



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 12:02 PM GMT

PDB ID : 3QMU
Title : Bovine glutamate dehydrogenase complexed with epicatechin-3-gallate (ECG)
Authors : Li, C.; Li, M.; Stanley, C.; Smith, T.J.
Deposited on : 2011-02-05
Resolution : 3.62 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

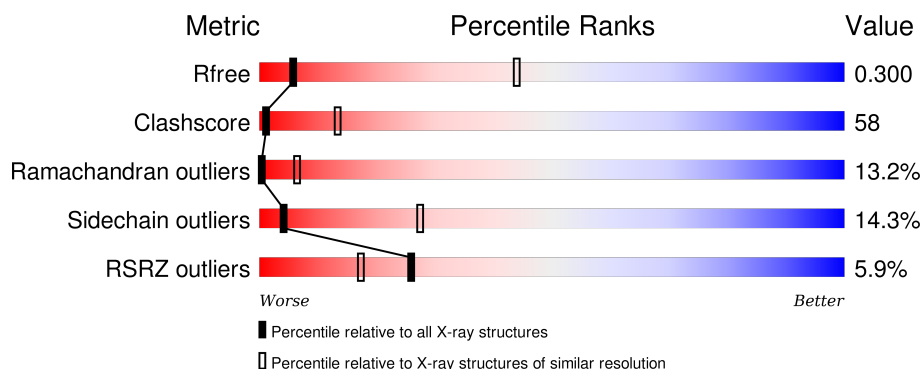
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.62 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	1093 (3.80-3.44)
Clashscore	102246	1043 (3.78-3.46)
Ramachandran outliers	100387	1003 (3.78-3.46)
Sidechain outliers	100360	1003 (3.78-3.46)
RSRZ outliers	91569	1100 (3.80-3.44)

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>8%</div> <div>26%</div> <div>55%</div> <div>18%</div> <div>..</div> </div>
1	B	501	<div> <div>7%</div> <div>25%</div> <div>56%</div> <div>17%</div> <div>..</div> </div>
1	C	501	<div> <div>6%</div> <div>27%</div> <div>54%</div> <div>17%</div> <div>..</div> </div>
1	D	501	<div> <div>6%</div> <div>25%</div> <div>56%</div> <div>17%</div> <div>..</div> </div>
1	E	501	<div> <div>8%</div> <div>24%</div> <div>56%</div> <div>18%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	501	
1	G	501	
1	H	501	
1	I	501	
1	J	501	
1	K	501	
1	L	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	NDP	B	552	-	-	-	X
3	XEG	B	601	-	-	X	-
3	XEG	D	601	-	-	-	X
3	XEG	F	601	-	-	X	-
3	XEG	G	601	-	-	X	-
3	XEG	H	601	-	-	X	-
3	XEG	I	601	-	-	-	X
3	XEG	J	601	-	-	X	-
3	XEG	K	601	-	-	X	-

2 Entry composition

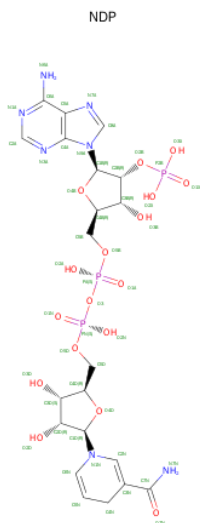
There are 3 unique types of molecules in this entry. The entry contains 47520 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

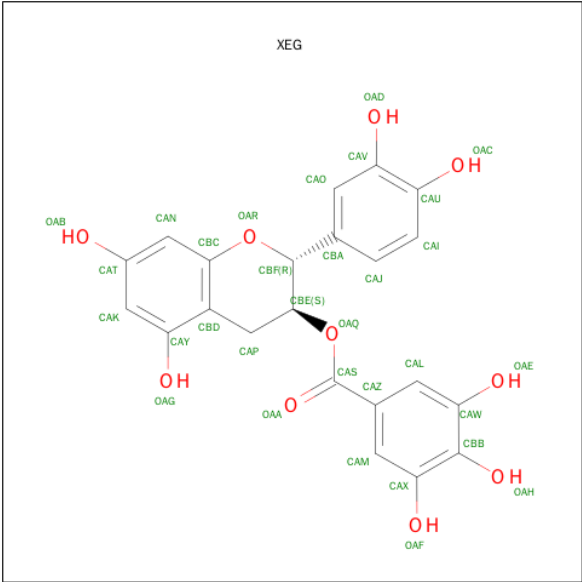
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	0	0	0
			3880	2454	679	728	19			
1	B	496	Total	C	N	O	S	0	0	0
			3880	2454	679	728	19			
1	C	496	Total	C	N	O	S	0	0	0
			3880	2454	679	728	19			
1	D	496	Total	C	N	O	S	0	0	0
			3880	2454	679	728	19			
1	E	496	Total	C	N	O	S	0	0	0
			3880	2454	679	728	19			
1	F	496	Total	C	N	O	S	0	0	0
			3880	2454	679	728	19			
1	G	496	Total	C	N	O	S	0	0	0
			3880	2454	679	728	19			
1	H	496	Total	C	N	O	S	0	0	0
			3880	2454	679	728	19			
1	I	496	Total	C	N	O	S	0	0	0
			3880	2454	679	728	19			
1	J	496	Total	C	N	O	S	0	0	0
			3880	2454	679	728	19			
1	K	496	Total	C	N	O	S	0	0	0
			3880	2454	679	728	19			
1	L	496	Total	C	N	O	S	0	0	0
			3880	2454	679	728	19			

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



2	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	B	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	C	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	D	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	E	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	F	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	G	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	H	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	I	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	J	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	K	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	L	1	Total 48	C 21	N 7	O 17	P 3	0	0

- Molecule 3 is (2R,3S)-2-(3,4-DIHYDROXYPHENYL)-5,7-DIHYDROXY-3,4-DIHYDRO-2-H-CHROMEN-3-YL 3,4,5-TRIHYDROXYBENZOATE (three-letter code: XEG) (formula: $C_{22}H_{18}O_{10}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			32	22	10		
3	B	1	Total	C	O	0	0
			32	22	10		
3	D	1	Total	C	O	0	0
			32	22	10		
3	D	1	Total	C	O	0	0
			32	22	10		
3	E	1	Total	C	O	0	0
			32	22	10		
3	F	1	Total	C	O	0	0
			32	22	10		
3	G	1	Total	C	O	0	0
			32	22	10		
3	H	1	Total	C	O	0	0
			32	22	10		
3	I	1	Total	C	O	0	0
			32	22	10		
3	J	1	Total	C	O	0	0
			32	22	10		
3	K	1	Total	C	O	0	0
			32	22	10		
3	L	1	Total	C	O	0	0
			32	22	10		

