



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 04:49 am GMT

PDB ID : 3MVQ
Title : Bovine Glutamate dehydrogenase complexed with zinc
Authors : Smith, T.J.; Li, M.
Deposited on : 2010-05-04
Resolution : 2.94 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

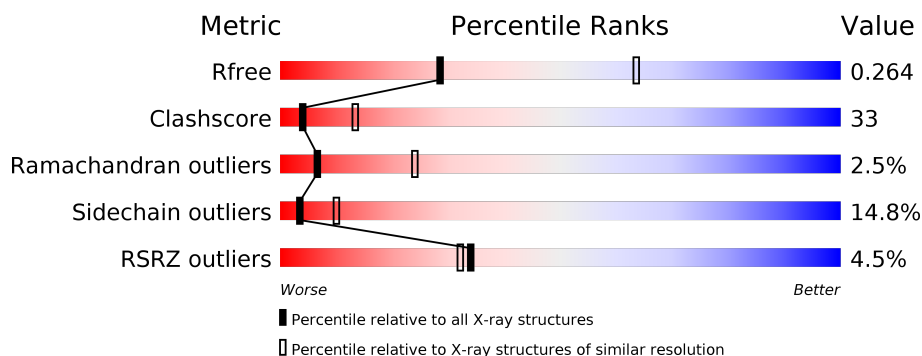
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.94 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	2289 (2.98-2.90)
Clashscore	112137	2543 (2.98-2.90)
Ramachandran outliers	110173	2475 (2.98-2.90)
Sidechain outliers	110143	2477 (2.98-2.90)
RSRZ outliers	101464	2301 (2.98-2.90)

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	501	<div> <div>4%</div> <div> <div>48%</div> <div>42%</div> <div>8%</div> </div> </div>
1	B	501	<div> <div>3%</div> <div> <div>46%</div> <div>44%</div> <div>9%</div> </div> </div>
1	C	501	<div> <div>7%</div> <div> <div>45%</div> <div>44%</div> <div>9%</div> </div> </div>
1	D	501	<div> <div>4%</div> <div> <div>49%</div> <div>41%</div> <div>8%</div> </div> </div>
1	E	501	<div> <div>4%</div> <div> <div>46%</div> <div>44%</div> <div>9%</div> </div> </div>
1	F	501	<div> <div>4%</div> <div> <div>45%</div> <div>45%</div> <div>10%</div> </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	GLU	C	502	-	-	X	-

2 Entry composition [i](#)

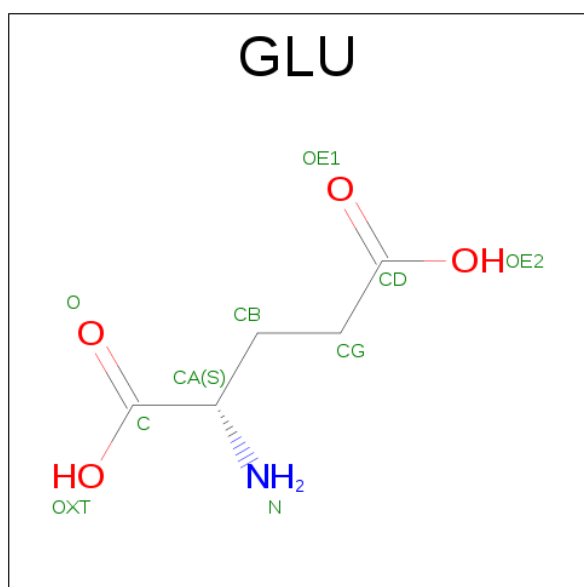
There are 5 unique types of molecules in this entry. The entry contains 23874 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glutamate dehydrogenase 1, mitochondrial.

