



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 18, 2026 – 01:48 PM UTC

PDB ID : 3BG3 / pdb_00003bg3
Title : Crystal Structure of Human Pyruvate Carboxylase (missing the biotin carboxylase domain at the N-terminus)
Authors : Xiang, S.; Tong, L.
Deposited on : 2007-11-26
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

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>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

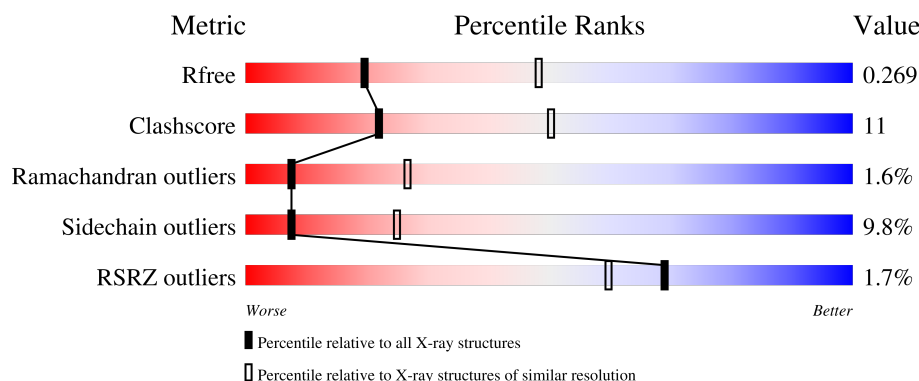
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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 ≥ 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	718	2% 67% 23% 5% 5%
1	B	718	2% 60% 21% • 16%
1	C	718	58% 23% • 16%
1	D	718	2% 67% 24% • 5%

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
3	PYR	C	2000	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19813 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 Pyruvate carboxylase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	680	Total	C	N	O	S	0	0	0
			5222	3314	895	978	35			
1	B	604	Total	C	N	O	S	0	0	0
			4663	2960	802	872	29			
1	C	604	Total	C	N	O	S	0	0	0
			4663	2960	802	872	29			
1	D	680	Total	C	N	O	S	0	0	0
			5222	3314	895	978	35			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	461	MET	-	expression tag	UNP P11498
A	462	GLY	-	expression tag	UNP P11498
A	463	SER	-	expression tag	UNP P11498
A	464	SER	-	expression tag	UNP P11498
A	465	HIS	-	expression tag	UNP P11498
A	466	HIS	-	expression tag	UNP P11498
A	467	HIS	-	expression tag	UNP P11498
A	468	HIS	-	expression tag	UNP P11498
A	469	HIS	-	expression tag	UNP P11498
A	470	HIS	-	expression tag	UNP P11498
A	471	SER	-	expression tag	UNP P11498
A	472	SER	-	expression tag	UNP P11498
A	473	GLY	-	expression tag	UNP P11498
A	474	LEU	-	expression tag	UNP P11498
A	475	VAL	-	expression tag	UNP P11498
A	476	PRO	-	expression tag	UNP P11498
A	477	ARG	-	expression tag	UNP P11498
A	478	GLY	-	expression tag	UNP P11498
A	479	SER	-	expression tag	UNP P11498
A	480	HIS	-	expression tag	UNP P11498
A	481	MET	-	expression tag	UNP P11498