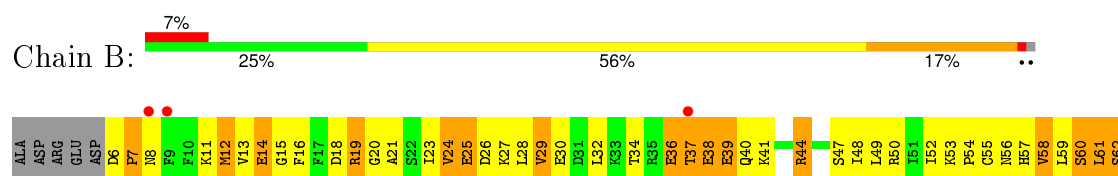
3 Residue-property plots

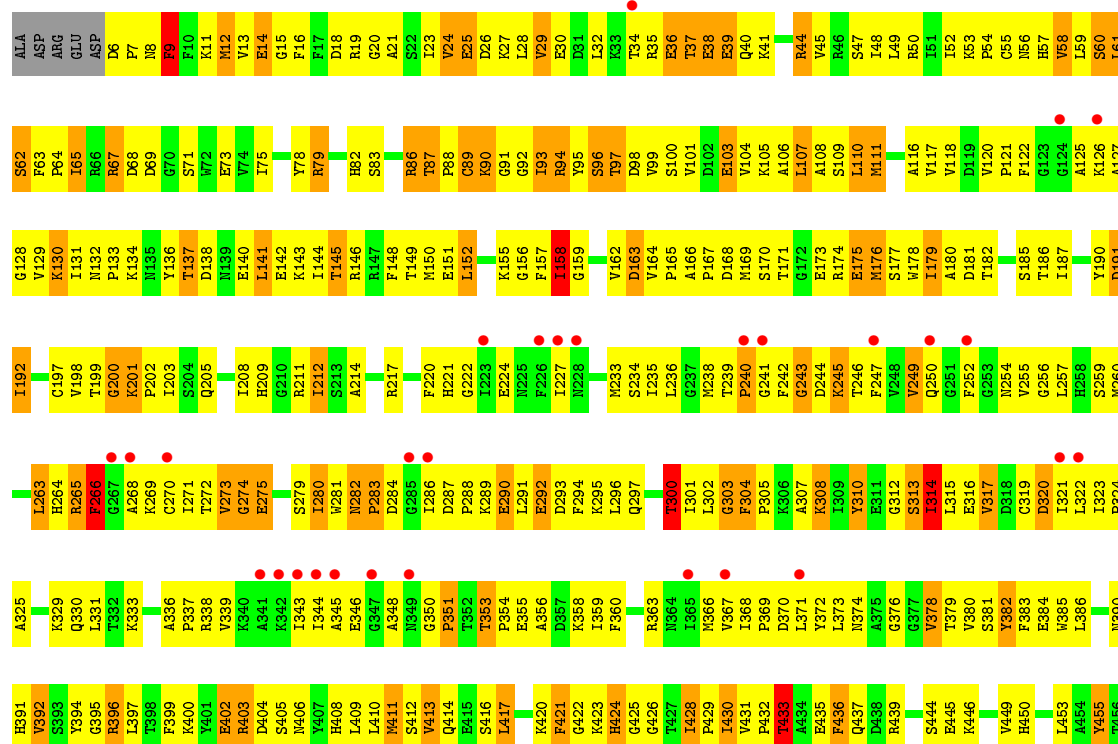
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