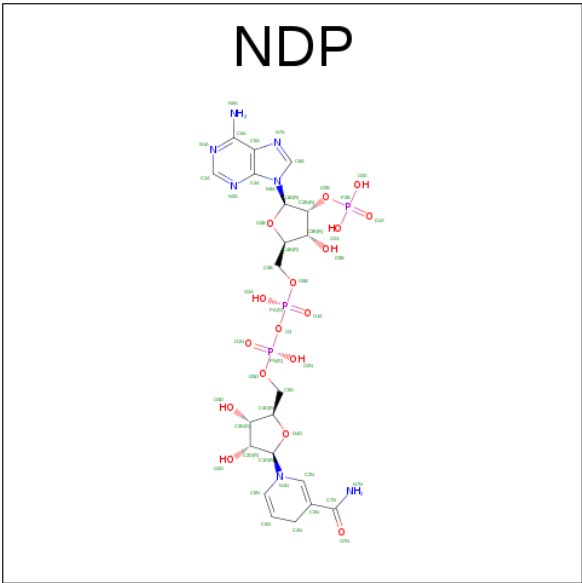
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	495	Total	C	N	O	S	0	0	0
			3880	2449	681	731	19			
1	B	495	Total	C	N	O	S	0	0	0
			3880	2449	681	731	19			
1	C	495	Total	C	N	O	S	0	0	0
			3880	2449	681	731	19			
1	D	495	Total	C	N	O	S	0	0	0
			3880	2449	681	731	19			
1	E	495	Total	C	N	O	S	0	0	0
			3880	2449	681	731	19			
1	F	501	Total	C	N	O	S	0	0	0
			3922	2476	687	740	19			

- Molecule 2 is GLUTAMIC ACID (three-letter code: GLU) (formula: C₅H₉NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	5	1	4		
2	B	1	Total	C	N	O	0	0
			10	5	1	4		
2	C	1	Total	C	N	O	0	0
			10	5	1	4		
2	D	1	Total	C	N	O	0	0
			10	5	1	4		
2	E	1	Total	C	N	O	0	0
			10	5	1	4		
2	F	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



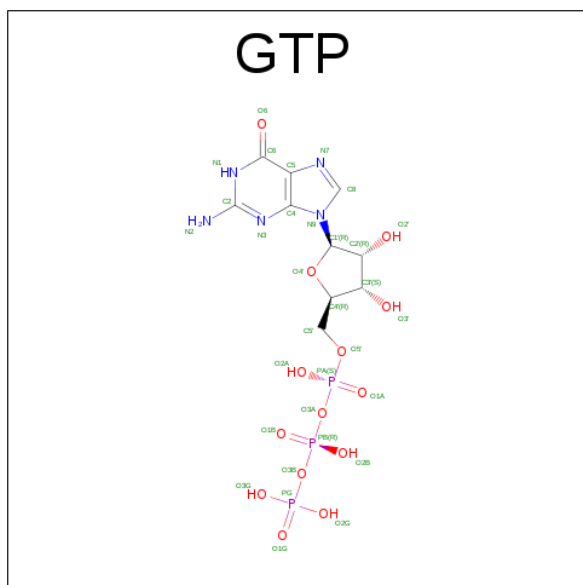
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	B	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	F	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	E	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	2	Total	Zn	0	0
			2	2		
5	E	2	Total	Zn	0	0
			2	2		

Continued on next page...

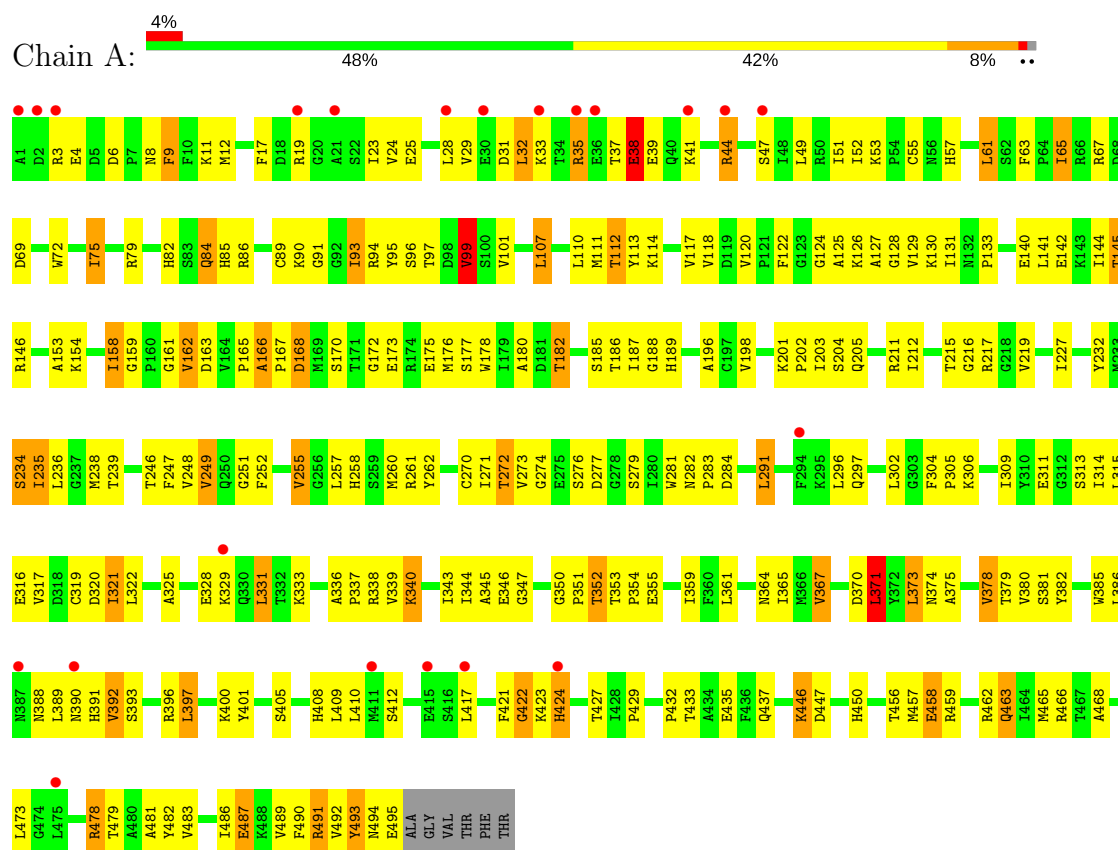
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total 2	Zn 2	0	0
5	C	3	Total 3	Zn 3	0	0
5	A	2	Total 2	Zn 2	0	0
5	F	1	Total 1	Zn 1	0	0