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Chain	Residue	Modelled	Actual	Comment	Reference
B	461	MET	-	expression tag	UNP P11498
B	462	GLY	-	expression tag	UNP P11498
B	463	SER	-	expression tag	UNP P11498
B	464	SER	-	expression tag	UNP P11498
B	465	HIS	-	expression tag	UNP P11498
B	466	HIS	-	expression tag	UNP P11498
B	467	HIS	-	expression tag	UNP P11498
B	468	HIS	-	expression tag	UNP P11498
B	469	HIS	-	expression tag	UNP P11498
B	470	HIS	-	expression tag	UNP P11498
B	471	SER	-	expression tag	UNP P11498
B	472	SER	-	expression tag	UNP P11498
B	473	GLY	-	expression tag	UNP P11498
B	474	LEU	-	expression tag	UNP P11498
B	475	VAL	-	expression tag	UNP P11498
B	476	PRO	-	expression tag	UNP P11498
B	477	ARG	-	expression tag	UNP P11498
B	478	GLY	-	expression tag	UNP P11498
B	479	SER	-	expression tag	UNP P11498
B	480	HIS	-	expression tag	UNP P11498
B	481	MET	-	expression tag	UNP P11498
C	461	MET	-	expression tag	UNP P11498
C	462	GLY	-	expression tag	UNP P11498
C	463	SER	-	expression tag	UNP P11498
C	464	SER	-	expression tag	UNP P11498
C	465	HIS	-	expression tag	UNP P11498
C	466	HIS	-	expression tag	UNP P11498
C	467	HIS	-	expression tag	UNP P11498
C	468	HIS	-	expression tag	UNP P11498
C	469	HIS	-	expression tag	UNP P11498
C	470	HIS	-	expression tag	UNP P11498
C	471	SER	-	expression tag	UNP P11498
C	472	SER	-	expression tag	UNP P11498
C	473	GLY	-	expression tag	UNP P11498
C	474	LEU	-	expression tag	UNP P11498
C	475	VAL	-	expression tag	UNP P11498
C	476	PRO	-	expression tag	UNP P11498
C	477	ARG	-	expression tag	UNP P11498
C	478	GLY	-	expression tag	UNP P11498
C	479	SER	-	expression tag	UNP P11498
C	480	HIS	-	expression tag	UNP P11498
C	481	MET	-	expression tag	UNP P11498

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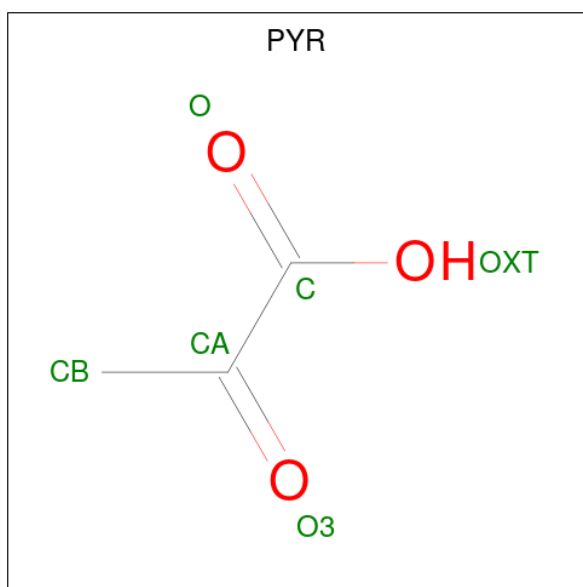
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Chain	Residue	Modelled	Actual	Comment	Reference
D	461	MET	-	expression tag	UNP P11498
D	462	GLY	-	expression tag	UNP P11498
D	463	SER	-	expression tag	UNP P11498
D	464	SER	-	expression tag	UNP P11498
D	465	HIS	-	expression tag	UNP P11498
D	466	HIS	-	expression tag	UNP P11498
D	467	HIS	-	expression tag	UNP P11498
D	468	HIS	-	expression tag	UNP P11498
D	469	HIS	-	expression tag	UNP P11498
D	470	HIS	-	expression tag	UNP P11498
D	471	SER	-	expression tag	UNP P11498
D	472	SER	-	expression tag	UNP P11498
D	473	GLY	-	expression tag	UNP P11498
D	474	LEU	-	expression tag	UNP P11498
D	475	VAL	-	expression tag	UNP P11498
D	476	PRO	-	expression tag	UNP P11498
D	477	ARG	-	expression tag	UNP P11498
D	478	GLY	-	expression tag	UNP P11498
D	479	SER	-	expression tag	UNP P11498
D	480	HIS	-	expression tag	UNP P11498
D	481	MET	-	expression tag	UNP P11498

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

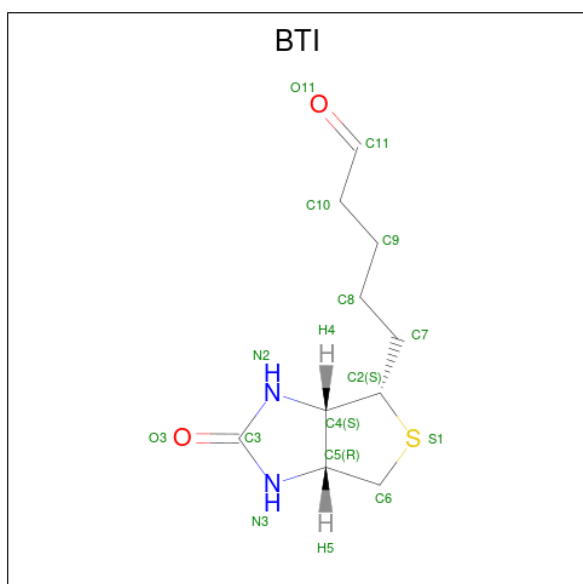
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mn 1 1	0	0
2	B	1	Total Mn 1 1	0	0
2	C	1	Total Mn 1 1	0	0
2	D	1	Total Mn 1 1	0	0