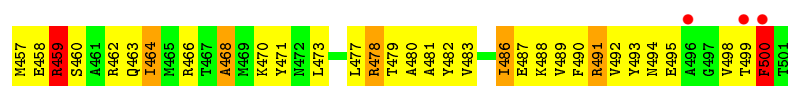
• Molecule 1: Glutamate dehydrogenase 1



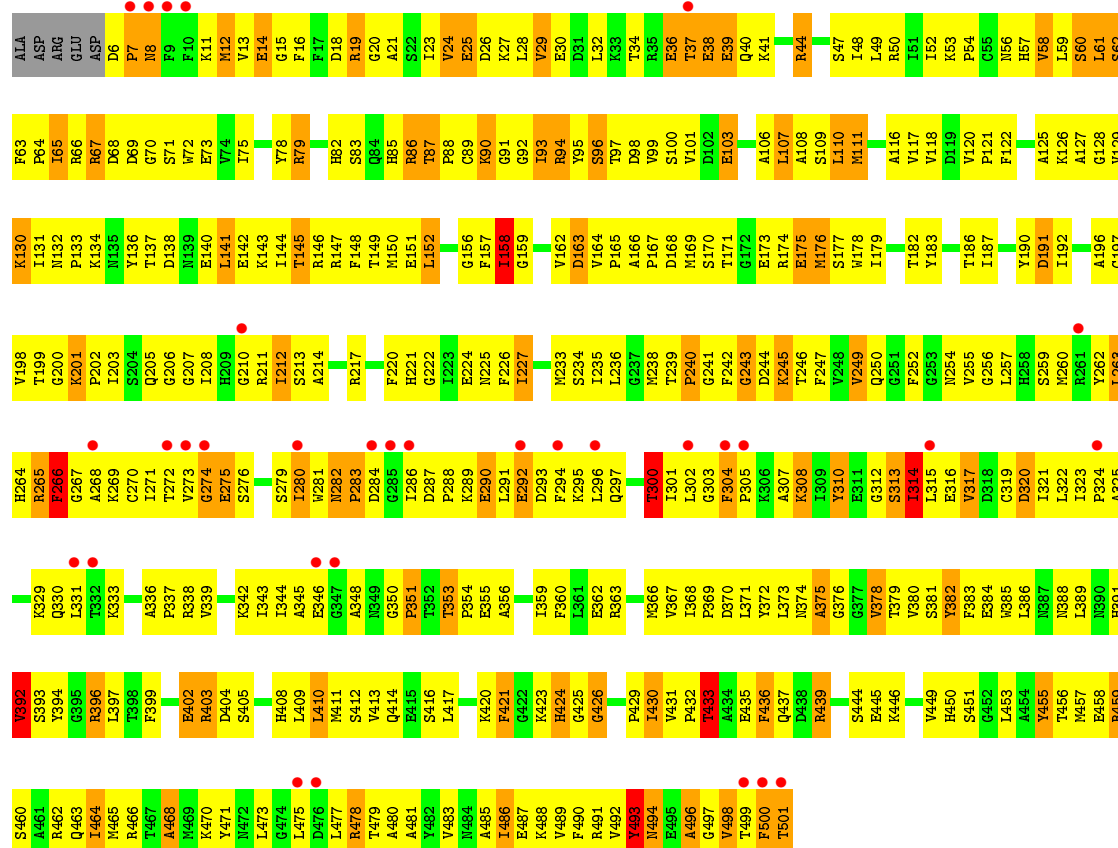
• Molecule 1: Glutamate dehydrogenase 1



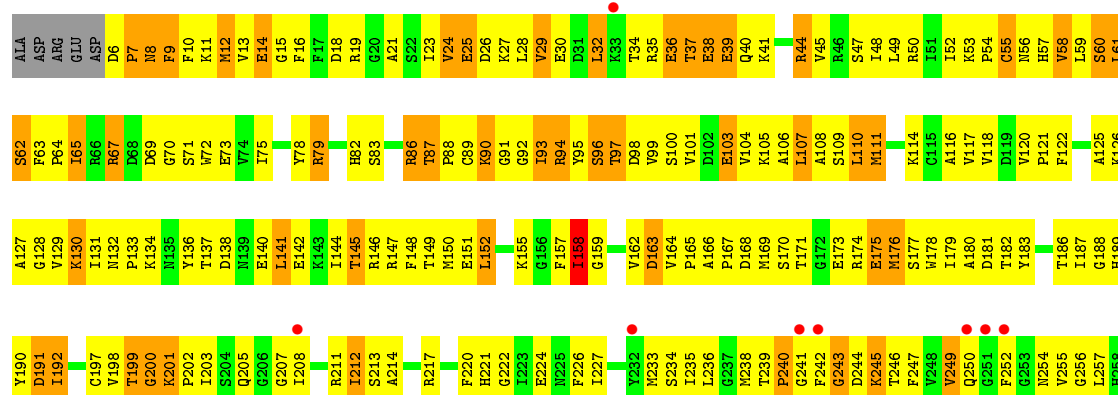


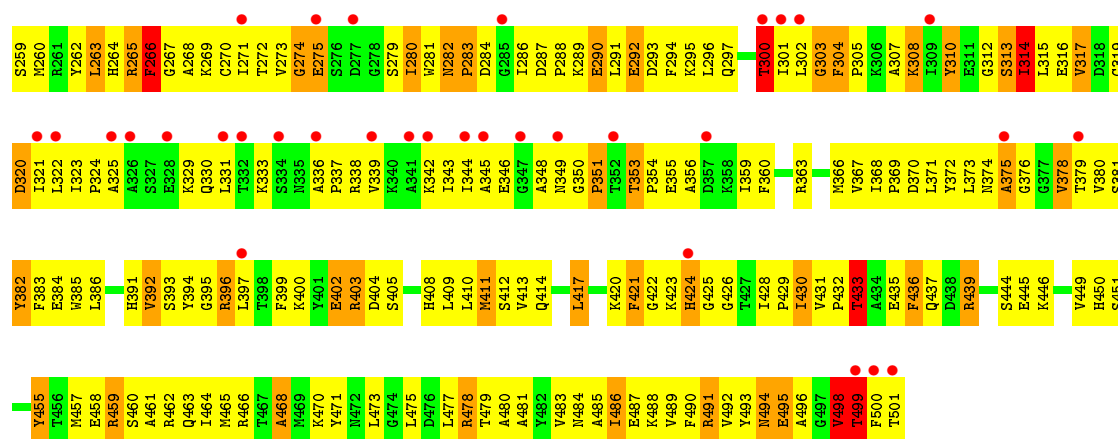


● Molecule 1: Glutamate dehydrogenase 1

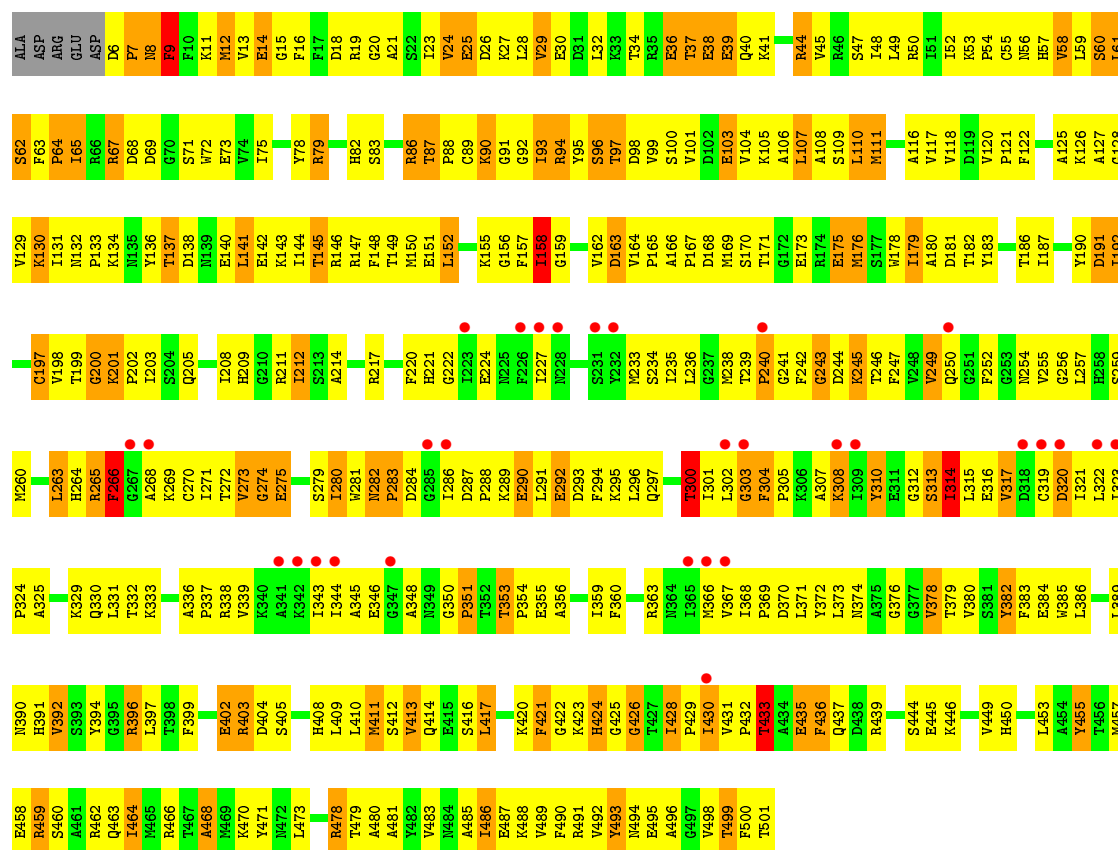


● Molecule 1: Glutamate dehydrogenase 1



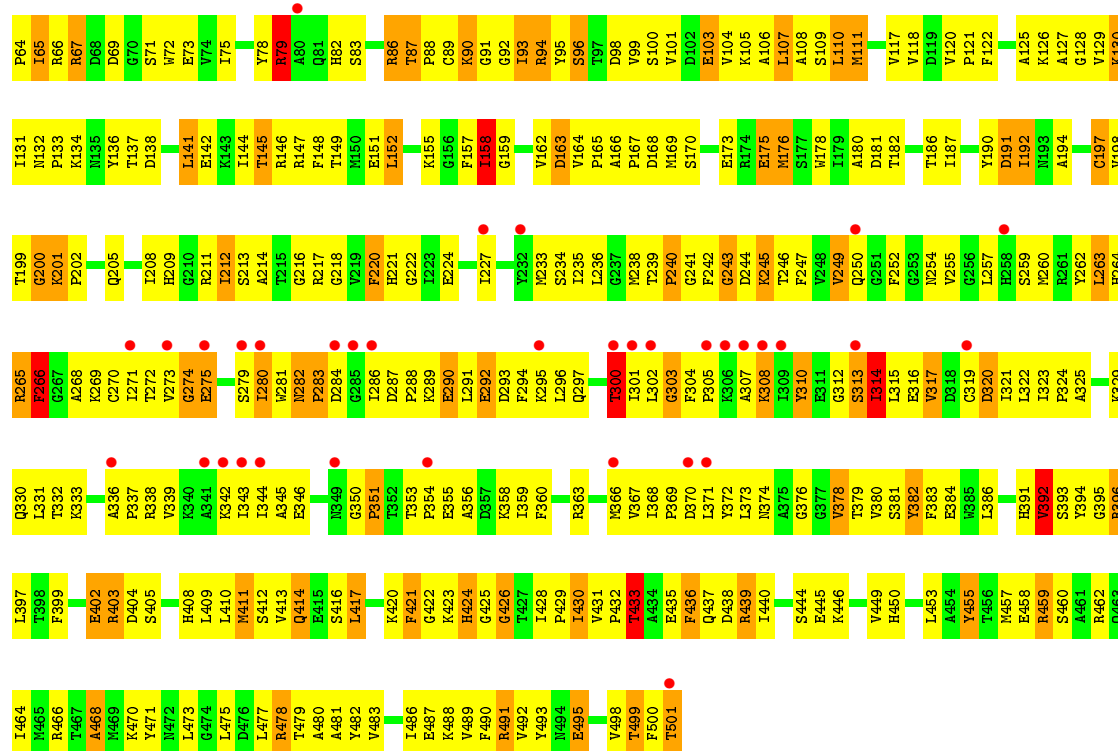


• Molecule 1: Glutamate dehydrogenase 1

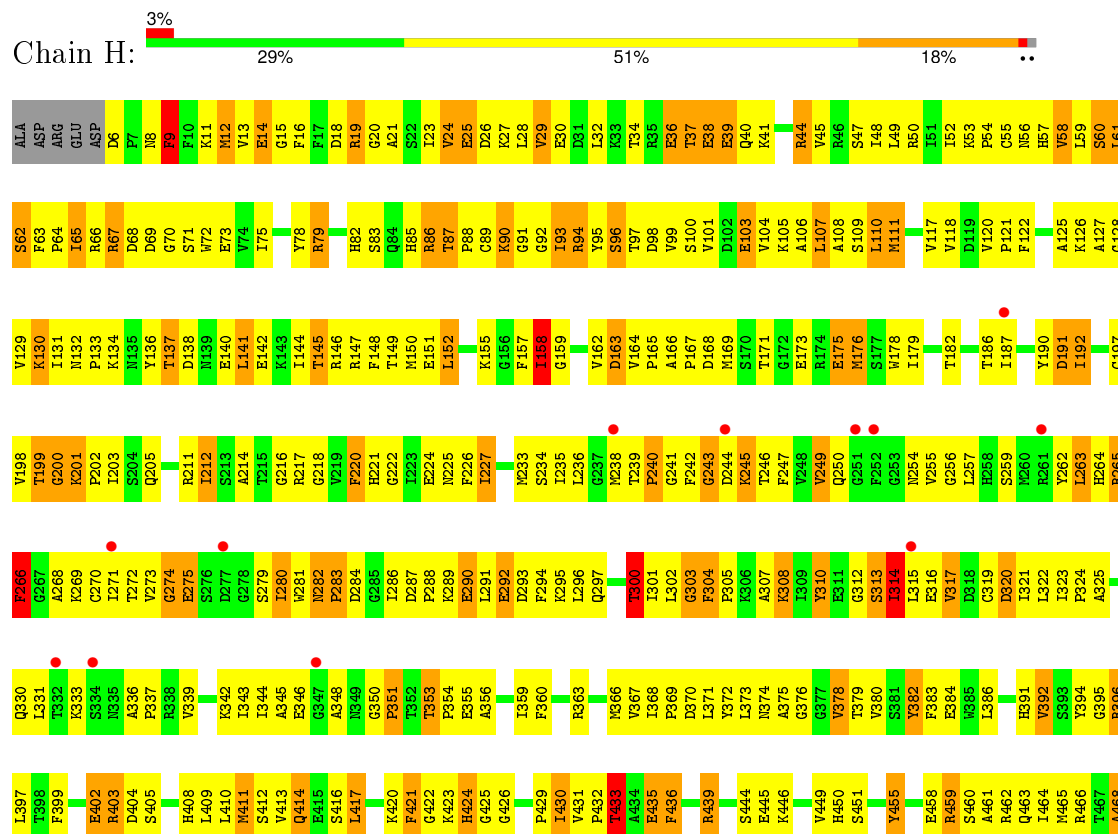


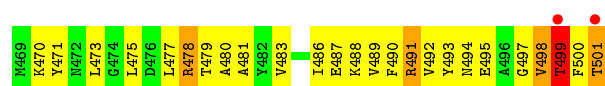
• Molecule 1: Glutamate dehydrogenase 1



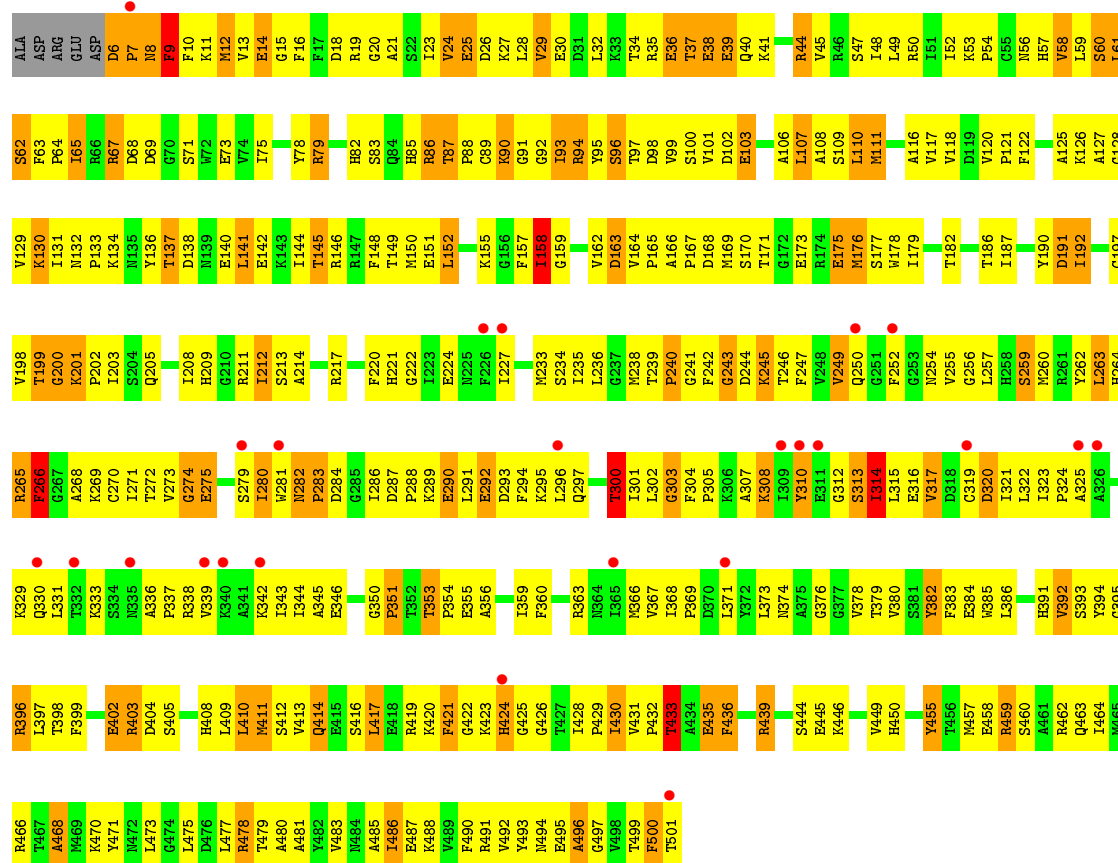


• Molecule 1: Glutamate dehydrogenase 1

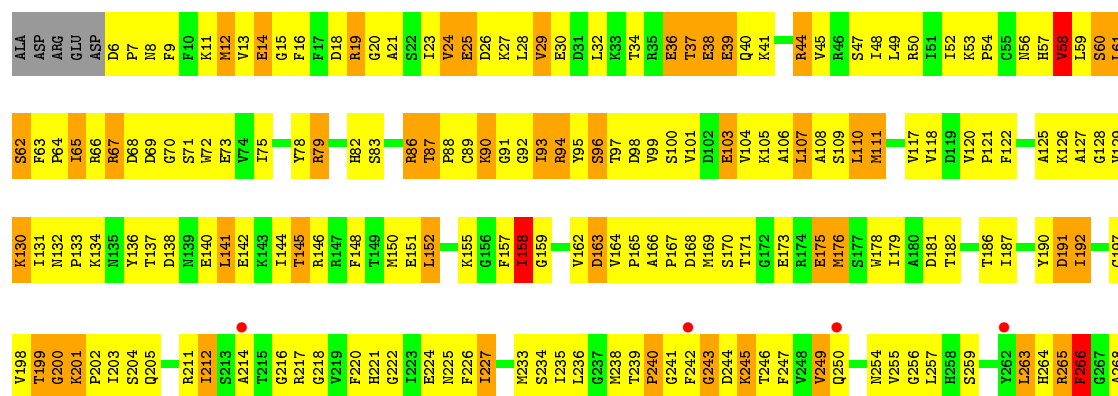


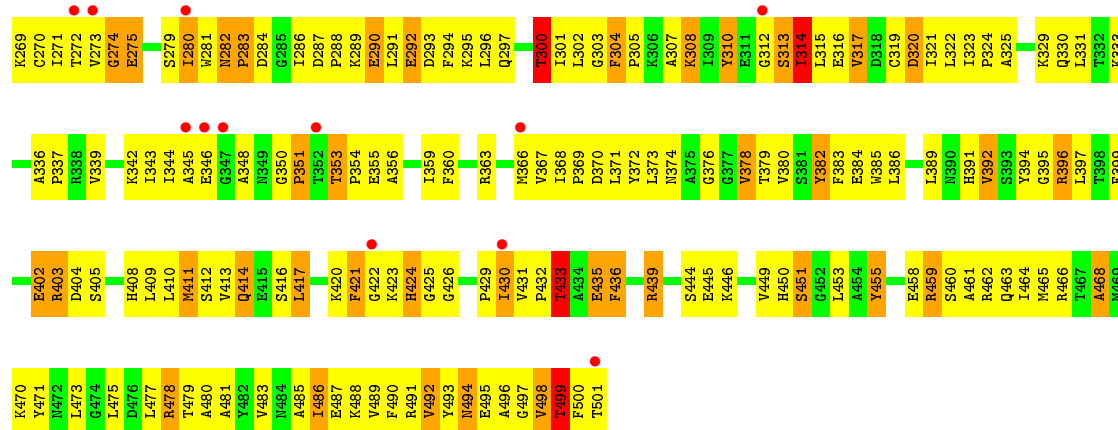


• Molecule 1: Glutamate dehydrogenase 1

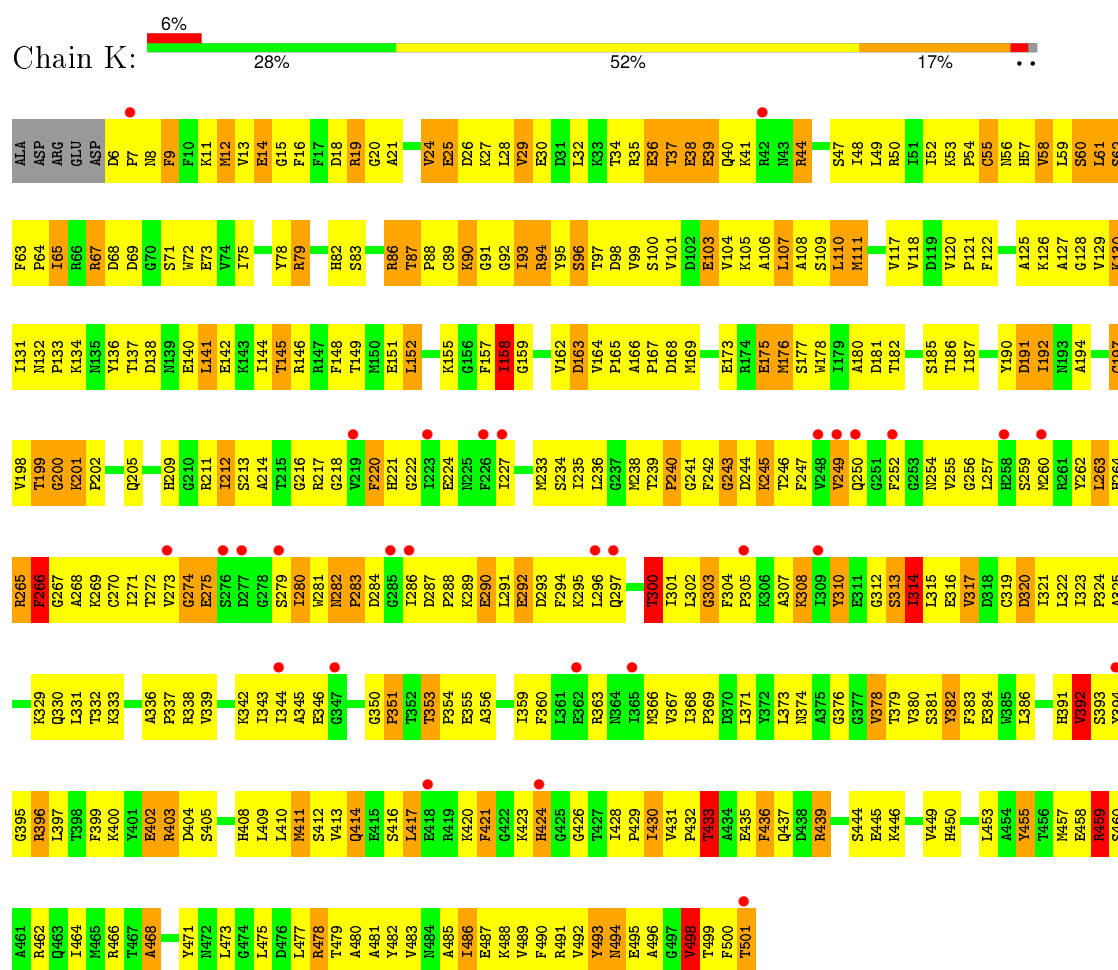


• Molecule 1: Glutamate dehydrogenase 1

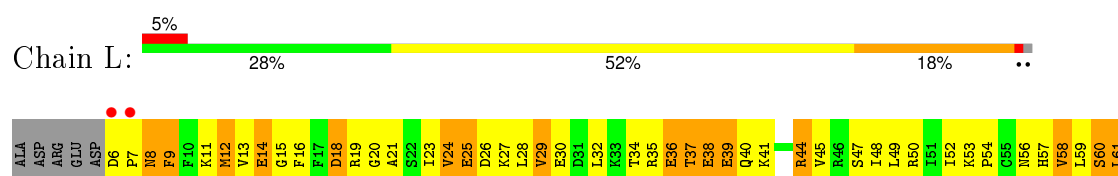




