



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 05:23 am GMT

PDB ID : 3DUF
Title : Snapshots of catalysis in the E1 subunit of the pyruvate dehydrogenase multi-enzyme complex
Authors : Pei, X.Y.; Titman, C.M.; Frank, R.A.W.; Leeper, F.J.; Luisi, B.F.
Deposited on : 2008-07-17
Resolution : 2.50 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

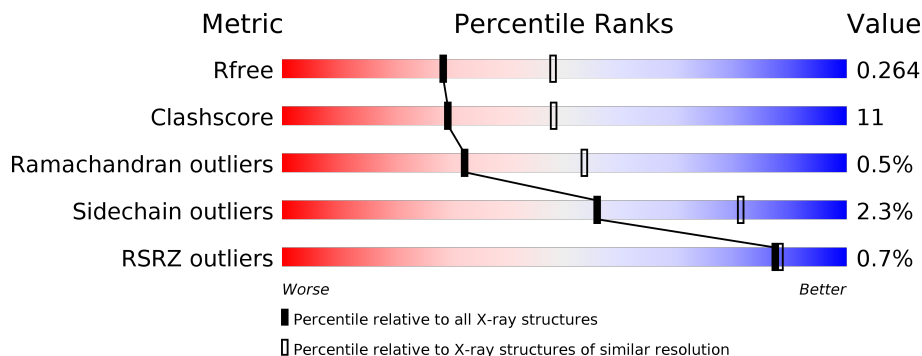
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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	369	<div> <div></div> <div>82%16%..</div> </div>
1	C	369	<div> <div>%</div> <div>81%17%..</div> </div>
1	E	369	<div> <div>2%</div> <div>75%22%..</div> </div>
1	G	369	<div> <div>%</div> <div>75%22%..</div> </div>
2	B	325	<div> <div></div> <div>81%18%. .</div> </div>
2	D	325	<div> <div>%</div> <div>83%16%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	325	<div> <div>%</div> <div> <div></div> <div>74%</div> <div>25%</div> </div> </div>
2	H	325	<div> <div></div> <div>78%</div> <div>21%</div> <div></div> </div>
3	I	428	<div> <div>5%</div> <div></div> <div>91%</div> </div>
3	J	428	<div> <div>%</div> <div>5%</div> <div></div> <div>92%</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
4	MG	D	1326	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 22480 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	365	Total	C	N	O	S	0	0	0
			2866	1832	488	538	8			
1	C	365	Total	C	N	O	S	0	0	0
			2845	1818	485	534	8			
1	E	365	Total	C	N	O	S	0	0	0
			2868	1832	488	540	8			
1	G	365	Total	C	N	O	S	0	0	0
			2881	1843	489	541	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	324	Total	C	N	O	S	0	0	0
			2488	1586	424	470	8			
2	D	324	Total	C	N	O	S	0	0	0
			2488	1586	424	470	8			
2	F	324	Total	C	N	O	S	0	0	0
			2486	1583	424	471	8			
2	H	324	Total	C	N	O	S	0	0	0
			2488	1586	424	470	8			

- Molecule 3 is a protein called Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	38	Total	C	N	O	S	0	0	0
			277	168	59	49	1			
3	J	36	Total	C	N	O	S	0	0	0
			263	160	51	51	1			

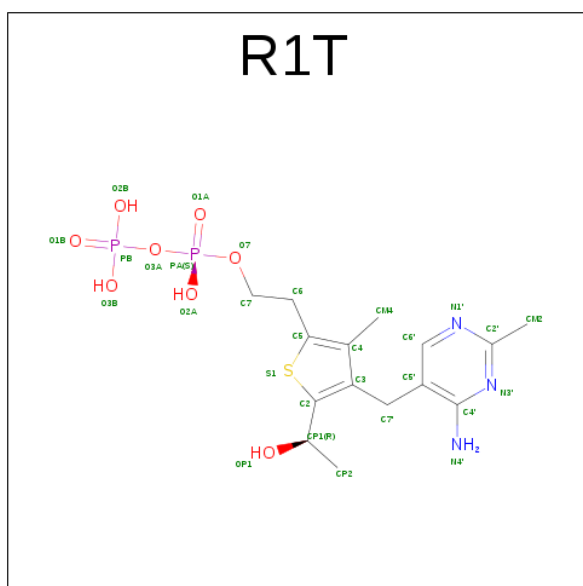
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total Mg 1 1	0	0
4	A	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0
4	E	1	Total Mg 1 1	0	0

