



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:31 AM GMT

PDB ID : 3EXE
Title : Crystal structure of the pyruvate dehydrogenase (E1p) component of human pyruvate dehydrogenase complex
Authors : Kato, M.; Wynn, R.M.; Chuang, J.L.; Tso, S.-C.; Machius, M.; Li, J.; Chuang, D.T.
Deposited on : 2008-10-16
Resolution : 1.98 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
<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

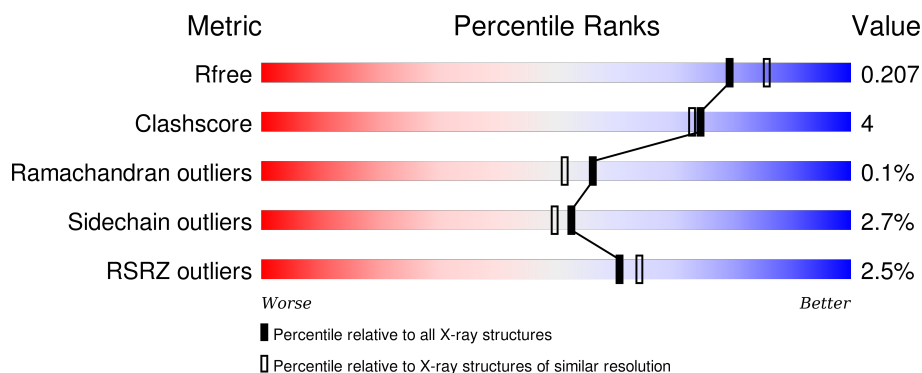
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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.



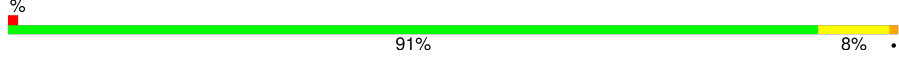
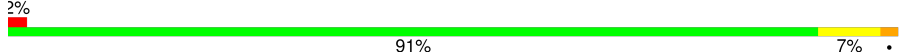
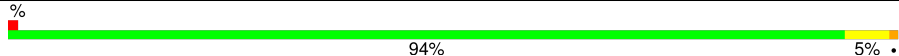
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	8664 (2.00-1.96)
Clashscore	102246	9905 (2.00-1.96)
Ramachandran outliers	100387	9792 (2.00-1.96)
Sidechain outliers	100360	9791 (2.00-1.96)
RSRZ outliers	91569	8679 (2.00-1.96)

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	382	<div> <div>2%</div> <div>84% 11% • 5%</div> </div>
1	C	382	<div> <div>2%</div> <div>84% 10% • 5%</div> </div>
1	E	382	<div> <div>4%</div> <div>80% 14% • 5%</div> </div>
1	G	382	<div> <div>4%</div> <div>83% 10% • 5%</div> </div>
2	B	329	<div> <div>2%</div> <div>90% 9% •</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	329	 91% 8%
2	F	329	 91% 7%
2	H	329	 94% 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
5	K	B	1003	-	-	-	X
5	K	D	1006	-	-	-	X
5	K	F	1009	-	-	-	X
5	K	H	1012	-	-	-	X
6	GOL	A	1101	-	-	-	X
6	GOL	C	1102	-	-	-	X
6	GOL	E	1103	-	-	-	X
6	GOL	G	1104	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 23831 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 dehydrogenase E1 component subunit alpha, somatic form, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	S	0	0	0
			2836	1780	499	532	25			
1	C	362	Total	C	N	O	S	0	0	0
			2823	1772	496	531	24			
1	E	361	Total	C	N	O	S	0	0	0
			2818	1769	495	530	24			
1	G	362	Total	C	N	O	S	0	0	0
			2826	1774	496	531	25			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	EXPRESSION TAG	UNP P08559
A	-19	GLY	-	EXPRESSION TAG	UNP P08559
A	-18	SER	-	EXPRESSION TAG	UNP P08559
A	-17	SER	-	EXPRESSION TAG	UNP P08559
A	-16	HIS	-	EXPRESSION TAG	UNP P08559
A	-15	HIS	-	EXPRESSION TAG	UNP P08559
A	-14	HIS	-	EXPRESSION TAG	UNP P08559
A	-13	HIS	-	EXPRESSION TAG	UNP P08559
A	-12	HIS	-	EXPRESSION TAG	UNP P08559
A	-11	HIS	-	EXPRESSION TAG	UNP P08559
A	-10	SER	-	EXPRESSION TAG	UNP P08559
A	-9	SER	-	EXPRESSION TAG	UNP P08559
A	-8	GLY	-	EXPRESSION TAG	UNP P08559
A	-7	LEU	-	EXPRESSION TAG	UNP P08559
A	-6	VAL	-	EXPRESSION TAG	UNP P08559
A	-5	PRO	-	EXPRESSION TAG	UNP P08559
A	-4	ARG	-	EXPRESSION TAG	UNP P08559
A	-3	GLY	-	EXPRESSION TAG	UNP P08559
A	-2	SER	-	EXPRESSION TAG	UNP P08559
A	-1	HIS	-	EXPRESSION TAG	UNP P08559