• Molecule 1: Glutamate dehydrogenase 1



• Molecule 1: Glutamate dehydrogenase 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	95.12Å 433.18Å 95.17Å 90.00° 118.74° 90.00°	Depositor
Resolution (Å)	49.71 – 3.62 49.71 – 3.62	Depositor EDS
% Data completeness (in resolution range)	95.0 (49.71-3.62) 95.0 (49.71-3.62)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 3.67Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_353)	Depositor
R, R_{free}	0.257 , 0.302 0.252 , 0.300	Depositor DCC
R_{free} test set	3755 reflections (5.46%)	DCC
Wilson B-factor (Å ²)	101.1	Xtriage
Anisotropy	0.399	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 112.7	EDS
Estimated twinning fraction	0.036 for -h-l,k,h 0.036 for l,k,-h-l 0.038 for h,-k,-h-l 0.036 for -h-l,-k,l 0.428 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 75039 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	47520	wwPDB-VP
Average B, all atoms (Å ²)	146.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: NDP, XEG

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	0.53	0/3963	0.64	0/5351
1	B	0.53	0/3963	0.67	0/5351
1	C	0.54	1/3963 (0.0%)	0.66	1/5351 (0.0%)
1	D	0.54	0/3963	0.66	0/5351
1	E	0.53	0/3963	0.64	0/5351
1	F	0.55	1/3963 (0.0%)	0.79	3/5351 (0.1%)
1	G	0.53	1/3963 (0.0%)	0.63	1/5351 (0.0%)
1	H	0.54	0/3963	0.63	0/5351
1	I	0.50	0/3963	0.63	0/5351
1	J	0.53	0/3963	0.63	0/5351
1	K	0.53	1/3963 (0.0%)	0.65	2/5351 (0.0%)
1	L	0.51	0/3963	0.63	0/5351
All	All	0.53	4/47556 (0.0%)	0.66	7/64212 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	197	CYS	CB-SG	-8.22	1.68	1.82
1	G	197	CYS	CB-SG	-7.69	1.69	1.82
1	F	197	CYS	CB-SG	-5.43	1.73	1.81
1	C	89	CYS	CB-SG	-5.40	1.73	1.81

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	459	ARG	NE-CZ-NH1	-22.15	109.22	120.30
1	F	459	ARG	NE-CZ-NH2	21.93	131.27	120.30
1	F	459	ARG	CD-NE-CZ	11.59	139.82	123.60