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

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

- Molecule 6 is 2-{4-[(4-AMINO-2-METHYLPYRIMIDIN-5-YL)METHYL]-5-[(1R)-1-HYDROXYETHYL]-3-METHYL-2-THIENYL}ETHYL TRIHYDROGEN DIPHOSPHATE (three-letter code: R1T) (formula: C₁₅H₂₃N₃O₈P₂S).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	E	1	Total	C	N	O	P	S	
			29	15	3	8	2	1	
6	G	1	Total	C	N	O	P	S	
			29	15	3	8	2	1	

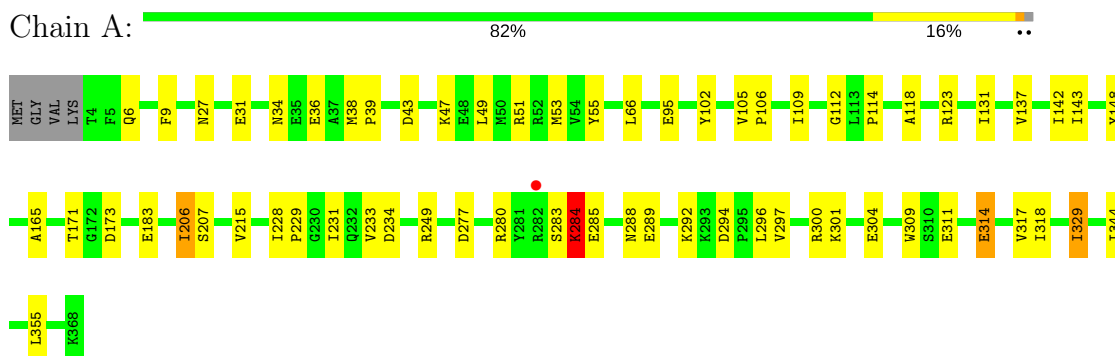
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	51	Total	O		
			51	51	0	0
7	B	43	Total	O		
			43	43	0	0
7	C	56	Total	O		
			56	56	0	0
7	D	48	Total	O		
			48	48	0	0
7	I	5	Total	O		
			5	5	0	0
7	E	54	Total	O		
			54	54	0	0
7	F	40	Total	O		
			40	40	0	0
7	G	47	Total	O		
			47	47	0	0
7	H	55	Total	O		
			55	55	0	0
7	J	8	Total	O		
			8	8	0	0

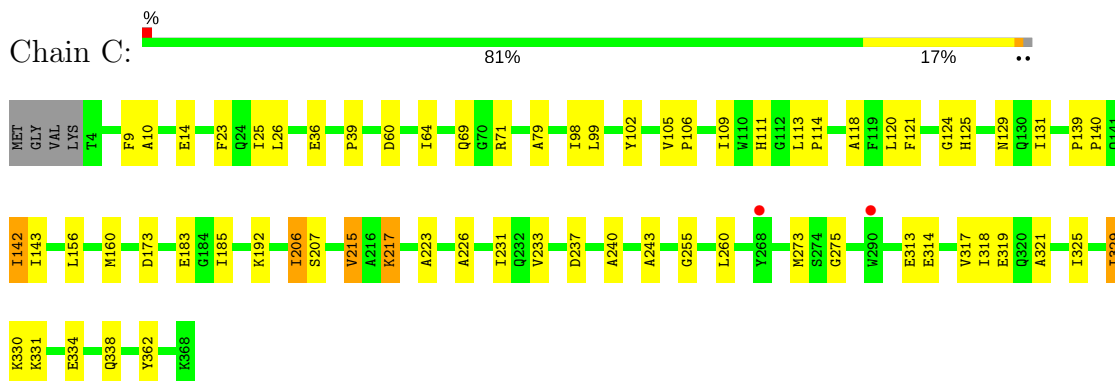
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

