



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:43 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

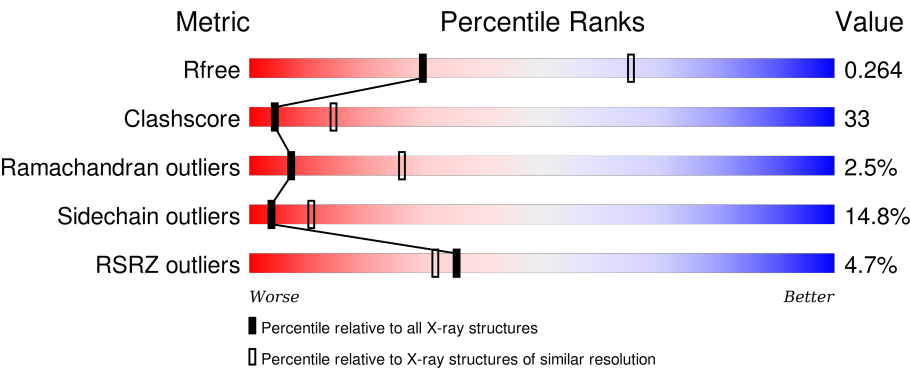
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.94 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}	91344	2057 (2.98-2.90)
Clashscore	102246	2308 (2.98-2.90)
Ramachandran outliers	100387	2245 (2.98-2.90)
Sidechain outliers	100360	2247 (2.98-2.90)
RSRZ outliers	91569	2065 (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	
1	B	501	
1	C	501	
1	D	501	
1	E	501	

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Mol	Chain	Length	Quality of chain
1	F	501	

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](#)

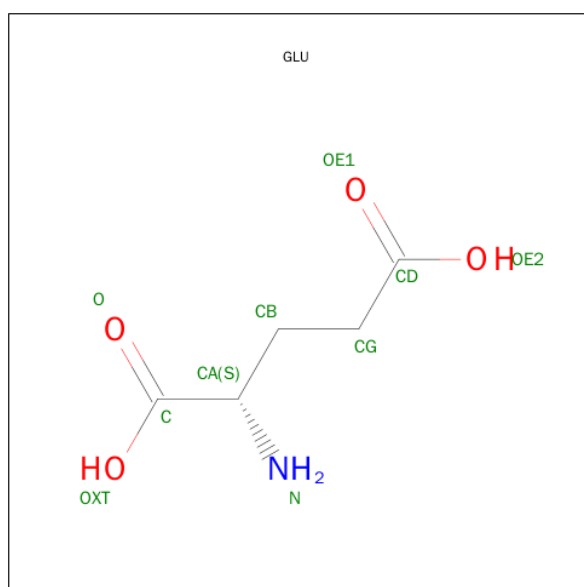
There are 5 unique types of molecules in this entry. The entry contains 23874 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

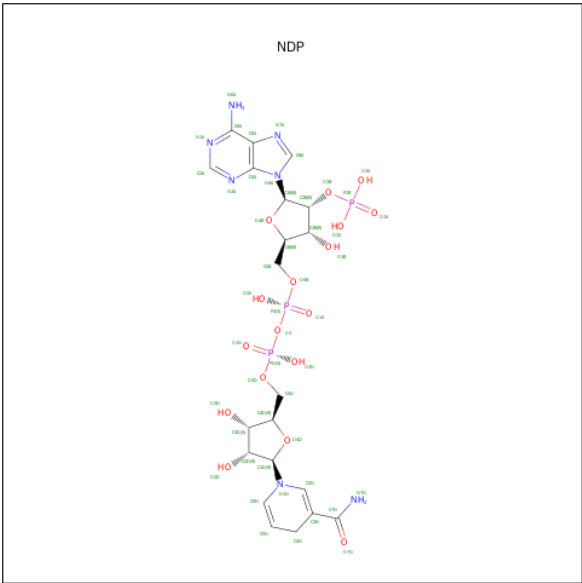
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	495	Total	C	N	O	S	0	0	0
			3880	2449	681	731	19			
1	B	495	Total	C	N	O	S	0	0	0
			3880	2449	681	731	19			
1	C	495	Total	C	N	O	S	0	0	0
			3880	2449	681	731	19			
1	D	495	Total	C	N	O	S	0	0	0
			3880	2449	681	731	19			
1	E	495	Total	C	N	O	S	0	0	0
			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).