1	K	459	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	C	459	ARG	NE-CZ-NH1	5.43	123.02	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	8	ASN	Peptide

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	3848	497	2
1	B	3880	0	3848	502	2
1	C	3880	0	3848	490	0
1	D	3880	0	3848	483	1
1	E	3880	0	3848	505	1
1	F	3880	0	3848	476	0
1	G	3880	0	3848	460	0
1	H	3880	0	3848	479	0
1	I	3880	0	3848	464	0
1	J	3880	0	3848	483	0
1	K	3880	0	3848	456	0
1	L	3880	0	3848	460	0
2	A	48	0	26	8	0
2	B	48	0	26	2	0
2	C	48	0	26	5	0
2	D	48	0	26	2	0
2	E	48	0	26	5	0
2	F	48	0	26	5	0
2	G	48	0	26	4	0
2	H	48	0	26	4	0
2	I	48	0	26	5	0
2	J	48	0	26	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	48	0	26	5	0
2	L	48	0	26	7	0
3	A	32	0	18	8	0
3	B	32	0	18	10	0
3	D	64	0	35	13	0
3	E	32	0	18	8	0
3	F	32	0	18	10	0
3	G	32	0	18	10	0
3	H	32	0	18	14	0
3	I	32	0	18	7	0
3	J	32	0	18	12	0
3	K	32	0	18	9	0
3	L	32	0	18	6	0
All	All	47520	0	46703	5482	3

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 58.