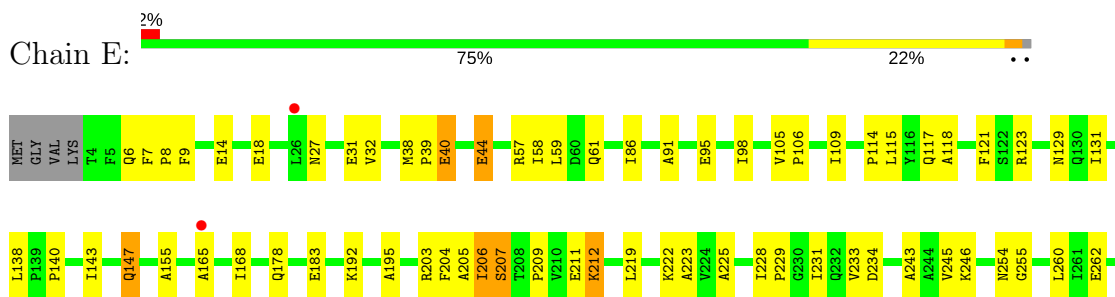
- Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha



- Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha

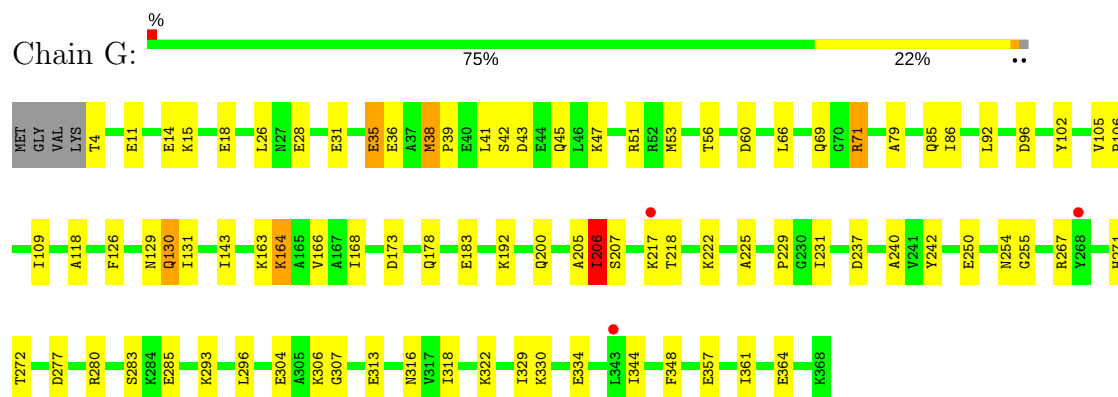


- Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha

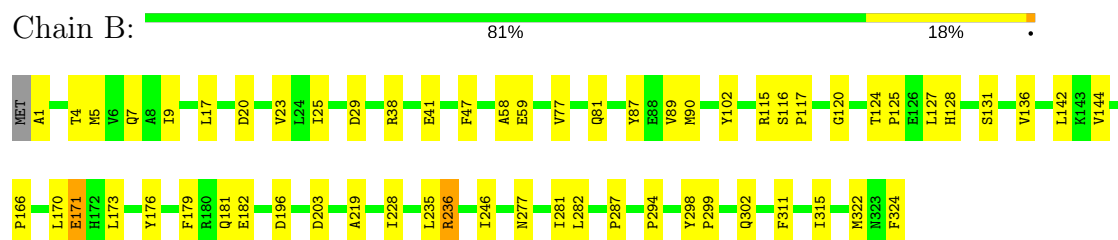