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	EXPRESSION TAG	UNP P08559
C	-20	MET	-	EXPRESSION TAG	UNP P08559
C	-19	GLY	-	EXPRESSION TAG	UNP P08559
C	-18	SER	-	EXPRESSION TAG	UNP P08559
C	-17	SER	-	EXPRESSION TAG	UNP P08559
C	-16	HIS	-	EXPRESSION TAG	UNP P08559
C	-15	HIS	-	EXPRESSION TAG	UNP P08559
C	-14	HIS	-	EXPRESSION TAG	UNP P08559
C	-13	HIS	-	EXPRESSION TAG	UNP P08559
C	-12	HIS	-	EXPRESSION TAG	UNP P08559
C	-11	HIS	-	EXPRESSION TAG	UNP P08559
C	-10	SER	-	EXPRESSION TAG	UNP P08559
C	-9	SER	-	EXPRESSION TAG	UNP P08559
C	-8	GLY	-	EXPRESSION TAG	UNP P08559
C	-7	LEU	-	EXPRESSION TAG	UNP P08559
C	-6	VAL	-	EXPRESSION TAG	UNP P08559
C	-5	PRO	-	EXPRESSION TAG	UNP P08559
C	-4	ARG	-	EXPRESSION TAG	UNP P08559
C	-3	GLY	-	EXPRESSION TAG	UNP P08559
C	-2	SER	-	EXPRESSION TAG	UNP P08559
C	-1	HIS	-	EXPRESSION TAG	UNP P08559
C	0	MET	-	EXPRESSION TAG	UNP P08559
E	-20	MET	-	EXPRESSION TAG	UNP P08559
E	-19	GLY	-	EXPRESSION TAG	UNP P08559
E	-18	SER	-	EXPRESSION TAG	UNP P08559
E	-17	SER	-	EXPRESSION TAG	UNP P08559
E	-16	HIS	-	EXPRESSION TAG	UNP P08559
E	-15	HIS	-	EXPRESSION TAG	UNP P08559
E	-14	HIS	-	EXPRESSION TAG	UNP P08559
E	-13	HIS	-	EXPRESSION TAG	UNP P08559
E	-12	HIS	-	EXPRESSION TAG	UNP P08559
E	-11	HIS	-	EXPRESSION TAG	UNP P08559
E	-10	SER	-	EXPRESSION TAG	UNP P08559
E	-9	SER	-	EXPRESSION TAG	UNP P08559
E	-8	GLY	-	EXPRESSION TAG	UNP P08559
E	-7	LEU	-	EXPRESSION TAG	UNP P08559
E	-6	VAL	-	EXPRESSION TAG	UNP P08559
E	-5	PRO	-	EXPRESSION TAG	UNP P08559
E	-4	ARG	-	EXPRESSION TAG	UNP P08559
E	-3	GLY	-	EXPRESSION TAG	UNP P08559
E	-2	SER	-	EXPRESSION TAG	UNP P08559
E	-1	HIS	-	EXPRESSION TAG	UNP P08559