- Molecule 3 is PYRUVIC ACID (CCD ID: PYR) (formula: C₃H₄O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is 5-(HEXAHYDRO-2-OXO-1H-THIENO[3,4-D]IMIDAZOL-6-YL)PENTANAL (CCD ID: BTI) (formula: C₁₀H₁₆N₂O₂S).

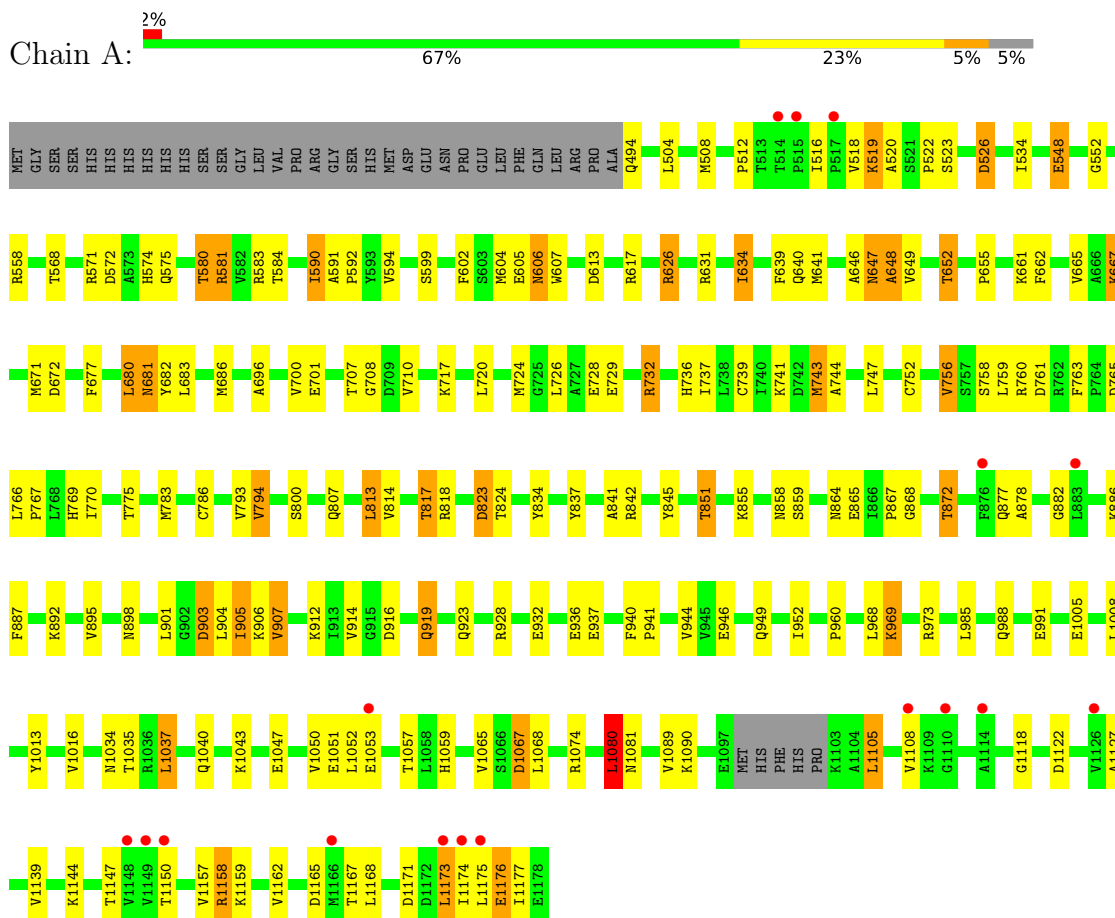