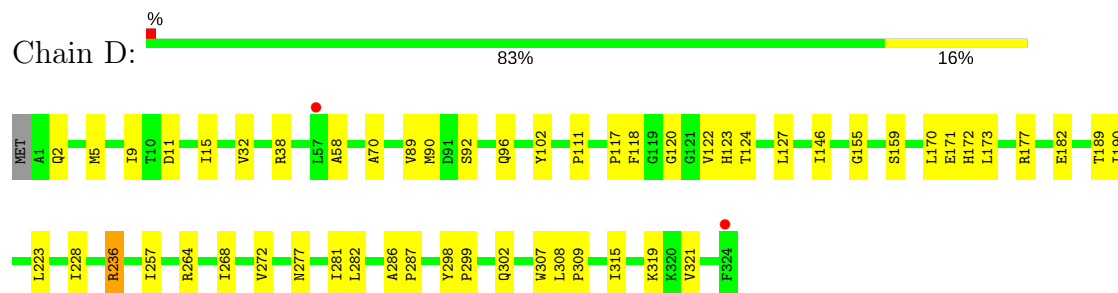
• Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha



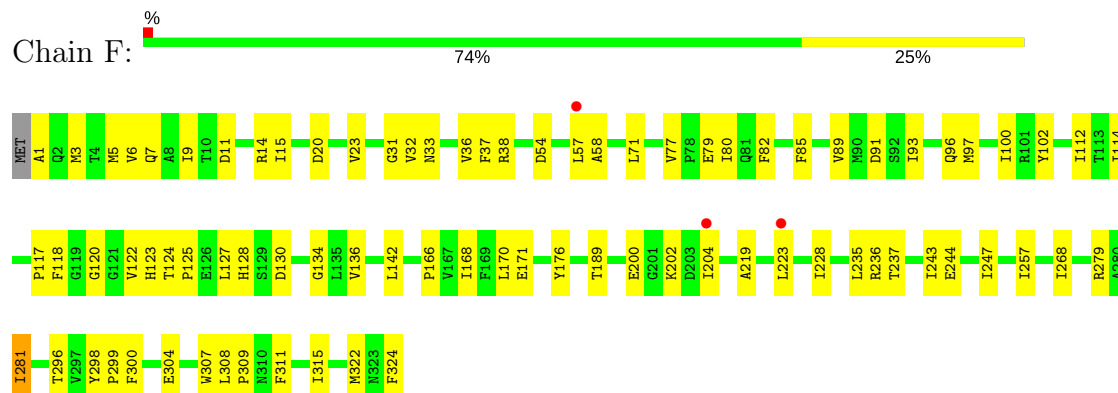
• Molecule 2: Pyruvate dehydrogenase E1 component subunit beta



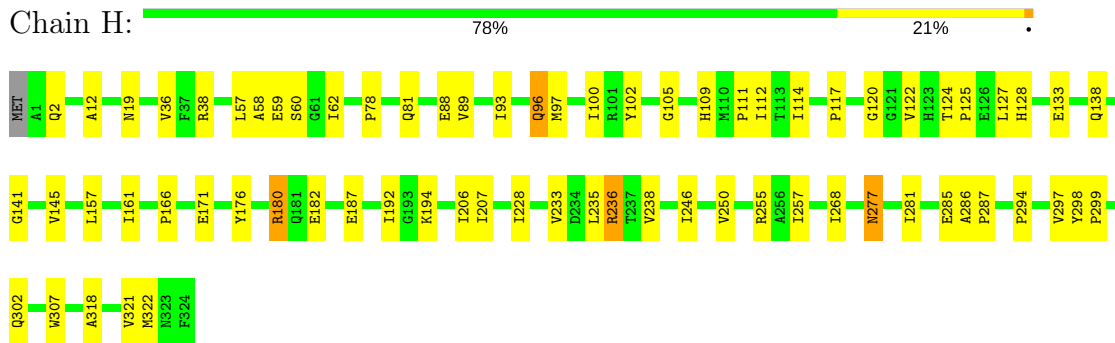
• Molecule 2: Pyruvate dehydrogenase E1 component subunit beta