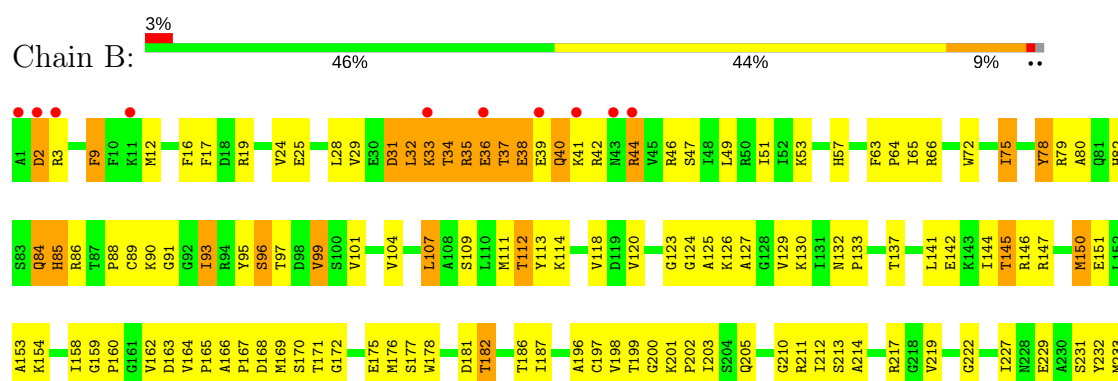
3 Residue-property plots

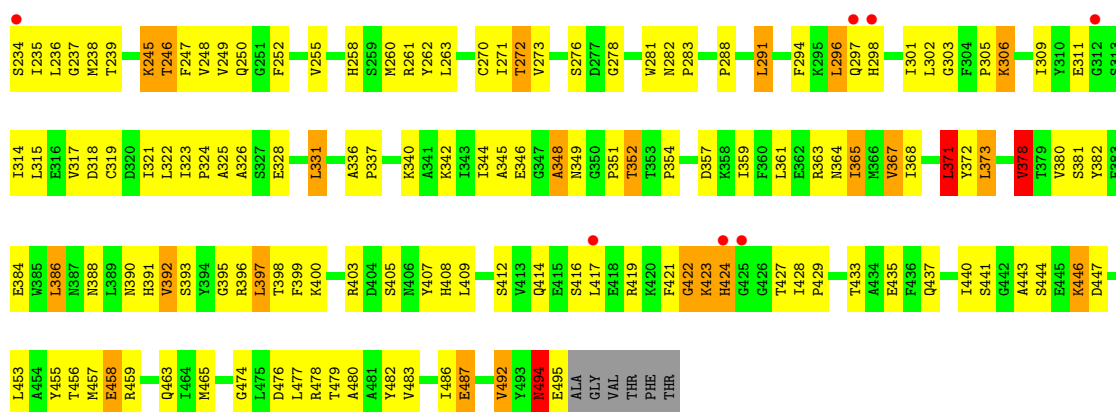
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Glutamate dehydrogenase 1, mitochondrial