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			15	10	2	2	1		

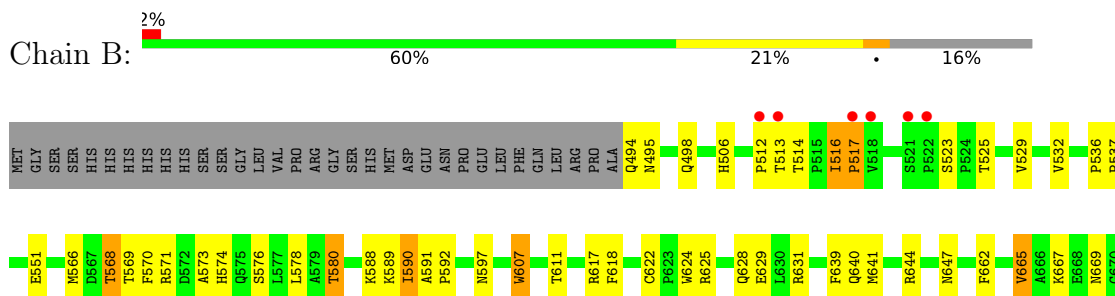
3 Residue-property plots

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.

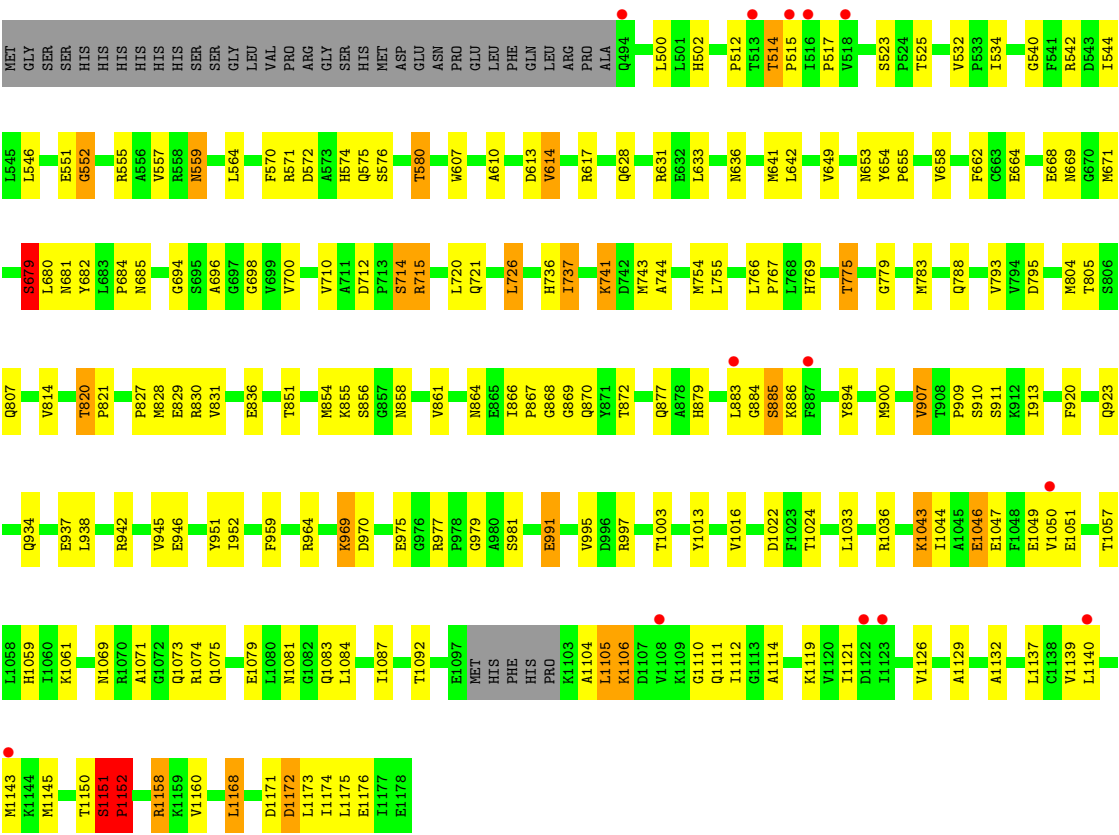
• Molecule 1: Pyruvate carboxylase, mitochondrial