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	0	MET	-	EXPRESSION TAG	UNP P08559
G	-20	MET	-	EXPRESSION TAG	UNP P08559
G	-19	GLY	-	EXPRESSION TAG	UNP P08559
G	-18	SER	-	EXPRESSION TAG	UNP P08559
G	-17	SER	-	EXPRESSION TAG	UNP P08559
G	-16	HIS	-	EXPRESSION TAG	UNP P08559
G	-15	HIS	-	EXPRESSION TAG	UNP P08559
G	-14	HIS	-	EXPRESSION TAG	UNP P08559
G	-13	HIS	-	EXPRESSION TAG	UNP P08559
G	-12	HIS	-	EXPRESSION TAG	UNP P08559
G	-11	HIS	-	EXPRESSION TAG	UNP P08559
G	-10	SER	-	EXPRESSION TAG	UNP P08559
G	-9	SER	-	EXPRESSION TAG	UNP P08559
G	-8	GLY	-	EXPRESSION TAG	UNP P08559
G	-7	LEU	-	EXPRESSION TAG	UNP P08559
G	-6	VAL	-	EXPRESSION TAG	UNP P08559
G	-5	PRO	-	EXPRESSION TAG	UNP P08559
G	-4	ARG	-	EXPRESSION TAG	UNP P08559
G	-3	GLY	-	EXPRESSION TAG	UNP P08559
G	-2	SER	-	EXPRESSION TAG	UNP P08559
G	-1	HIS	-	EXPRESSION TAG	UNP P08559
G	0	MET	-	EXPRESSION TAG	UNP P08559

- Molecule 2 is a protein called Pyruvate dehydrogenase E1 component subunit beta, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	329	Total	C	N	O	S	0	0	0
			2519	1604	427	469	19			
2	D	329	Total	C	N	O	S	0	0	0
			2519	1604	427	469	19			
2	F	329	Total	C	N	O	S	0	0	0
			2519	1604	427	469	19			
2	H	329	Total	C	N	O	S	0	0	0
			2519	1604	427	469	19			

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

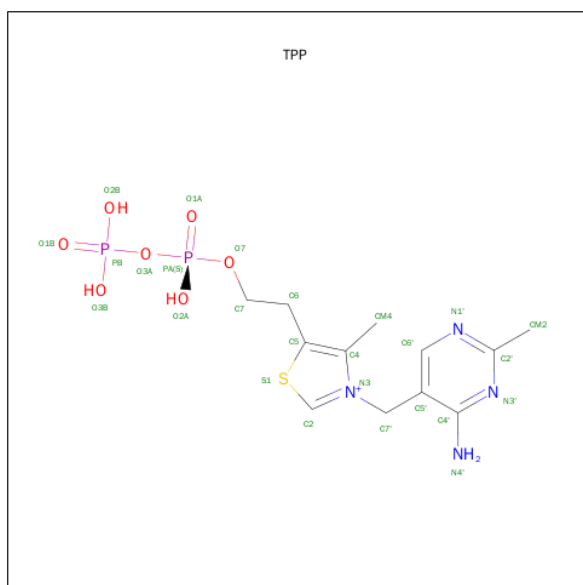
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Mn	0	0
			1	1		
3	A	1	Total	Mn	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	Mn	0	0
			1	1		
3	E	1	Total	Mn	0	0
			1	1		

- Molecule 4 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: C₁₂H₁₉N₄O₇P₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	C	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
4	A	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
4	G	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
4	E	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