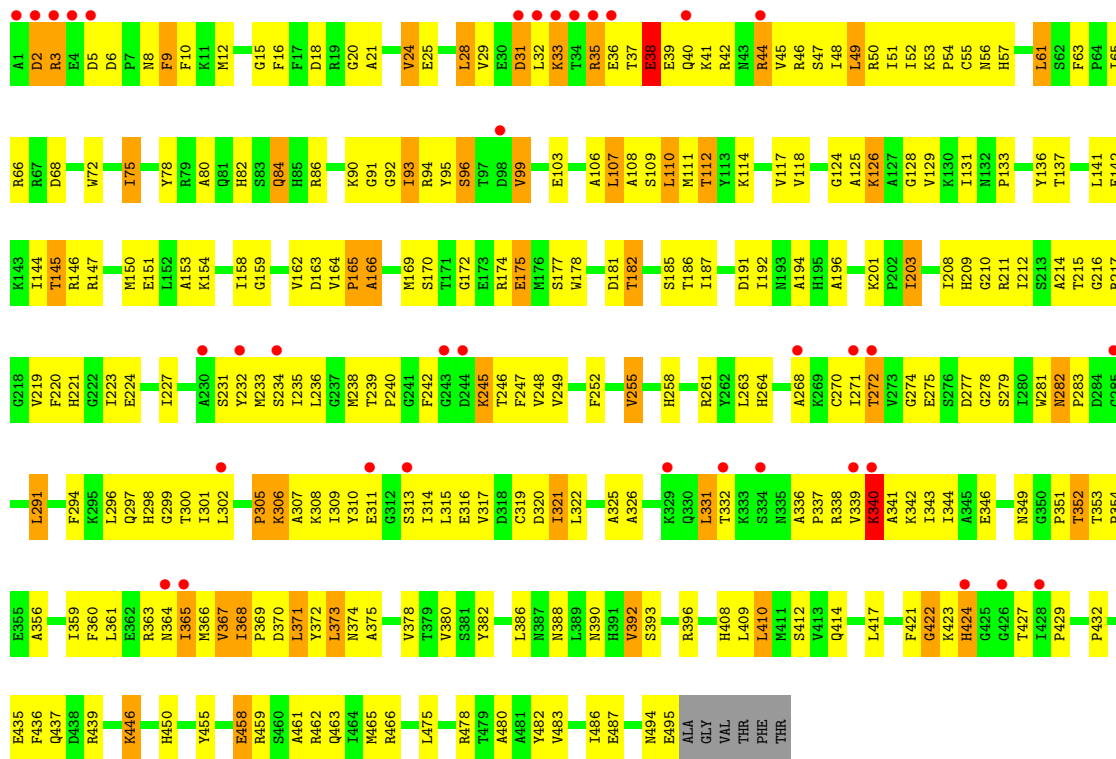


- Molecule 1: Glutamate dehydrogenase 1, mitochondrial

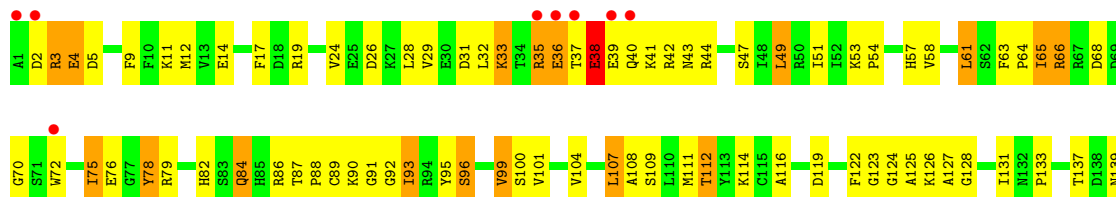


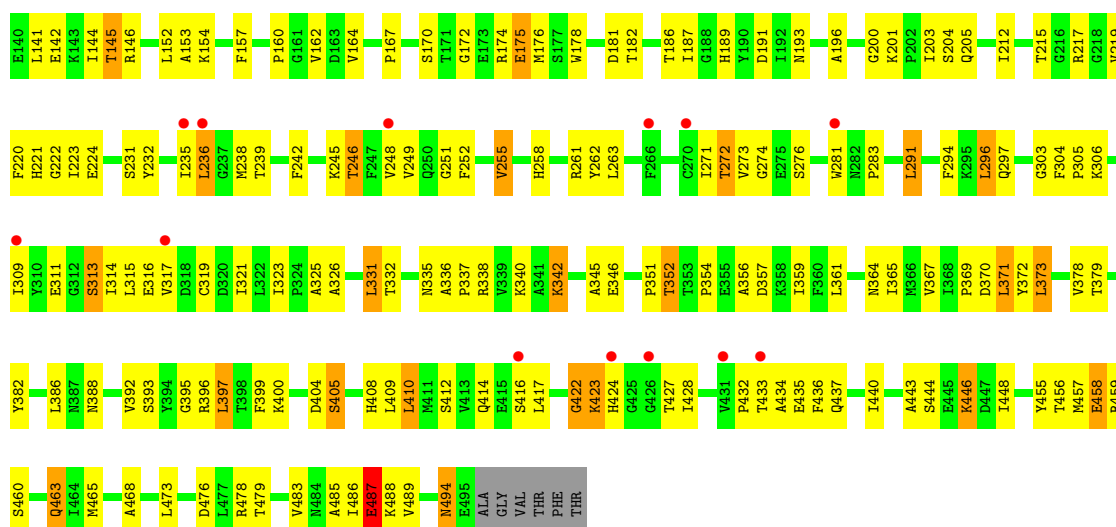


● Molecule 1: Glutamate dehydrogenase 1, mitochondrial



● Molecule 1: Glutamate dehydrogenase 1, mitochondrial

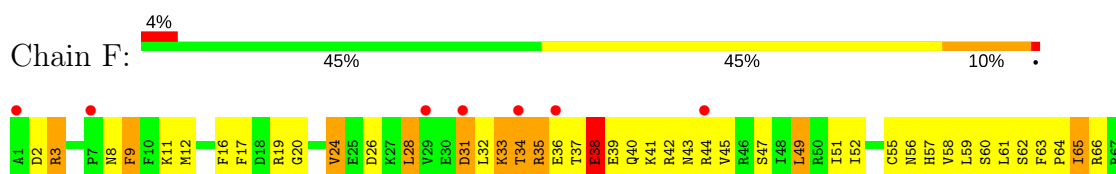




• Molecule 1: Glutamate dehydrogenase 1, mitochondrial



• Molecule 1: Glutamate dehydrogenase 1, mitochondrial



Y455	Y456	T457	V378	E311	V219	K143	D68
T456	V380	S313	I379	G312	I227	I144	W72
M457	S381	I314	S380	S313	T145	R146	I75
E458	Y382	L315	Y382	I314	R147	F148	E76
R459	F383	E316	F382	L315	A230	T149	G77
A461	E384	V317	E383	E316	Y232	M150	Y78
R462	W385	D318	F384	V317	W233	E151	R79
M465	L386	C319	W385	D318	S234	L152	H82
R466	N387	D320	N386	C319	L236	A153	S83
L476	N388	I321	N387	D320	T239	I158	O84
R478	V392	L322	V392	I321	F242	G159	H85
T479	S393	A325	S393	L322	G243	V162	R86
T479	G395	E328	G395	A325	D244	D163	C89
A480	R396	L331	R396	E328	K245	V164	K90
A481	L397	A336	L397	L331	T246	P165	G91
A482	T398	P337	T398	A336	F247	A166	G92
V483	F399	R338	F399	P337	V249	P167	I93