• Molecule 1: Pyruvate carboxylase, mitochondrial







4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.27Å 173.32Å 118.19Å 90.00° 95.87° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 30.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.7 (30.00-2.80) 94.6 (30.00-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 2.76Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.216 , 0.271 0.216 , 0.269	Depositor DCC
R_{free} test set	3954 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å ²)	69.3	Xtriage
Anisotropy	0.375	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 37.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	19813	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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: KCX, MN, PYR, BTI

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	0.63	4/5322 (0.1%)	0.95	2/7211 (0.0%)
1	B	0.67	5/4759 (0.1%)	0.95	2/6456 (0.0%)
1	C	0.61	2/4759 (0.0%)	0.93	1/6456 (0.0%)
1	D	0.67	6/5322 (0.1%)	0.95	6/7211 (0.1%)
All	All	0.64	17/20162 (0.1%)	0.95	11/27334 (0.0%)

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1066	SER	CB-OG	11.38	1.65	1.42
1	B	973	ARG	CZ-NH1	11.17	1.48	1.32
1	A	973	ARG	CD-NE	8.79	1.58	1.46
1	B	973	ARG	NE-CZ	6.82	1.40	1.33
1	D	991	GLU	CD-OE2	6.72	1.38	1.25

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1106	LYS	N-CA-C	6.95	120.71	112.93
1	C	1094	ALA	N-CA-C	-6.13	105.28	112.89
1	A	952	ILE	N-CA-C	-5.88	107.53	113.47
1	D	552	GLY	O-C-N	5.81	127.76	122.18
1	D	698	GLY	N-CA-C	5.80	120.49	112.37

There are no chirality outliers.

There are no planarity outliers.

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	5222	0	5216	120	0
1	B	4663	0	4609	106	0
1	C	4663	0	4608	98	0
1	D	5222	0	5217	105	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	6	0	0	0	0
3	B	6	0	0	0	0
3	C	6	0	0	0	0
3	D	6	0	0	0	0
4	A	15	0	15	0	0
All	All	19813	0	19665	421	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 11.

The worst 5 of 421 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1066:SER:OG	1:B:1066:SER:CB	1.64	1.45
1:C:870:GLN:HE22	1:C:911:SER:HB2	1.17	1.07
1:B:568:THR:HG21	1:B:807:GLN:NE2	1.82	0.94
1:A:851:THR:HG21	1:D:855:LYS:HD2	1.47	0.94
1:B:641:MET:HE3	1:B:671:MET:HG2	1.51	0.91

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	675/718 (94%)	612 (91%)	50 (7%)	13 (2%)	6	22
1	B	601/718 (84%)	542 (90%)	54 (9%)	5 (1%)	16	44
1	C	601/718 (84%)	543 (90%)	47 (8%)	11 (2%)	6	23
1	D	675/718 (94%)	603 (89%)	59 (9%)	13 (2%)	6	22
All	All	2552/2872 (89%)	2300 (90%)	210 (8%)	42 (2%)	7	27

5 of 42 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1165	ASP
1	B	1055	GLY
1	C	496	ARG
1	D	1110	GLY
1	D	1152	PRO

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	559/593 (94%)	499 (89%)	60 (11%)	6	21
1	B	496/593 (84%)	448 (90%)	48 (10%)	8	25
1	C	496/593 (84%)	445 (90%)	51 (10%)	7	23
1	D	559/593 (94%)	512 (92%)	47 (8%)	10	32
All	All	2110/2372 (89%)	1904 (90%)	206 (10%)	7	25

5 of 206 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	601	LEU
1	C	924	ASN

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Mol	Chain	Res	Type
1	D	1074	ARG
1	C	630	LEU
1	C	726	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 79 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1040	GLN
1	D	864	ASN
1	C	1075	GLN
1	D	575	GLN
1	D	1073	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	KCX	D	741	2	10,11,12	0.77	0	6,12,14	2.40	1 (16%)
1	KCX	A	741	2	10,11,12	1.14	2 (20%)	6,12,14	1.22	1 (16%)
1	KCX	B	741	2	10,11,12	0.98	0	6,12,14	1.36	1 (16%)
1	KCX	C	741	2	10,11,12	0.92	0	6,12,14	2.00	1 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	D	741	2	-	0/9/10/12	-
1	KCX	A	741	2	-	1/9/10/12	-
1	KCX	B	741	2	-	1/9/10/12	-
1	KCX	C	741	2	-	0/9/10/12	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	741	KCX	OQ1-CX	2.08	1.25	1.21
1	A	741	KCX	CE-NZ	2.04	1.50	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	741	KCX	OQ1-CX-NZ	-5.39	116.73	124.92
1	C	741	KCX	OQ1-CX-NZ	-4.69	117.80	124.92
1	B	741	KCX	OQ1-CX-NZ	-2.97	120.42	124.92
1	A	741	KCX	OQ1-CX-NZ	-2.78	120.69	124.92