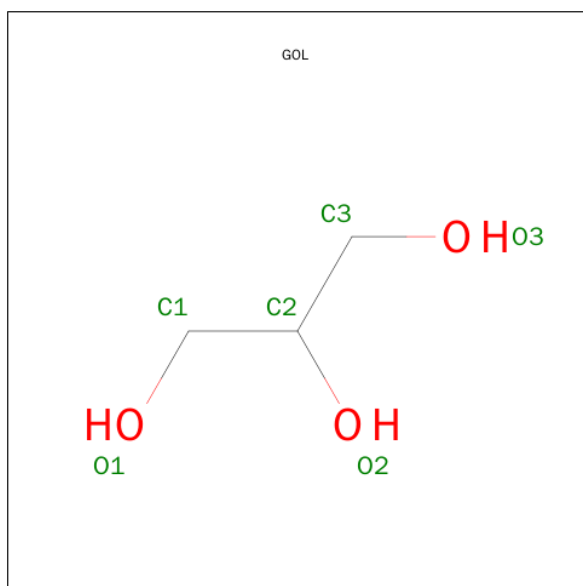
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	1	Total	K	0	0
			1	1		
5	B	1	Total	K	0	0
			1	1		
5	D	1	Total	K	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	F	1	Total K 1 1	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 6 3 3	0	0
6	C	1	Total C O 6 3 3	0	0
6	E	1	Total C O 6 3 3	0	0
6	G	1	Total C O 6 3 3	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	329	Total O 329 329	0	0
7	B	257	Total O 257 257	0	0
7	C	301	Total O 301 301	0	0
7	D	289	Total O 289 289	0	0

Continued on next page...

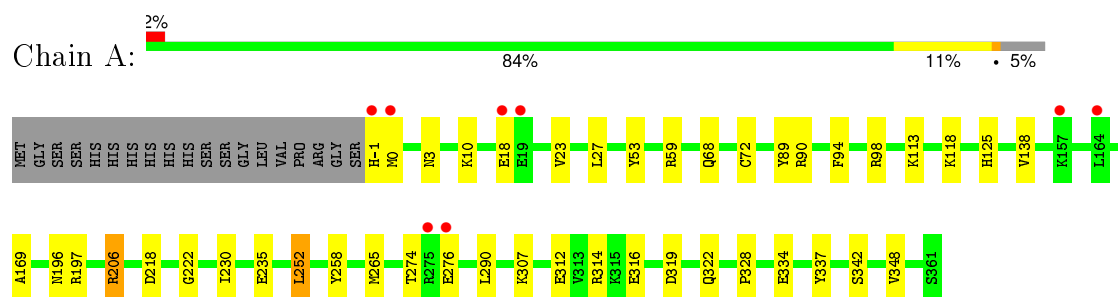
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	E	287	Total 287	O 287	0	0
7	F	255	Total 255	O 255	0	0
7	G	317	Total 317	O 317	0	0
7	H	281	Total 281	O 281	0	0

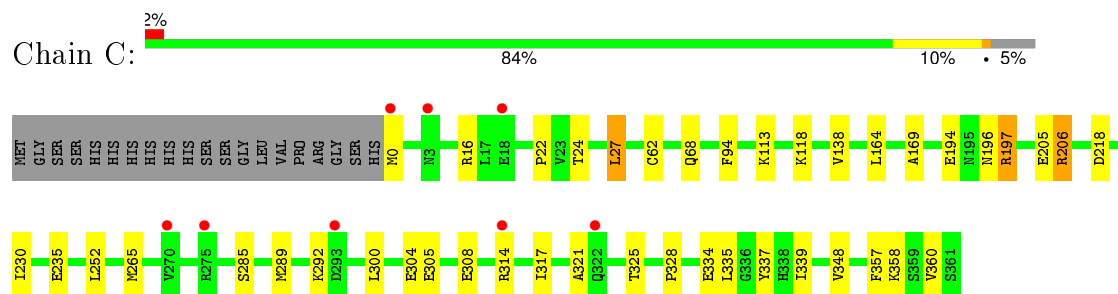
3 Residue-property plots

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.