I486	K400	V339	K400	R338	F252	S170	R94
E487	Y401	K340	Y401	V339	V255	T171	Y95
R491	R403	A341	R403	K340	G256	G172	S96
M494	H408	K342	M494	A341	H258	E173	T97
E495	L409	I343	E495	K342	R261	R174	D98
A496	L410	I344	A496	I343	V262	E175	Y99
C497	M411	A345	C497	I344	L263	M176	S100
V498	S412	E346	V498	A345	H264	S177	V101
T499	S416	C347	T499	E346	C270	W178	E103
F500	L417	N349	F500	C347	L271	D181	L107
T501	E418	G350	T501	N349	T272	T182	A108
	R419	P351		G350	V273	I186	S109
	K420	T352		P351		I187	L110
	F421	T353		T352		G188	M111
	G422	P354		T353		H189	T112
	K423	D357		P354		A196	Y113
	H424	K358		D357		C197	K114
	G425	I359		K358		V198	V117
	T427	F360		I359		T199	V118
	T428	L361		F360		G200	G123
	P429	E362		L361		K201	G124
	T430	N363		E362		P202	A125
	V431	I365		N363		I203	K126
	P432	M366		I365		S204	A127
	T433	V367		M366		G128	G128
	A434	I368		V367		V129	V129
	E435	P369		I368		K130	K130
	F436	D370		P369		R211	I131
	Q437	Y371		D370		I212	N132
	D438	Y372		Y371		S213	P133
	R439	L373		Y372		A214	A214
	K445	N374		L373		T215	T137
	D447	A375		N374		G216	L141
	I448			A375		R217	L141
						G218	E142