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	741	KCX	O-C-CA-CB
1	B	741	KCX	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	741	KCX	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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	PYR	C	2000	-	5,5,5	3.03	3 (60%)	3,6,6	2.11	2 (66%)
4	BTI	A	2100	1	15,16,16	1.66	2 (13%)	20,21,21	2.07	2 (10%)
3	PYR	B	2000	-	5,5,5	2.99	3 (60%)	3,6,6	2.30	2 (66%)
3	PYR	D	2000	-	5,5,5	3.15	3 (60%)	3,6,6	1.93	1 (33%)
3	PYR	A	2000	-	5,5,5	3.07	3 (60%)	3,6,6	1.82	2 (66%)

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	PYR	C	2000	-	-	3/4/4/4	-
4	BTI	A	2100	1	-	2/6/27/27	0/2/2/2
3	PYR	B	2000	-	-	0/4/4/4	-
3	PYR	D	2000	-	-	1/4/4/4	-
3	PYR	A	2000	-	-	0/4/4/4	-

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2100	BTI	O3-C3	4.64	1.33	1.23
3	A	2000	PYR	CA-C	-4.45	1.39	1.54
3	D	2000	PYR	CA-C	-4.42	1.39	1.54
3	D	2000	PYR	O3-CA	4.23	1.32	1.23
3	C	2000	PYR	CA-C	-4.10	1.40	1.54

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2100	BTI	C6-C5-N3	-6.68	104.57	113.18
4	A	2100	BTI	C2-C4-N2	-5.17	107.87	113.34
3	B	2000	PYR	OXT-C-O	-2.85	117.10	123.90
3	D	2000	PYR	OXT-C-CA	2.69	121.05	113.59

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	C	2000	PYR	OXT-C-CA	2.67	121.00	113.59

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	2000	PYR	O-C-CA-CB
3	C	2000	PYR	OXT-C-CA-CB
3	D	2000	PYR	OXT-C-CA-CB
4	A	2100	BTI	C11-C10-C9-C8
4	A	2100	BTI	C2-C7-C8-C9

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	679/718 (94%)	0.03	17 (2%) 58 48	49, 89, 174, 254	0
1	B	603/718 (83%)	-0.04	12 (1%) 65 56	55, 89, 135, 163	0
1	C	603/718 (83%)	-0.07	2 (0%) 90 86	57, 91, 140, 165	0
1	D	679/718 (94%)	-0.04	13 (1%) 66 57	51, 87, 159, 257	0
All	All	2564/2872 (89%)	-0.03	44 (1%) 69 60	49, 89, 151, 257	0

The worst 5 of 44 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1108	VAL	4.3
1	A	1150	THR	4.2
1	C	648	ALA	3.9
1	A	1175	LEU	3.6
1	D	1108	VAL	3.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
1	KCX	C	741	12/13	0.95	0.10	70,72,74,75	0
1	KCX	B	741	12/13	0.96	0.08	64,66,68,68	0
1	KCX	A	741	12/13	0.97	0.08	66,69,70,70	0
1	KCX	D	741	12/13	0.97	0.07	54,60,63,64	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
3	PYR	C	2000	6/6	0.84	0.19	88,89,91,91	0
3	PYR	B	2000	6/6	0.85	0.14	72,74,74,74	0
4	BTI	A	2100	15/15	0.90	0.11	89,92,93,94	0
3	PYR	D	2000	6/6	0.91	0.18	76,77,77,79	0
3	PYR	A	2000	6/6	0.92	0.10	75,76,77,79	0
2	MN	C	2001	1/1	0.96	0.05	77,77,77,77	0
2	MN	B	2001	1/1	0.96	0.06	68,68,68,68	0
2	MN	A	2001	1/1	0.97	0.06	72,72,72,72	0
2	MN	D	2001	1/1	0.98	0.05	68,68,68,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.