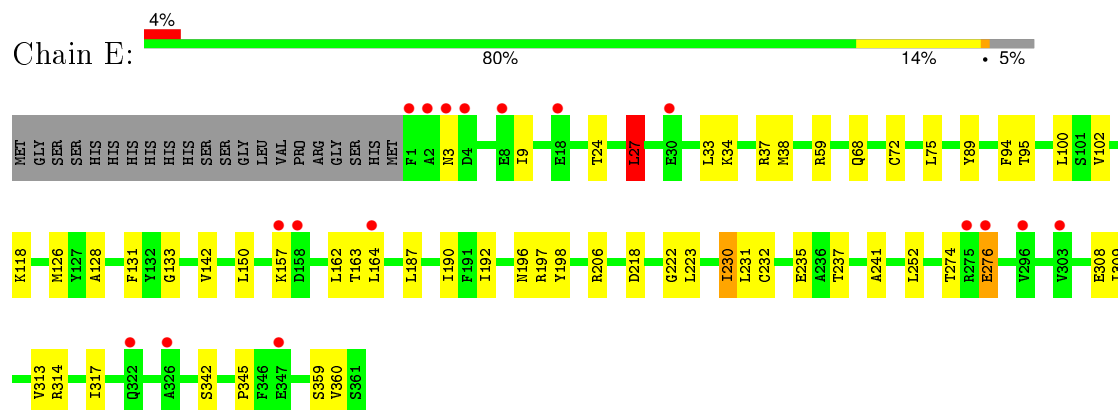
- Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha, somatic form, mitochondrial



- Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha, somatic form, mitochondrial

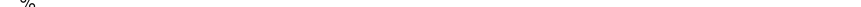


- Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha, somatic form, mitochondrial

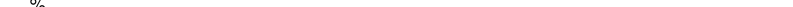



- Chain G:
-
- 83% 4% 10% 5%
- | Amino Acid | Frequency (%) |
|------------|---------------|
| MET | 0.1 |
| GLY | 0.1 |
| SER | 0.1 |
| SER | 0.1 |
| HIS | 0.1 |
| HIS | 0.1 |
| HIS | 0.1 |
| HIS | 0.1 |
| HIS | 0.1 |
| SER | 0.1 |
| SER | 0.1 |
| GLY | 0.1 |
| LEU | 0.1 |
| VAL | 0.1 |
| PRO | 0.1 |
| ARG | 0.1 |
| GLY | 0.1 |
| SER | 0.1 |
| HIS | 0.1 |
| NO | 0.1 |
| D4 | 0.1 |
| A5 | 0.1 |
| T6 | 0.1 |
| F7 | 0.1 |
| B8 | 0.1 |
| R16 | 0.1 |
| L17 | 0.1 |
| E18 | 0.1 |
| E19 | 0.1 |
| T24 | 0.1 |
| L27 | 0.1 |
| P39 | 0.1 |
| Q68 | 0.1 |
| B69 | 0.1 |
| L75 | 0.1 |
| Y89 | 0.1 |
| T95 | 0.1 |
| L100 | 0.1 |
| K113 | 0.1 |
| K118 | 0.1 |
| H128 | 0.1 |
| M126 | 0.1 |
| Y127 | 0.1 |
| L150 | 0.1 |
| K157 | 0.1 |
| D158 | 0.1 |
| L162 | 0.1 |
| T192 | 0.1 |
| M196 | 0.1 |
| E205 | 0.1 |
| R206 | 0.1 |
| R216 | 0.1 |
| G217 | 0.1 |
| D218 | 0.1 |
| G222 | 0.1 |
| T230 | 0.1 |
| T237 | 0.1 |
| L252 | 0.1 |
| V270 | 0.1 |
| T274 | 0.1 |
| R275 | 0.1 |
| E276 | 0.1 |
| Q279 | 0.1 |
| S283 | 0.1 |
| R284 | 0.1 |
| S285 | 0.1 |
| D286 | 0.1 |
| M289 | 0.1 |
| L300 | 0.1 |
| R314 | 0.1 |
| Q322 | 0.1 |
| P330 | 0.1 |
| P331 | 0.1 |
| L332 | 0.1 |
| E333 | 0.1 |
| E334 | 0.1 |
| L339 | 0.1 |
| S342 | 0.1 |
| D343 | 0.1 |
| E347 | 0.1 |
| V348 | 0.1 |
| W354 | 0.1 |
| S361 | 0.1 |