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	121.11Å 98.76Å 165.64Å 90.00° 101.55° 90.00°	Depositor
Resolution (Å)	45.88 – 2.94 47.44 – 2.94	Depositor EDS
% Data completeness (in resolution range)	92.9 (45.88-2.94) 93.0 (47.44-2.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.76 (at 2.96Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_353)	Depositor
R, R_{free}	0.223 , 0.262 0.203 , 0.264	Depositor DCC
R_{free} test set	3821 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	34.5	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 35.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	23874	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, NDP, ZN

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	0.46	0/3962	0.65	0/5348
1	B	0.46	0/3962	0.64	1/5348 (0.0%)
1	C	0.46	0/3962	0.63	0/5348
1	D	0.48	0/3962	0.63	0/5348
1	E	0.47	0/3962	0.63	0/5348
1	F	0.48	0/4005	0.65	0/5406
All	All	0.47	0/23815	0.64	1/32146 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	378	VAL	CB-CA-C	-5.01	101.88	111.40

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	3880	0	3843	281	0
1	B	3880	0	3843	278	0
1	C	3880	0	3843	292	0
1	D	3880	0	3843	237	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3880	0	3843	274	0
1	F	3922	0	3883	282	0
2	A	10	0	5	3	0
2	B	10	0	5	3	0
2	C	10	0	5	5	0
2	D	10	0	5	1	0
2	E	10	0	5	3	0
2	F	10	0	5	2	0
3	A	48	0	26	4	0
3	B	48	0	26	7	0
3	C	48	0	26	5	0
3	D	48	0	26	3	0
3	E	48	0	26	5	0
3	F	48	0	26	5	0
4	A	32	0	12	1	0
4	B	32	0	12	0	0
4	C	32	0	12	1	0
4	D	32	0	12	0	0
4	E	32	0	12	1	0
4	F	32	0	12	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	3	0	0	0	0
5	D	2	0	0	0	0
5	E	2	0	0	0	0
5	F	1	0	0	0	0
All	All	23874	0	23356	1557	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 33.

The worst 5 of 1557 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:F:93:ILE:HD11	1:F:95:TYR:CE1	1.78	1.18
1:C:38:GLU:HG2	1:C:39:GLU:N	1.58	1.13
1:D:392:VAL:HG11	1:D:397:LEU:HD11	1.27	1.12
1:F:38:GLU:HG2	1:F:39:GLU:H	1.00	1.09
1:E:38:GLU:HG2	1:E:39:GLU:H	0.96	1.09

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	493/501 (98%)	428 (87%)	52 (10%)	13 (3%)	6	23
1	B	493/501 (98%)	429 (87%)	49 (10%)	15 (3%)	5	19
1	C	493/501 (98%)	424 (86%)	55 (11%)	14 (3%)	6	21
1	D	493/501 (98%)	427 (87%)	57 (12%)	9 (2%)	10	33
1	E	493/501 (98%)	427 (87%)	56 (11%)	10 (2%)	9	30
1	F	499/501 (100%)	424 (85%)	62 (12%)	13 (3%)	6	23
All	All	2964/3006 (99%)	2559 (86%)	331 (11%)	74 (2%)	6	24

5 of 74 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	GLU
1	A	371	LEU
1	B	34	THR
1	B	37	THR
1	B	38	GLU

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	416/420 (99%)	356 (86%)	60 (14%)	4	10
1	B	416/420 (99%)	353 (85%)	63 (15%)	3	9
1	C	416/420 (99%)	358 (86%)	58 (14%)	4	12