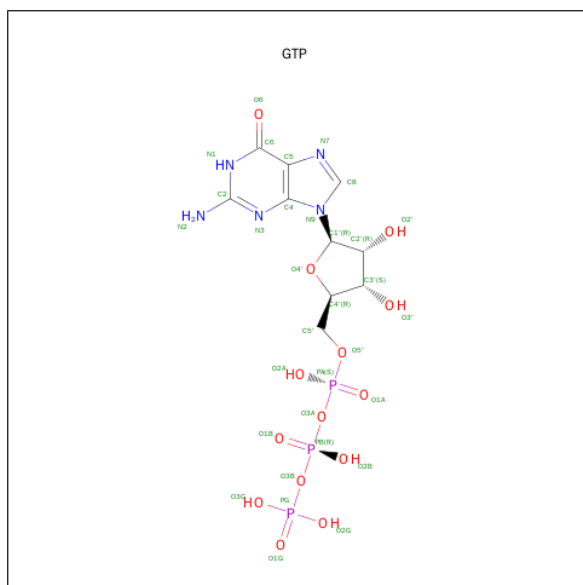
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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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		

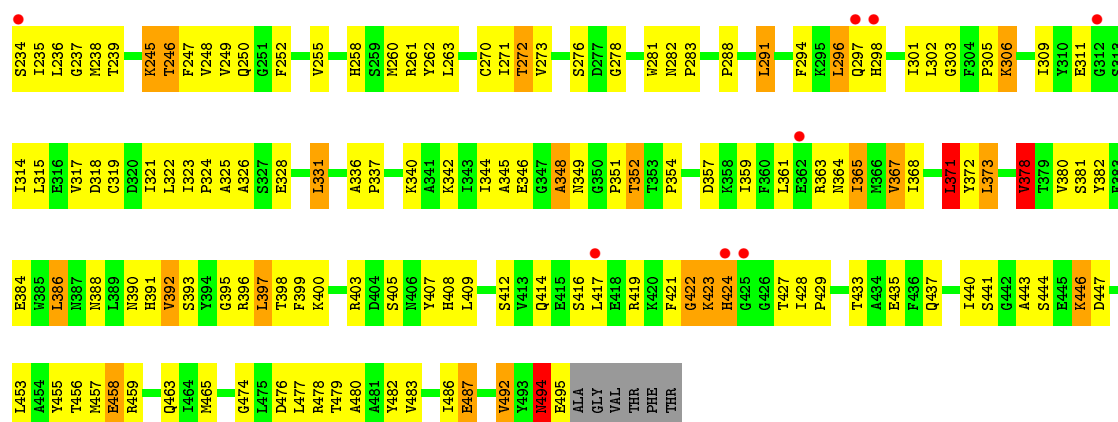
- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