The worst 5 of 5482 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:E:371:LEU:HD23	1:E:481:ALA:HB1	1.26	1.15
1:D:24:VAL:HG13	1:D:483:VAL:HG13	1.26	1.13
1:I:408:HIS:HB3	1:K:436:PHE:CD2	1.82	1.13
1:G:436:PHE:CD2	1:L:408:HIS:HB3	1.85	1.12
1:F:99:VAL:HG11	1:F:128:GLY:HA3	1.34	1.10

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:362:GLU:O	1:E:38:GLU:OE2[1_556]	2.11	0.09
1:A:38:GLU:OE2	1:B:362:GLU:O[1_455]	2.12	0.08
1:A:36:GLU:OE2	1:B:362:GLU:O[1_455]	2.17	0.03

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	494/501 (99%)	313 (63%)	113 (23%)	68 (14%)	0	6
1	B	494/501 (99%)	322 (65%)	104 (21%)	68 (14%)	0	6
1	C	494/501 (99%)	321 (65%)	107 (22%)	66 (13%)	0	6
1	D	494/501 (99%)	318 (64%)	112 (23%)	64 (13%)	0	7
1	E	494/501 (99%)	313 (63%)	113 (23%)	68 (14%)	0	6
1	F	494/501 (99%)	319 (65%)	111 (22%)	64 (13%)	0	7
1	G	494/501 (99%)	325 (66%)	106 (22%)	63 (13%)	0	7
1	H	494/501 (99%)	322 (65%)	106 (22%)	66 (13%)	0	6
1	I	494/501 (99%)	321 (65%)	108 (22%)	65 (13%)	0	6
1	J	494/501 (99%)	321 (65%)	110 (22%)	63 (13%)	0	7
1	K	494/501 (99%)	324 (66%)	108 (22%)	62 (13%)	0	7
1	L	494/501 (99%)	320 (65%)	111 (22%)	63 (13%)	0	7
All	All	5928/6012 (99%)	3839 (65%)	1309 (22%)	780 (13%)	0	6

5 of 780 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	PRO
1	A	12	MET
1	A	30	GLU
1	A	62	SER
1	A	87	THR

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%)	357 (86%)	59 (14%)	4	28
1	B	416/420 (99%)	360 (86%)	56 (14%)	5	30
1	C	416/420 (99%)	358 (86%)	58 (14%)	4	28
1	D	416/420 (99%)	356 (86%)	60 (14%)	4	27
1	E	416/420 (99%)	356 (86%)	60 (14%)	4	27
1	F	416/420 (99%)	355 (85%)	61 (15%)	4	26
1	G	416/420 (99%)	357 (86%)	59 (14%)	4	28
1	H	416/420 (99%)	357 (86%)	59 (14%)	4	28
1	I	416/420 (99%)	357 (86%)	59 (14%)	4	28
1	J	416/420 (99%)	354 (85%)	62 (15%)	4	25
1	K	416/420 (99%)	358 (86%)	58 (14%)	4	28
1	L	416/420 (99%)	354 (85%)	62 (15%)	4	25
All	All	4992/5040 (99%)	4279 (86%)	713 (14%)	4	27

5 of 713 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	192	ILE
1	G	382	TYR
1	L	36	GLU
1	F	310	TYR
1	G	58	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 111 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	297	GLN
1	H	82	HIS
1	L	8	ASN
1	F	330	GLN
1	G	254	ASN

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 ⓘ

24 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NDP	A	552	-	42,52,52	1.63	4 (9%)	55,80,80	2.04	5 (9%)
3	XEG	A	601	-	35,35,35	1.31	4 (11%)	52,52,52	1.20	3 (5%)
2	NDP	B	552	-	42,52,52	1.61	5 (11%)	55,80,80	2.09	4 (7%)
3	XEG	B	601	-	35,35,35	1.27	3 (8%)	52,52,52	1.33	4 (7%)
2	NDP	C	552	-	42,52,52	1.59	4 (9%)	55,80,80	1.99	4 (7%)
3	XEG	D	502	-	35,35,35	1.25	2 (5%)	52,52,52	1.39	6 (11%)
2	NDP	D	552	-	42,52,52	1.59	5 (11%)	55,80,80	2.09	4 (7%)
3	XEG	D	601	-	35,35,35	1.42	4 (11%)	52,52,52	1.37	9 (17%)
2	NDP	E	552	-	42,52,52	1.61	5 (11%)	55,80,80	2.03	5 (9%)
3	XEG	E	601	-	35,35,35	1.31	3 (8%)	52,52,52	1.20	4 (7%)
2	NDP	F	552	-	42,52,52	1.58	4 (9%)	55,80,80	1.98	4 (7%)
3	XEG	F	601	-	35,35,35	1.36	5 (14%)	52,52,52	1.35	7 (13%)
2	NDP	G	552	-	42,52,52	1.61	4 (9%)	55,80,80	2.02	4 (7%)
3	XEG	G	601	-	35,35,35	1.42	4 (11%)	52,52,52	1.27	4 (7%)
2	NDP	H	552	-	42,52,52	1.54	4 (9%)	55,80,80	1.90	4 (7%)
3	XEG	H	601	-	35,35,35	1.27	3 (8%)	52,52,52	1.45	7 (13%)
2	NDP	I	552	-	42,52,52	1.62	5 (11%)	55,80,80	2.03	4 (7%)
3	XEG	I	601	-	35,35,35	1.46	6 (17%)	52,52,52	1.35	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NDP	J	552	-	42,52,52	1.53	4 (9%)	55,80,80	1.93	3 (5%)
3	XEG	J	601	-	35,35,35	1.26	3 (8%)	52,52,52	1.47	9 (17%)
2	NDP	K	552	-	42,52,52	1.60	4 (9%)	55,80,80	2.01	3 (5%)
3	XEG	K	601	-	35,35,35	1.42	4 (11%)	52,52,52	1.20	3 (5%)
2	NDP	L	552	-	42,52,52	1.61	5 (11%)	55,80,80	2.05	3 (5%)
3	XEG	L	601	-	35,35,35	1.49	7 (20%)	52,52,52	1.33	7 (13%)

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	NDP	A	552	-	-	0/30/77/77	0/5/5/5
3	XEG	A	601	-	-	2/12/24/24	0/4/4/4
2	NDP	B	552	-	-	0/30/77/77	0/5/5/5
3	XEG	B	601	-	-	2/12/24/24	0/4/4/4
2	NDP	C	552	-	-	0/30/77/77	0/5/5/5
3	XEG	D	502	-	-	2/12/24/24	0/4/4/4
2	NDP	D	552	-	-	0/30/77/77	0/5/5/5
3	XEG	D	601	-	-	2/12/24/24	0/4/4/4
2	NDP	E	552	-	-	0/30/77/77	0/5/5/5
3	XEG	E	601	-	-	2/12/24/24	0/4/4/4
2	NDP	F	552	-	-	0/30/77/77	0/5/5/5
3	XEG	F	601	-	-	2/12/24/24	0/4/4/4
2	NDP	G	552	-	-	0/30/77/77	0/5/5/5
3	XEG	G	601	-	-	2/12/24/24	0/4/4/4
2	NDP	H	552	-	-	0/30/77/77	0/5/5/5
3	XEG	H	601	-	-	2/12/24/24	0/4/4/4
2	NDP	I	552	-	-	0/30/77/77	0/5/5/5
3	XEG	I	601	-	-	2/12/24/24	0/4/4/4
2	NDP	J	552	-	-	0/30/77/77	0/5/5/5
3	XEG	J	601	-	-	2/12/24/24	0/4/4/4
2	NDP	K	552	-	-	0/30/77/77	0/5/5/5
3	XEG	K	601	-	-	2/12/24/24	0/4/4/4
2	NDP	L	552	-	-	0/30/77/77	0/5/5/5
3	XEG	L	601	-	-	2/12/24/24	0/4/4/4