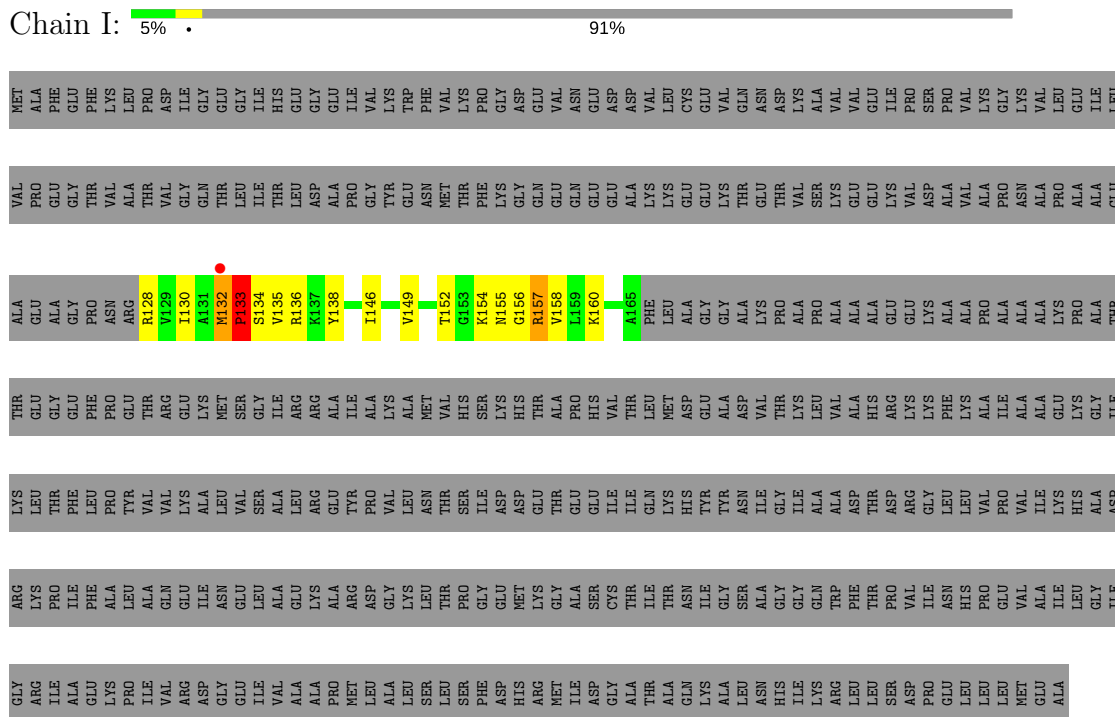
• Molecule 2: Pyruvate dehydrogenase E1 component subunit beta



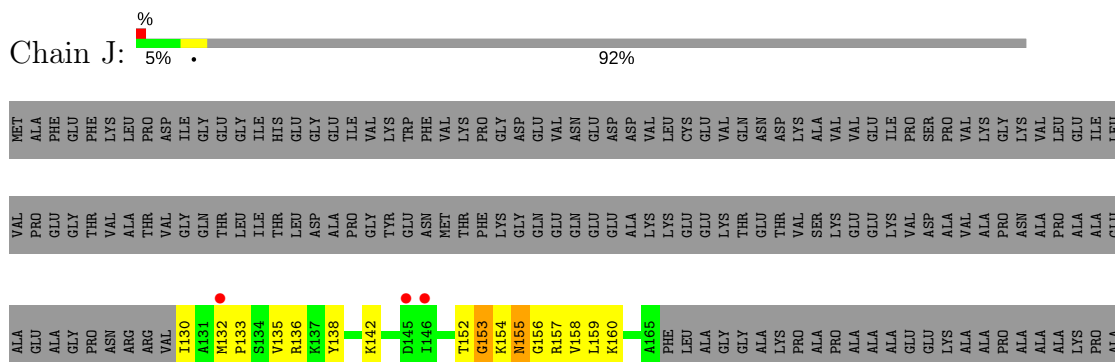
- Molecule 2: Pyruvate dehydrogenase E1 component subunit beta