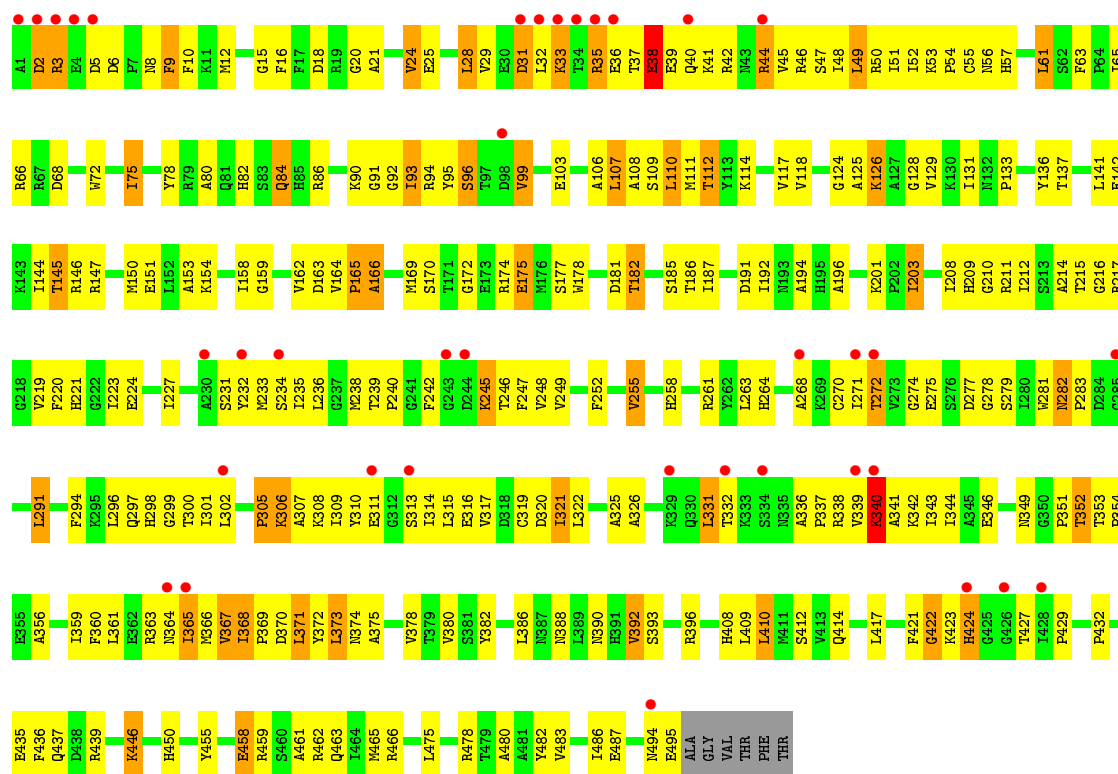
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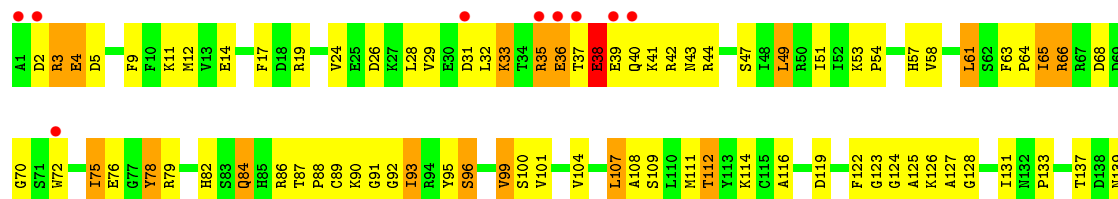
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total 2	Zn 2	0	0
5	C	3	Total 3	Zn 3	0	0
5	A	2	Total 2	Zn 2	0	0
5	F	1	Total 1	Zn 1	0	0