- Chain B:
-
- 2% 90% 9%
- L1 T4 D84 K38 R75 L107 I112 V113 F114 M118 F132 E151 M164 M172 M175 P179 F180 E181 F182 P183 A186 F191 L192 Q203 I207 R214 P215 S227 E232 M237 R242 M246 V260 T261 V262
- I279 V295 I313 F314 Q315 K325 L329

- Chain D: 

- Chain F:
-
- 91% 7% 2%
- Legend: Polar (Green), Non-polar (Yellow), Special (Orange)

- Chain H:  94% 5%
- 

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	103.57Å 129.62Å 124.30Å 90.00° 92.48° 90.00°	Depositor
Resolution (Å)	50.00 – 1.98 31.66 – 1.98	Depositor EDS
% Data completeness (in resolution range)	98.7 (50.00-1.98) 98.8 (31.66-1.98)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.4	Depositor
R, R_{free}	0.158 , 0.206 0.159 , 0.207	Depositor DCC
R_{free} test set	11272 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	19.6	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 47.0	EDS
Estimated twinning fraction	0.016 for -h,-l,-k 0.013 for -h,l,k 0.127 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 224961 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	23831	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% 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: GOL, K, MN, TPP

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	1.02	1/2893 (0.0%)	0.93	6/3895 (0.2%)
1	C	0.97	2/2879 (0.1%)	0.90	6/3877 (0.2%)
1	E	0.96	1/2874 (0.0%)	0.88	4/3870 (0.1%)
1	G	0.93	1/2882 (0.0%)	0.88	6/3880 (0.2%)
2	B	1.00	1/2574 (0.0%)	0.85	3/3488 (0.1%)
2	D	1.08	2/2574 (0.1%)	0.92	6/3488 (0.2%)
2	F	0.92	1/2574 (0.0%)	0.84	2/3488 (0.1%)
2	H	1.00	0/2574	0.85	1/3488 (0.0%)
All	All	0.99	9/21824 (0.0%)	0.88	34/29474 (0.1%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	250	GLU	CD-OE2	6.00	1.32	1.25
1	C	194	GLU	CG-CD	5.89	1.60	1.51
2	B	151	GLU	CB-CG	-5.83	1.41	1.52
2	F	169	VAL	CB-CG1	5.70	1.64	1.52
2	D	168	VAL	CB-CG2	5.39	1.64	1.52

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	206	ARG	NE-CZ-NH1	10.90	125.75	120.30
1	E	206	ARG	NE-CZ-NH2	-10.41	115.09	120.30
1	E	206	ARG	NE-CZ-NH1	10.41	125.51	120.30
1	A	206	ARG	NE-CZ-NH2	-10.19	115.21	120.30
2	D	214	ARG	NE-CZ-NH1	9.69	125.15	120.30

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	2836	0	2791	25	0
1	C	2823	0	2777	25	0
1	E	2818	0	2775	32	0
1	G	2826	0	2784	28	0
2	B	2519	0	2517	19	0
2	D	2519	0	2517	12	0
2	F	2519	0	2517	21	0
2	H	2519	0	2517	11	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
4	A	26	0	16	3	0
4	C	26	0	16	0	0
4	E	26	0	16	1	0
4	G	26	0	16	2	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
5	F	1	0	0	0	0
5	H	1	0	0	0	0
6	A	6	0	8	0	0
6	C	6	0	8	1	0
6	E	6	0	8	0	0
6	G	6	0	8	0	0
7	A	329	0	0	10	0
7	B	257	0	0	5	0
7	C	301	0	0	8	0
7	D	289	0	0	2	0
7	E	287	0	0	5	0
7	F	255	0	0	2	0
7	G	317	0	0	5	0
7	H	281	0	0	1	0
All	All	23831	0	21291	169	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 4.