- Molecule 3: Dihydrolipoylysine-residue acetyltransferase component of pyruvate dehydrogenase complex



- Molecule 3: Dihydrolipoylysine-residue acetyltransferase component of pyruvate dehydrogenase complex



ILE	ASP	ILE	THR
ARG	ARG	LYS	THR
GLY	LYS	LEU	GLU
ILE	PRO	THR	GLY
ILE	ILE	PHE	GLU
GLU	PHE	LEU	PHE
LYS	GLU	PRO	PRO
PRO	LEU	THR	GLU
ILE	ALA	VAL	THR
VAL	GLN	VAL	ARG
ARG	GLU	LYS	GLU
ASP	ILE	ALA	LYS
GLY	ASN	LEU	MET
GLU	GLU	VAL	SER
ILE	LEU	SER	GLY
VAL	ALA	ALA	ILE
ALA	GLU	LEU	ARG
ALA	LYS	ARG	ARG
PRO	ALA	GLU	ILE
MET	ARG	TYR	ILE
LEU	ASP	PRO	ALA
ALA	GLY	VAL	LYS
LEU	LYS	LEU	ALA
SER	LEU	ASN	MET
LEU	THR	THR	VAL
SER	PRO	SER	HIS
PHE	GLY	ILE	SER
ASP	GLU	ASP	LYS
HIS	MET	ASP	HIS
ARG	LYS	GLU	THR
MET	GLY	THR	ALA
ILE	ALA	GLU	PRO
ASP	SER	GLU	HIS
GLY	CYS	ILE	VAL
ALA	THR	ILE	THR
THR	ILE	GLN	LEU
THR	THR	LYS	MET
GLN	ASN	HIS	ASP
LYS	ILE	TYR	GLU
ALA	GLY	TYR	ALA
LEU	SER	ASN	ASP
ASN	ALA	ILE	VAL
HIS	GLY	GLY	THR
ILE	GLY	ILE	LYS
LYS	GLN	ALA	LEU
ARG	TRP	ALA	VAL
LEU	PHE	ASP	ALA
LEU	THR	THR	HIS
SER	PRO	ASP	ARG
ASP	VAL	ARG	LYS
PRO	ILE	GLY	LYS
GLU	ASN	LEU	PHE
LEU	HIS	LEU	LYS
LEU	PRO	VAL	ALA
LEU	GLU	PRO	ILE
MET	VAL	VAL	ILE
GLU	ALA	ILE	ALA
ALA	ILE	LYS	GLU
	LEU	HIS	GLY
	GLY	ALA	THR

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.25Å 232.00Å 92.61Å 90.00° 90.74° 90.00°	Depositor
Resolution (Å)	59.44 – 2.50 59.45 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.9 (59.44-2.50) 98.8 (59.45-2.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.25 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.188 , 0.263 0.189 , 0.264	Depositor DCC
R_{free} test set	5027 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	43.0	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 24.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.074 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	22480	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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: K, MG, R1T

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	0/2929	0.59	1/3961 (0.0%)
1	C	0.38	0/2908	0.57	0/3937
1	E	0.35	0/2930	0.57	2/3963 (0.1%)
1	G	0.37	0/2944	0.59	1/3980 (0.0%)
2	B	0.37	0/2534	0.64	1/3437 (0.0%)
2	D	0.39	0/2534	0.65	2/3437 (0.1%)
2	F	0.35	0/2532	0.61	0/3433
2	H	0.36	0/2534	0.62	2/3437 (0.1%)
3	I	0.32	0/278	0.67	0/369
3	J	0.30	0/264	0.76	1/351 (0.3%)
All	All	0.37	0/22387	0.60	10/30305 (0.0%)

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	207	SER	N-CA-CB	-7.11	99.84	110.50
1	A	284	LYS	CB-CA-C	-6.65	97.10	110.40
2	D	236	ARG	CB-CA-C	-6.55	97.30	110.40
2	B	236	ARG	CB-CA-C	-6.46	97.48	110.40
1	E	207	SER	N-CA-C	6.30	128.01	111.00