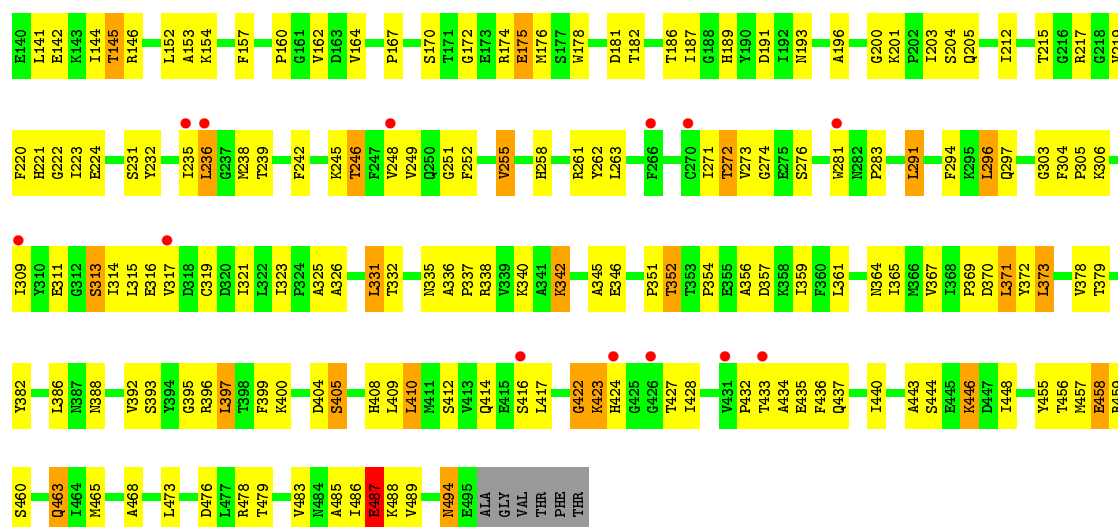


• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

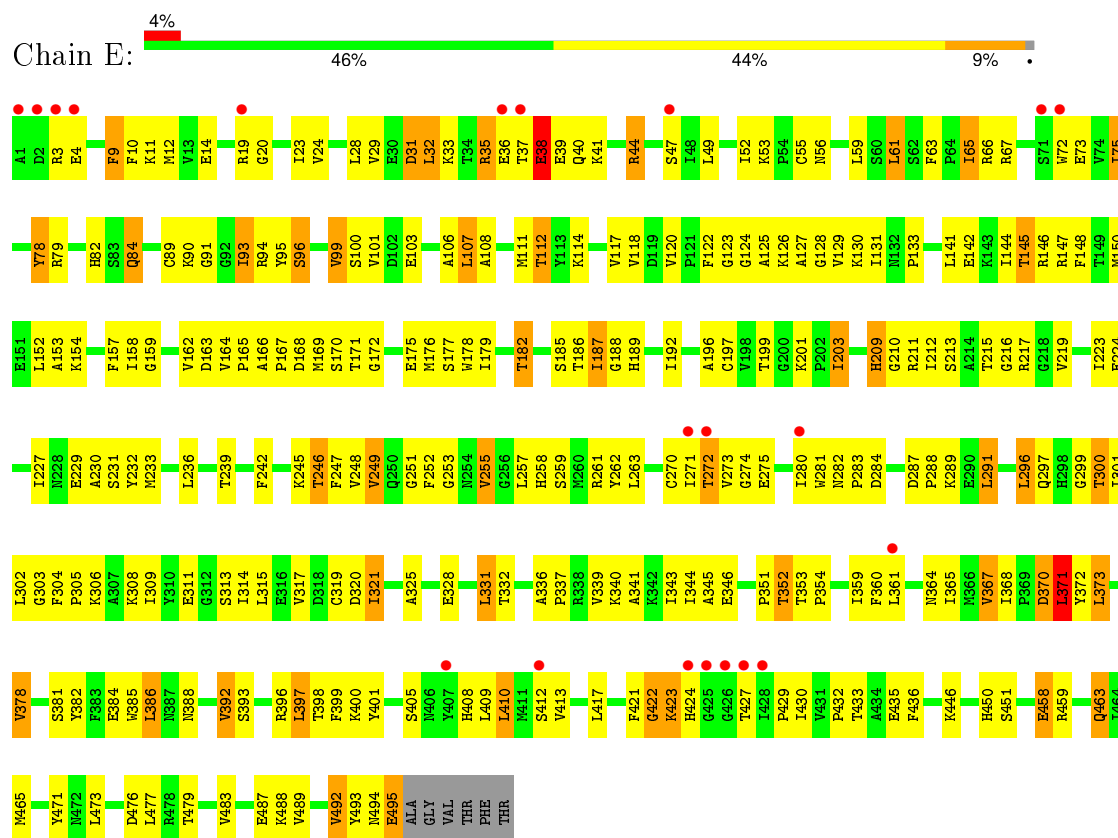


• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

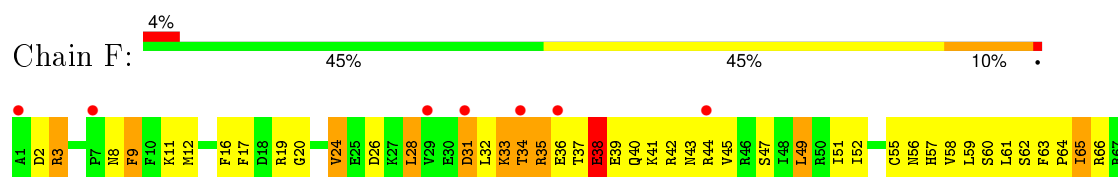




• Molecule 1: Glutamate dehydrogenase 1, mitochondrial



• Molecule 1: Glutamate dehydrogenase 1, mitochondrial



Y455	V378	E311	Y219	K143	D68
T456	T379	G312	I227	I144	
M457	V380	S313		T145	W72
E458	S381	I314	A230	R146	I75
R459	Y382	I315	S231	F147	E76
S460	F383	E316	Y232	T148	T77
A461	E384	V317	T233	T149	Y78
R462	T385	D318	S234	M150	R79
	L386	C319	L235	E151	
M465	N387	D320	L236	A153	H82
R466	N388	I321			S83
		L322	T239	I158	O84
L475	V392			G159	H85
	S393	A325	F242		R86
R478	Y394		G243	V162	
T479	C395	E328	D244	D163	C89
A480	R396	I329	K245	V164	X90
A481	L397	L331	T246	P165	G91
A482	T398		F247	A166	G92
V483	F399	A336	V248	P167	I93
	K400	R337	V249		R94
I486	Y401	R338		S170	Y95
E487	E402	V339	F252	T171	S96
	R403	K340		G172	T97
R491		A341	V255	E173	D98
	R408	R342	G256	R174	Y99
M494	L409	I343	H258	E175	S100
E495	L410	I344		M176	
A496	M411	A345	R261	S177	V101
A497	S412	E346	T262	W178	D102
		C347	L263		E103
T499	S416	A348	H264	D181	L107
F500	L417	N349		T182	A108
T501	E418	G350	C270	T186	S109
	R419	P351	I271	I187	L110
	K420	T352	T272	G188	M111
	F421	T353	V273	H189	T112
	G422	P354			Y113
	K423	D357	L280	A196	K114
	R424	K358	N281	C197	
		I359	N282	V198	V117
	G425	F360	P283	T199	V118
	T427	L361	I286	G200	
	T428	E362	D287	K201	G123
	P429	R363	P288	P202	G124