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	416/420 (99%)	352 (85%)	64 (15%)	3	9
1	E	416/420 (99%)	355 (85%)	61 (15%)	3	10
1	F	420/420 (100%)	356 (85%)	64 (15%)	3	9
All	All	2500/2520 (99%)	2130 (85%)	370 (15%)	3	10

5 of 370 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	367	VAL
1	D	212	ILE
1	F	306	LYS
1	C	386	LEU
1	D	38	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	258	HIS
1	D	388	ASN
1	F	388	ASN
1	C	388	ASN
1	D	82	HIS

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

Of 30 ligands modelled in this entry, 12 are monoatomic - leaving 18 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$
2	GLU	A	502	-	1,9,9	0.31	0	1,11,11	0.38	0
4	GTP	A	503	5	27,34,34	1.31	3 (11%)	27,54,54	2.02	7 (25%)
3	NDP	A	552	-	43,52,52	1.49	5 (11%)	49,80,80	1.63	4 (8%)
2	GLU	B	502	-	1,9,9	0.23	0	1,11,11	0.10	0
4	GTP	B	503	5	27,34,34	1.10	2 (7%)	27,54,54	2.06	9 (33%)
3	NDP	B	552	-	43,52,52	1.55	4 (9%)	49,80,80	1.76	2 (4%)
2	GLU	C	502	-	1,9,9	0.55	0	1,11,11	0.29	0
4	GTP	C	503	5	27,34,34	0.94	1 (3%)	27,54,54	1.69	4 (14%)
3	NDP	C	552	-	43,52,52	1.60	4 (9%)	49,80,80	1.66	2 (4%)
2	GLU	D	502	-	1,9,9	0.08	0	1,11,11	0.67	0
4	GTP	D	503	5	27,34,34	0.96	1 (3%)	27,54,54	1.74	6 (22%)
3	NDP	D	552	-	43,52,52	1.52	4 (9%)	49,80,80	1.72	4 (8%)
2	GLU	E	502	-	1,9,9	0.20	0	1,11,11	0.10	0
4	GTP	E	503	5	27,34,34	1.04	2 (7%)	27,54,54	1.95	8 (29%)
3	NDP	E	552	-	43,52,52	1.56	5 (11%)	49,80,80	1.75	3 (6%)
2	GLU	F	502	-	1,9,9	0.40	0	1,11,11	0.17	0
4	GTP	F	503	5	27,34,34	1.00	1 (3%)	27,54,54	1.80	6 (22%)
3	NDP	F	552	-	43,52,52	1.50	3 (6%)	49,80,80	1.66	2 (4%)

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
2	GLU	A	502	-	-	0/3/9/9	0/0/0/0
4	GTP	A	503	5	-	0/18/38/38	0/3/3/3
3	NDP	A	552	-	-	0/30/77/77	0/5/5/5
2	GLU	B	502	-	-	0/3/9/9	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GTP	B	503	5	-	0/18/38/38	0/3/3/3
3	NDP	B	552	-	-	0/30/77/77	0/5/5/5
2	GLU	C	502	-	-	0/3/9/9	0/0/0/0
4	GTP	C	503	5	-	0/18/38/38	0/3/3/3
3	NDP	C	552	-	-	0/30/77/77	0/5/5/5
2	GLU	D	502	-	-	0/3/9/9	0/0/0/0
4	GTP	D	503	5	-	0/18/38/38	0/3/3/3
3	NDP	D	552	-	-	0/30/77/77	0/5/5/5
2	GLU	E	502	-	-	0/3/9/9	0/0/0/0
4	GTP	E	503	5	-	0/18/38/38	0/3/3/3
3	NDP	E	552	-	-	0/30/77/77	0/5/5/5
2	GLU	F	502	-	-	0/3/9/9	0/0/0/0
4	GTP	F	503	5	-	0/18/38/38	0/3/3/3
3	NDP	F	552	-	-	0/30/77/77	0/5/5/5

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	GTP	O4'-C4'	-2.31	1.39	1.45
4	B	503	GTP	C2-N1	2.01	1.39	1.35
3	A	552	NDP	C2N-C3N	2.06	1.40	1.34
4	E	503	GTP	C2-N1	2.06	1.39	1.35
3	E	552	NDP	C2N-C3N	2.15	1.41	1.34