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	2866	0	2818	53	0
1	C	2845	0	2776	52	0
1	E	2868	0	2825	89	0
1	G	2881	0	2844	71	0
2	B	2488	0	2515	43	0
2	D	2488	0	2515	42	0
2	F	2486	0	2506	60	0
2	H	2488	0	2515	59	0
3	I	277	0	277	28	0
3	J	263	0	259	25	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
6	A	29	0	20	2	0
6	C	29	0	20	2	0
6	E	29	0	20	6	0
6	G	29	0	20	5	0
7	A	51	0	0	2	0
7	B	43	0	0	3	0
7	C	56	0	0	1	0
7	D	48	0	0	3	0
7	E	54	0	0	6	0
7	F	40	0	0	2	0
7	G	47	0	0	5	0
7	H	55	0	0	2	0
7	I	5	0	0	0	0
7	J	8	0	0	0	0
All	All	22480	0	21930	476	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 476 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)
6:E:1370:R1T:N4'	6:E:1370:R1T:HP22	1.35	1.41
6:E:1370:R1T:CP2	6:E:1370:R1T:H4'2	1.64	1.08
1:E:115:LEU:HD21	1:E:325:ILE:HD13	1.36	1.03
1:E:206:ILE:HG22	1:E:207:SER:H	1.23	1.01
1:E:143:ILE:HD11	2:H:127:LEU:HD13	1.45	0.98

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	363/369 (98%)	351 (97%)	10 (3%)	2 (1%)	28	48
1	C	363/369 (98%)	350 (96%)	11 (3%)	2 (1%)	28	48
1	E	363/369 (98%)	344 (95%)	17 (5%)	2 (1%)	28	48
1	G	363/369 (98%)	349 (96%)	13 (4%)	1 (0%)	44	66
2	B	322/325 (99%)	308 (96%)	13 (4%)	1 (0%)	44	66
2	D	322/325 (99%)	307 (95%)	14 (4%)	1 (0%)	44	66
2	F	322/325 (99%)	307 (95%)	13 (4%)	2 (1%)	28	48
2	H	322/325 (99%)	307 (95%)	15 (5%)	0	100	100
3	I	36/428 (8%)	29 (81%)	6 (17%)	1 (3%)	6	8
3	J	34/428 (8%)	31 (91%)	2 (6%)	1 (3%)	5	7
All	All	2810/3632 (77%)	2683 (96%)	114 (4%)	13 (0%)	32	53

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	284	LYS
2	B	236	ARG
3	I	133	PRO

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Mol	Chain	Res	Type
1	G	206	ILE
3	J	153	GLY

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	294/305 (96%)	289 (98%)	5 (2%)	66	87
1	C	289/305 (95%)	281 (97%)	8 (3%)	49	76
1	E	295/305 (97%)	286 (97%)	9 (3%)	45	73
1	G	297/305 (97%)	288 (97%)	9 (3%)	46	74
2	B	263/264 (100%)	258 (98%)	5 (2%)	62	85
2	D	263/264 (100%)	262 (100%)	1 (0%)	93	98
2	F	262/264 (99%)	256 (98%)	6 (2%)	56	81
2	H	263/264 (100%)	258 (98%)	5 (2%)	62	85
3	I	25/341 (7%)	21 (84%)	4 (16%)	3	5
3	J	25/341 (7%)	25 (100%)	0	100	100
All	All	2276/2958 (77%)	2224 (98%)	52 (2%)	56	81

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	6	GLN
1	E	254	ASN
2	H	81	GLN
1	E	40	GLU
1	E	147	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	315	ASN