	T430	N364		I203	A125
	V431	I365	L291	S204	K126
	P432	M366		G128	A127
	T433	V367	F294	Q205	
	A434	I368	K295	G210	V129
	E435	P369	L296	R211	K130
	F436	D370	Q297	I212	I131
	Q437	L371	H298	S213	N132
	D438	Y372		A214	P133
	R439	L373		T215	
		N374	F304	G216	T137
	R446	D447	P305	R217	
	T448		K306	E142	L141

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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 75931 reflections (0.001%)	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, 0.375 respectively for untwinned datasets, and 0.333, 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: 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 [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	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

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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 [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	493/501 (98%)	428 (87%)	52 (10%)	13 (3%)	7	25
1	B	493/501 (98%)	429 (87%)	49 (10%)	15 (3%)	5	21
1	C	493/501 (98%)	424 (86%)	55 (11%)	14 (3%)	6	23
1	D	493/501 (98%)	427 (87%)	57 (12%)	9 (2%)	11	36
1	E	493/501 (98%)	427 (87%)	56 (11%)	10 (2%)	9	33
1	F	499/501 (100%)	424 (85%)	62 (12%)	13 (3%)	7	25
All	All	2964/3006 (99%)	2559 (86%)	331 (11%)	74 (2%)	7	26

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 [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	416/420 (99%)	356 (86%)	60 (14%)	4	11
1	B	416/420 (99%)	353 (85%)	63 (15%)	3	10
1	C	416/420 (99%)	358 (86%)	58 (14%)	4	12

