	5	ASN
1	C	76	ASN
1	D	90	GLN
1	E	5	ASN
1	E	8	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	KIV	A	275	2	4,7,7	2.53	1 (25%)	4,9,9	2.17	2 (50%)
3	KIV	B	275	2	4,7,7	2.39	1 (25%)	4,9,9	2.62	2 (50%)
3	KIV	D	275	2	4,7,7	2.56	1 (25%)	4,9,9	2.27	3 (75%)
3	KIV	E	275	2	4,7,7	2.29	1 (25%)	4,9,9	2.66	2 (50%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	KIV	A	275	2	-	0/4/8/8	0/0/0/0
3	KIV	B	275	2	-	0/4/8/8	0/0/0/0
3	KIV	D	275	2	-	0/4/8/8	0/0/0/0
3	KIV	E	275	2	-	0/4/8/8	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	275	KIV	C3-C2	4.38	1.57	1.51
3	B	275	KIV	C3-C2	4.66	1.57	1.51
3	D	275	KIV	C3-C2	4.74	1.57	1.51
3	A	275	KIV	C3-C2	4.81	1.57	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	275	KIV	C5-C3-C2	-3.33	103.60	110.32
3	B	275	KIV	C5-C3-C2	-2.79	104.69	110.32
3	D	275	KIV	C5-C3-C2	-2.71	104.86	110.32
3	A	275	KIV	C5-C3-C2	-2.45	105.38	110.32
3	D	275	KIV	C4-C3-C2	2.46	115.27	110.32
3	D	275	KIV	O3-C2-C3	2.65	123.69	117.64
3	A	275	KIV	C4-C3-C2	3.24	116.83	110.32
3	E	275	KIV	C4-C3-C2	3.86	118.08	110.32
3	B	275	KIV	C4-C3-C2	4.40	119.17	110.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	275	KIV	2	0

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	235/275 (85%)	-0.12	3 (1%) 79 84	13, 21, 34, 47	0
1	B	247/275 (89%)	-0.04	12 (4%) 33 42	13, 21, 43, 51	0
1	C	231/275 (84%)	-0.15	2 (0%) 85 88	10, 20, 33, 45	0
1	D	247/275 (89%)	-0.01	14 (5%) 27 35	12, 20, 47, 56	0
1	E	234/275 (85%)	0.27	10 (4%) 39 48	16, 30, 46, 61	0
All	All	1194/1375 (86%)	-0.01	41 (3%) 49 58	10, 22, 42, 61	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	222	GLY	6.4
1	E	223	LYS	5.8
1	E	221	PRO	5.4
1	D	149	TYR	5.4
1	E	224	THR	4.7
1	D	221	PRO	4.5
1	D	224	THR	3.9
1	D	223	LYS	3.7
1	C	221	PRO	3.7
1	D	156	GLY	3.4
1	B	156	GLY	3.3
1	B	155	GLY	3.3
1	D	146	PHE	3.2
1	D	154	ARG	3.1
1	B	151	VAL	3.0
1	D	147	GLY	2.9
1	B	223	LYS	2.9
1	B	222	GLY	2.8
1	B	150	LYS	2.8
1	E	181	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	0	SER	2.8
1	D	150	LYS	2.7
1	A	260	ILE	2.7
1	D	148	GLY	2.7
1	B	149	TYR	2.6
1	C	224	THR	2.5
1	B	182	LEU	2.5
1	D	155	GLY	2.5
1	D	153	GLY	2.4
1	E	1	LEU	2.4
1	A	224	THR	2.4
1	B	224	THR	2.3
1	A	221	PRO	2.2
1	D	222	GLY	2.2
1	E	0	SER	2.2
1	E	205	ASP	2.2
1	B	154	ARG	2.2
1	E	182	LEU	2.1
1	D	220	PHE	2.1
1	E	76	ASN	2.1
1	B	221	PRO	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	NA	E	274	1/1	0.93	0.21	7.77	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	KIV	A	275	8/8	0.91	0.20	7.74	31,33,33,33	0
2	NA	B	274	1/1	0.97	0.17	6.31	31,31,31,31	0
3	KIV	D	275	8/8	0.94	0.14	5.17	30,30,31,32	0
3	KIV	E	275	8/8	0.89	0.23	4.35	34,35,35,36	0
3	KIV	B	275	8/8	0.94	0.12	1.72	28,29,30,31	0
2	NA	A	274	1/1	0.91	0.12	1.28	35,35,35,35	0
2	NA	D	274	1/1	0.98	0.07	-3.09	32,32,32,32	0

6.5 Other polymers

There are no such residues in this entry.