The worst 5 of 169 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:319:ASP:HB2	7:A:4036:HOH:O	1.40	1.17
1:G:68:GLN:HE22	1:G:196:ASN:HD22	1.13	0.94
1:E:118:LYS:HE3	2:F:105:GLY:O	1.68	0.92
1:C:68:GLN:HE22	1:C:196:ASN:HD22	1.08	0.91
1:E:276:GLU:HG2	7:E:3567:HOH:O	1.72	0.90

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	361/382 (94%)	349 (97%)	11 (3%)	1 (0%)	46	39
1	C	360/382 (94%)	350 (97%)	9 (2%)	1 (0%)	46	39
1	E	359/382 (94%)	348 (97%)	10 (3%)	1 (0%)	46	39
1	G	360/382 (94%)	347 (96%)	12 (3%)	1 (0%)	46	39
2	B	327/329 (99%)	317 (97%)	10 (3%)	0	100	100
2	D	327/329 (99%)	316 (97%)	11 (3%)	0	100	100
2	F	327/329 (99%)	317 (97%)	10 (3%)	0	100	100
2	H	327/329 (99%)	316 (97%)	11 (3%)	0	100	100
All	All	2748/2844 (97%)	2660 (97%)	84 (3%)	4 (0%)	56	51

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	218	ASP
1	C	218	ASP
1	E	218	ASP
1	G	218	ASP

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	296/312 (95%)	289 (98%)	7 (2%)	57	55
1	C	294/312 (94%)	287 (98%)	7 (2%)	57	55
1	E	294/312 (94%)	285 (97%)	9 (3%)	47	43
1	G	295/312 (95%)	284 (96%)	11 (4%)	41	35
2	B	268/268 (100%)	263 (98%)	5 (2%)	65	65
2	D	268/268 (100%)	263 (98%)	5 (2%)	65	65
2	F	268/268 (100%)	259 (97%)	9 (3%)	44	39
2	H	268/268 (100%)	261 (97%)	7 (3%)	54	51
All	All	2251/2320 (97%)	2191 (97%)	60 (3%)	52	50

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	33	LEU
2	F	2	GLN
2	H	157	ILE
1	E	235	GLU
2	F	182	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	353	GLN
1	E	68	GLN
1	G	299	ASN
2	D	237	ASN
2	D	328	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	TPP	A	1005	3	20,27,27	1.20	2 (10%)	31,40,40	2.14	9 (29%)
6	GOL	A	1101	-	5,5,5	0.34	0	5,5,5	0.72	0
4	TPP	C	1002	3	20,27,27	1.49	4 (20%)	31,40,40	1.82	9 (29%)
6	GOL	C	1102	-	5,5,5	0.73	0	5,5,5	0.79	0
4	TPP	E	1011	3	20,27,27	1.81	6 (30%)	31,40,40	1.97	11 (35%)
6	GOL	E	1103	-	5,5,5	0.37	0	5,5,5	0.76	0
4	TPP	G	1008	3	20,27,27	1.38	5 (25%)	31,40,40	2.04	10 (32%)
6	GOL	G	1104	-	5,5,5	0.57	0	5,5,5	0.69	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	TPP	A	1005	3	-	0/16/17/17	0/2/2/2
6	GOL	A	1101	-	-	0/4/4/4	0/0/0/0
4	TPP	C	1002	3	-	0/16/17/17	0/2/2/2
6	GOL	C	1102	-	-	0/4/4/4	0/0/0/0
4	TPP	E	1011	3	-	0/16/17/17	0/2/2/2
6	GOL	E	1103	-	-	0/4/4/4	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	TPP	G	1008	3	-	0/16/17/17	0/2/2/2
6	GOL	G	1104	-	-	0/4/4/4	0/0/0/0