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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%)	4	11
1	F	420/420 (100%)	356 (85%)	64 (15%)	3	10
All	All	2500/2520 (99%)	2130 (85%)	370 (15%)	4	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 ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 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	-	3,9,9	0.42	0	2,11,11	0.16	0
4	GTP	A	503	5	25,34,34	1.26	3 (12%)	34,54,54	1.99	9 (26%)
3	NDP	A	552	-	42,52,52	1.51	5 (11%)	55,80,80	1.89	6 (10%)
2	GLU	B	502	-	3,9,9	0.45	0	2,11,11	0.13	0
4	GTP	B	503	5	25,34,34	1.06	2 (8%)	34,54,54	1.98	12 (35%)
3	NDP	B	552	-	42,52,52	1.55	5 (11%)	55,80,80	1.93	3 (5%)
2	GLU	C	502	-	3,9,9	0.46	0	2,11,11	0.34	0
4	GTP	C	503	5	25,34,34	0.92	1 (4%)	34,54,54	1.72	6 (17%)
3	NDP	C	552	-	42,52,52	1.60	5 (11%)	55,80,80	1.79	3 (5%)
2	GLU	D	502	-	3,9,9	0.30	0	2,11,11	0.13	0
4	GTP	D	503	5	25,34,34	0.95	1 (4%)	34,54,54	1.74	8 (23%)
3	NDP	D	552	-	42,52,52	1.53	5 (11%)	55,80,80	1.95	5 (9%)
2	GLU	E	502	-	3,9,9	0.38	0	2,11,11	0.16	0
4	GTP	E	503	5	25,34,34	1.06	2 (8%)	34,54,54	1.97	10 (29%)
3	NDP	E	552	-	42,52,52	1.57	5 (11%)	55,80,80	1.97	6 (10%)
2	GLU	F	502	-	3,9,9	0.47	0	2,11,11	0.33	0
4	GTP	F	503	5	25,34,34	0.99	1 (4%)	34,54,54	1.97	10 (29%)
3	NDP	F	552	-	42,52,52	1.52	4 (9%)	55,80,80	1.80	3 (5%)

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

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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 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	GTP	O4'-C4'	-2.27	1.39	1.45
4	B	503	GTP	C2-N1	2.04	1.39	1.35
3	D	552	NDP	C2N-C3N	2.08	1.39	1.34
3	C	552	NDP	C2N-C3N	2.08	1.39	1.34
4	E	503	GTP	C2-N1	2.09	1.39	1.35

The worst 5 of 81 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	552	NDP	N3A-C2A-N1A	-12.13	119.61	128.89
3	E	552	NDP	N3A-C2A-N1A	-11.72	119.92	128.89
3	D	552	NDP	N3A-C2A-N1A	-11.36	120.20	128.89
3	F	552	NDP	N3A-C2A-N1A	-11.11	120.39	128.89
3	C	552	NDP	N3A-C2A-N1A	-11.00	120.47	128.89

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

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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%)	0.14	23 (4%)	36	32	15, 32, 68, 127	0
1	B	495/501 (98%)	0.15	18 (3%)	46	42	17, 34, 71, 128	0
1	C	495/501 (98%)	0.29	37 (7%)	17	13	18, 38, 71, 129	0
1	D	495/501 (98%)	0.12	22 (4%)	38	34	15, 32, 71, 131	0
1	E	495/501 (98%)	0.13	21 (4%)	40	36	16, 32, 71, 126	0
1	F	501/501 (100%)	-0.02	19 (3%)	44	40	14, 29, 73, 130	0
All	All	2976/3006 (99%)	0.13	140 (4%)	35	32	14, 32, 72, 131	0

The worst 5 of 140 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	424	HIS	8.2
1	B	2	ASP	7.7
1	E	424	HIS	7.1
1	C	3	ARG	6.9
1	F	424	HIS	6.6

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
2	GLU	F	502	10/10	0.95	0.19	1.31	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	0.69	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	-0.26	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	-0.37	19,26,31,31	0
5	ZN	B	505	1/1	0.97	0.17	-0.40	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	-0.48	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	-4.43	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 [i](#)

There are no such residues in this entry.