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Mol	Chain	Res	Type
2	F	138	GLN
2	H	138	GLN
2	F	7	GLN
2	F	33	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 7 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	$\# Z > 2$
6	R1T	A	1370	4	25,30,30	1.10	1 (4%)	30,45,45	1.53	6 (20%)
6	R1T	C	1370	4	25,30,30	1.10	1 (4%)	30,45,45	1.53	4 (13%)
6	R1T	E	1370	4	25,30,30	6.06	12 (48%)	30,45,45	1.82	10 (33%)
6	R1T	G	1370	4	25,30,30	6.22	14 (56%)	30,45,45	1.62	8 (26%)

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
6	R1T	A	1370	4	-	0/16/21/21	0/2/2/2
6	R1T	C	1370	4	-	0/16/21/21	0/2/2/2
6	R1T	E	1370	4	-	0/16/21/21	0/2/2/2
6	R1T	G	1370	4	-	0/16/21/21	0/2/2/2

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	1370	R1T	C5-S1	-21.86	1.33	1.74
6	E	1370	R1T	C2-S1	-21.24	1.34	1.74
6	G	1370	R1T	C2-S1	-17.63	1.41	1.74
6	E	1370	R1T	C5-S1	-16.50	1.43	1.74
6	G	1370	R1T	C7'-C5'	-6.92	1.39	1.52

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	1370	R1T	O3A-PB-O1B	-3.67	88.86	111.44
6	G	1370	R1T	C5'-C6'-N1'	-3.59	117.80	123.87
6	E	1370	R1T	CP2-CP1-C2	-3.21	106.77	112.17
6	A	1370	R1T	N1'-C2'-N3'	-3.02	120.36	125.59
6	E	1370	R1T	C7'-C5'-C6'	-3.02	117.56	121.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1370	R1T	2	0
6	C	1370	R1T	2	0
6	E	1370	R1T	6	0
6	G	1370	R1T	5	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 [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	365/369 (98%)	-0.37	1 (0%) 93 94	24, 37, 63, 80	2 (0%)
1	C	365/369 (98%)	-0.36	2 (0%) 90 91	20, 37, 63, 90	2 (0%)
1	E	365/369 (98%)	-0.24	6 (1%) 72 73	24, 45, 75, 96	2 (0%)
1	G	365/369 (98%)	-0.28	3 (0%) 86 86	28, 42, 66, 81	2 (0%)
2	B	324/325 (99%)	-0.34	0 100 100	21, 38, 57, 65	0
2	D	324/325 (99%)	-0.38	2 (0%) 89 89	22, 34, 50, 61	0
2	F	324/325 (99%)	-0.20	3 (0%) 84 85	28, 43, 60, 69	0
2	H	324/325 (99%)	-0.31	0 100 100	24, 38, 53, 63	0
3	I	38/428 (8%)	0.26	1 (2%) 56 59	52, 68, 84, 93	0
3	J	36/428 (8%)	0.24	3 (8%) 12 12	54, 71, 89, 96	0
All	All	2830/3632 (77%)	-0.30	21 (0%) 87 88	20, 40, 65, 96	8 (0%)

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	132	MET	4.6
3	J	145	ASP	4.0
1	E	165	ALA	2.9
1	C	290	TRP	2.8
2	F	223	LEU	2.7

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 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
4	MG	D	1326	1/1	0.90	0.27	2.54	64,64,64,64	0
4	MG	C	1368	1/1	0.97	0.18	1.99	33,33,33,33	0
4	MG	A	1368	1/1	0.98	0.16	0.71	17,17,17,17	0
4	MG	E	1371	1/1	0.97	0.13	0.26	37,37,37,37	0
6	R1T	C	1370	29/29	0.98	0.16	0.21	19,31,38,43	0
5	K	D	1325	1/1	0.99	0.12	-0.16	32,32,32,32	0
6	R1T	A	1370	29/29	0.98	0.12	-0.51	15,27,37,43	0
6	R1T	E	1370	29/29	0.97	0.11	-0.75	25,36,50,54	0
6	R1T	G	1370	29/29	0.97	0.12	-0.78	20,34,45,63	0
5	K	B	1325	1/1	0.98	0.12	-0.91	52,52,52,52	0
4	MG	G	1371	1/1	0.96	0.08	-1.25	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.