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	552	NDP	N3A-C2A-N1A	-10.62	119.61	128.86
3	E	552	NDP	N3A-C2A-N1A	-10.26	119.92	128.86
3	D	552	NDP	N3A-C2A-N1A	-9.94	120.20	128.86
3	F	552	NDP	N3A-C2A-N1A	-9.73	120.39	128.86
3	C	552	NDP	N3A-C2A-N1A	-9.63	120.47	128.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	502	GLU	3	0
4	A	503	GTP	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	552	NDP	4	0
2	B	502	GLU	3	0
3	B	552	NDP	7	0
2	C	502	GLU	5	0
4	C	503	GTP	1	0
3	C	552	NDP	5	0
2	D	502	GLU	1	0
3	D	552	NDP	3	0
2	E	502	GLU	3	0
4	E	503	GTP	1	0
3	E	552	NDP	5	0
2	F	502	GLU	2	0
3	F	552	NDP	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	495/501 (98%)	0.13	22 (4%) 35 33	15, 32, 68, 127	0
1	B	495/501 (98%)	0.13	17 (3%) 46 43	17, 34, 71, 128	0
1	C	495/501 (98%)	0.28	36 (7%) 16 13	18, 38, 71, 129	0
1	D	495/501 (98%)	0.10	21 (4%) 37 34	15, 32, 71, 131	0
1	E	495/501 (98%)	0.12	20 (4%) 39 37	16, 32, 71, 126	0
1	F	501/501 (100%)	-0.03	19 (3%) 41 39	14, 29, 73, 130	0
All	All	2976/3006 (99%)	0.12	135 (4%) 34 32	14, 32, 72, 131	0

The worst 5 of 135 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	424	HIS	8.1
1	B	2	ASP	7.5
1	C	3	ARG	7.2
1	E	424	HIS	7.0
1	F	424	HIS	6.5

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

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	GLU	F	502	10/10	0.95	0.19	1.36	19,20,26,26	0
2	GLU	D	502	10/10	0.94	0.19	0.96	20,24,26,33	0
2	GLU	C	502	10/10	0.95	0.17	0.68	25,31,33,34	0
2	GLU	B	502	10/10	0.95	0.17	0.26	22,26,31,31	0
5	ZN	C	506	1/1	0.96	0.19	0.03	46,46,46,46	0
2	GLU	E	502	10/10	0.94	0.17	-0.23	20,29,33,35	0
3	NDP	A	552	48/48	0.96	0.16	-0.30	18,27,36,44	0
2	GLU	A	502	10/10	0.95	0.16	-0.38	19,26,31,31	0
5	ZN	B	505	1/1	0.97	0.17	-0.41	43,43,43,43	0
5	ZN	F	504	1/1	0.97	0.18	-0.43	37,37,37,37	0
3	NDP	D	552	48/48	0.97	0.15	-0.45	17,27,38,46	0
3	NDP	F	552	48/48	0.97	0.15	-0.49	14,21,32,35	0
3	NDP	C	552	48/48	0.94	0.17	-0.58	23,39,55,60	0
3	NDP	B	552	48/48	0.97	0.14	-0.58	24,32,39,42	0
5	ZN	D	505	1/1	0.95	0.15	-0.70	42,42,42,42	0
4	GTP	D	503	32/32	0.96	0.16	-0.80	19,33,40,42	0
3	NDP	E	552	48/48	0.95	0.15	-0.98	22,30,44,54	0
4	GTP	E	503	32/32	0.96	0.15	-1.07	16,27,33,38	0
4	GTP	B	503	32/32	0.96	0.14	-1.25	24,36,43,48	0
4	GTP	A	503	32/32	0.96	0.14	-1.27	24,34,37,44	0
4	GTP	C	503	32/32	0.94	0.15	-1.44	27,41,51,62	0
4	GTP	F	503	32/32	0.97	0.12	-1.98	18,23,35,45	0
5	ZN	E	505	1/1	0.93	0.13	-2.13	37,37,37,37	0
5	ZN	A	505	1/1	0.98	0.11	-2.61	31,31,31,31	0
5	ZN	C	504	1/1	0.95	0.06	-3.74	63,63,63,63	0
5	ZN	C	505	1/1	0.95	0.05	-4.41	55,55,55,55	0
5	ZN	D	504	1/1	0.92	0.08	-	65,65,65,65	0
5	ZN	B	504	1/1	0.97	0.04	-	64,64,64,64	0
5	ZN	E	504	1/1	0.99	0.07	-	50,50,50,50	0
5	ZN	A	504	1/1	0.95	0.08	-	58,58,58,58	0

6.5 Other polymers

There are no such residues in this entry.