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1002	TPP	C4-N3	-3.57	1.36	1.39
4	E	1011	TPP	C4-N3	-3.32	1.36	1.39
4	G	1008	TPP	C7'-N3	-2.25	1.44	1.48
4	G	1008	TPP	PA-O2A	-2.09	1.46	1.54
4	E	1011	TPP	C7'-N3	-2.08	1.44	1.48

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1005	TPP	C5'-C7'-N3	-5.09	104.82	113.33
4	G	1008	TPP	C5'-C7'-N3	-5.06	104.88	113.33
4	C	1002	TPP	C5'-C7'-N3	-5.04	104.90	113.33
4	A	1005	TPP	N1'-C2'-N3'	-4.44	117.38	125.60
4	G	1008	TPP	N1'-C2'-N3'	-4.41	117.45	125.60

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1005	TPP	3	0
6	C	1102	GOL	1	0
4	E	1011	TPP	1	0
4	G	1008	TPP	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	363/382 (95%)	0.20	8 (2%) 65 68	9, 17, 26, 40	0
1	C	362/382 (94%)	0.31	8 (2%) 65 68	12, 17, 26, 34	0
1	E	361/382 (94%)	0.39	17 (4%) 35 39	12, 17, 26, 35	0
1	G	362/382 (94%)	0.21	15 (4%) 41 45	11, 17, 25, 33	0
2	B	329/329 (100%)	0.14	5 (1%) 76 79	12, 16, 25, 36	0
2	D	329/329 (100%)	0.11	4 (1%) 81 83	11, 16, 24, 34	0
2	F	329/329 (100%)	0.23	8 (2%) 62 66	10, 16, 24, 33	0
2	H	329/329 (100%)	0.08	4 (1%) 81 83	12, 16, 24, 31	0
All	All	2764/2844 (97%)	0.21	69 (2%) 61 64	9, 16, 26, 40	0

The worst 5 of 69 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	1	LEU	5.9
2	D	1	LEU	5.3
2	B	1	LEU	4.4
1	E	2	ALA	4.1
1	E	1	PHE	4.0

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 [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. 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
6	GOL	E	1103	6/6	0.86	0.30	9.73	35,40,42,43	0
6	GOL	A	1101	6/6	0.90	0.18	7.22	32,33,34,34	0
5	K	F	1009	1/1	0.98	0.28	6.02	40,40,40,40	0
5	K	B	1003	1/1	0.99	0.15	4.52	34,34,34,34	0
5	K	D	1006	1/1	0.98	0.21	4.13	27,27,27,27	0
6	GOL	C	1102	6/6	0.92	0.21	4.09	26,32,33,34	0
6	GOL	G	1104	6/6	0.90	0.18	3.87	31,35,37,40	0
5	K	H	1012	1/1	0.91	0.18	2.67	34,34,34,34	0
4	TPP	G	1008	26/26	0.98	0.09	-1.10	7,11,15,16	0
4	TPP	E	1011	26/26	0.97	0.09	-1.33	6,11,16,19	0
4	TPP	A	1005	26/26	0.97	0.09	-1.35	5,9,14,16	0
4	TPP	C	1002	26/26	0.97	0.08	-1.74	6,9,14,18	0
3	MN	C	1001	1/1	1.00	0.04	-3.59	10,10,10,10	0
3	MN	A	1004	1/1	1.00	0.04	-3.79	10,10,10,10	0
3	MN	G	1007	1/1	1.00	0.04	-4.13	12,12,12,12	0
3	MN	E	1010	1/1	0.99	0.05	-4.35	12,12,12,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.