The worst 5 of 101 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	601	XEG	OAR-CBF	-4.32	1.37	1.45
3	J	601	XEG	OAR-CBF	-4.31	1.37	1.45
3	L	601	XEG	OAR-CBF	-3.71	1.38	1.45
3	I	601	XEG	OAR-CBF	-3.70	1.38	1.45
3	D	502	XEG	OAR-CBF	-3.58	1.38	1.45

The worst 5 of 116 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	552	NDP	N3A-C2A-N1A	-12.63	119.22	128.89
2	D	552	NDP	N3A-C2A-N1A	-12.55	119.29	128.89
2	L	552	NDP	N3A-C2A-N1A	-12.19	119.56	128.89
2	I	552	NDP	N3A-C2A-N1A	-11.95	119.74	128.89
2	A	552	NDP	N3A-C2A-N1A	-11.71	119.92	128.89

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	L	601	XEG	CBE-OAQ-CAS-OAA
3	D	502	XEG	CBE-OAQ-CAS-OAA
3	I	601	XEG	CBE-OAQ-CAS-OAA
3	F	601	XEG	CBE-OAQ-CAS-OAA
3	A	601	XEG	CBE-OAQ-CAS-OAA

There are no ring outliers.

24 monomers are involved in 161 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	552	NDP	8	0
3	A	601	XEG	8	0
2	B	552	NDP	2	0
3	B	601	XEG	10	0
2	C	552	NDP	5	0
3	D	502	XEG	8	0
2	D	552	NDP	2	0
3	D	601	XEG	5	0
2	E	552	NDP	5	0
3	E	601	XEG	8	0
2	F	552	NDP	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	601	XEG	10	0
2	G	552	NDP	4	0
3	G	601	XEG	10	0
2	H	552	NDP	4	0
3	H	601	XEG	14	0
2	I	552	NDP	5	0
3	I	601	XEG	7	0
2	J	552	NDP	2	0
3	J	601	XEG	12	0
2	K	552	NDP	5	0
3	K	601	XEG	9	0
2	L	552	NDP	7	0
3	L	601	XEG	6	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 ⓘ

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(Å²)	Q<0.9
1	A	496/501 (99%)	0.25	41 (8%)	14	10	63, 122, 279, 367	0
1	B	496/501 (99%)	0.21	34 (6%)	20	13	63, 121, 276, 367	0
1	C	496/501 (99%)	0.25	32 (6%)	22	15	62, 121, 277, 365	0
1	D	496/501 (99%)	0.25	32 (6%)	22	15	61, 122, 276, 369	0
1	E	496/501 (99%)	0.37	41 (8%)	14	10	64, 122, 279, 366	0
1	F	496/501 (99%)	0.23	30 (6%)	25	17	62, 121, 278, 365	0
1	G	496/501 (99%)	0.28	35 (7%)	19	13	61, 120, 278, 368	0
1	H	496/501 (99%)	0.07	14 (2%)	56	42	60, 120, 276, 365	0
1	I	496/501 (99%)	0.09	24 (4%)	34	23	59, 121, 278, 365	0
1	J	496/501 (99%)	0.10	16 (3%)	51	37	61, 120, 276, 364	0
1	K	496/501 (99%)	0.23	30 (6%)	25	17	62, 122, 279, 368	0
1	L	496/501 (99%)	0.13	23 (4%)	36	25	60, 121, 278, 366	0
All	All	5952/6012 (99%)	0.21	352 (5%)	26	17	59, 121, 278, 369	0

The worst 5 of 352 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	285	GLY	13.7
1	E	501	THR	9.7
1	G	308	LYS	9.5
1	F	342	LYS	9.4
1	K	285	GLY	9.1

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 ⓘ

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
3	XEG	D	601	32/32	0.51	0.56	2.88	100,132,151,156	0
3	XEG	I	601	32/32	0.79	0.55	2.44	96,132,147,159	0
3	XEG	L	601	32/32	0.63	0.40	1.84	92,132,145,155	0
3	XEG	H	601	32/32	0.76	0.36	1.47	97,130,150,154	0
3	XEG	K	601	32/32	0.79	0.29	0.94	102,130,147,149	0
2	NDP	B	552	48/48	0.61	0.42	0.92	140,186,224,364	0
3	XEG	J	601	32/32	0.84	0.27	0.70	96,130,150,156	0
3	XEG	A	601	32/32	0.78	0.29	0.68	99,134,143,145	0
3	XEG	G	601	32/32	0.85	0.28	0.55	100,132,145,147	0
2	NDP	F	552	48/48	0.81	0.34	0.22	136,176,207,282	0
3	XEG	E	601	32/32	0.79	0.23	0.15	103,133,146,148	0
3	XEG	D	502	32/32	0.86	0.24	-0.10	89,132,147,152	0
3	XEG	B	601	32/32	0.86	0.22	-0.15	90,132,147,149	0
2	NDP	D	552	48/48	0.74	0.30	-0.16	140,184,224,364	0
2	NDP	I	552	48/48	0.79	0.28	-0.18	139,178,205,364	0
3	XEG	F	601	32/32	0.75	0.27	-0.18	101,132,147,148	0
2	NDP	C	552	48/48	0.81	0.32	-0.35	139,176,207,305	0
2	NDP	G	552	48/48	0.78	0.26	-0.41	134,178,204,311	0
2	NDP	L	552	48/48	0.82	0.22	-0.48	137,179,207,364	0
2	NDP	J	552	48/48	0.78	0.25	-0.51	123,184,207,309	0
2	NDP	H	552	48/48	0.75	0.25	-0.55	131,184,207,312	0
2	NDP	E	552	48/48	0.71	0.30	-0.65	139,181,209,278	0
2	NDP	K	552	48/48	0.79	0.26	-0.65	137,179,205,315	0
2	NDP	A	552	48/48	0.76	0.24	-0.68	138,182,210,364	0

6.5 Other polymers ⓘ

There are no such residues in this entry.