



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 6, 2025 – 04:13 PM EDT

PDB ID : 9YIS / pdb_00009yis
Title : Crystal structure of glutamate dehydrogenase from Babesia microti
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2025-10-02
Resolution : 2.18 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

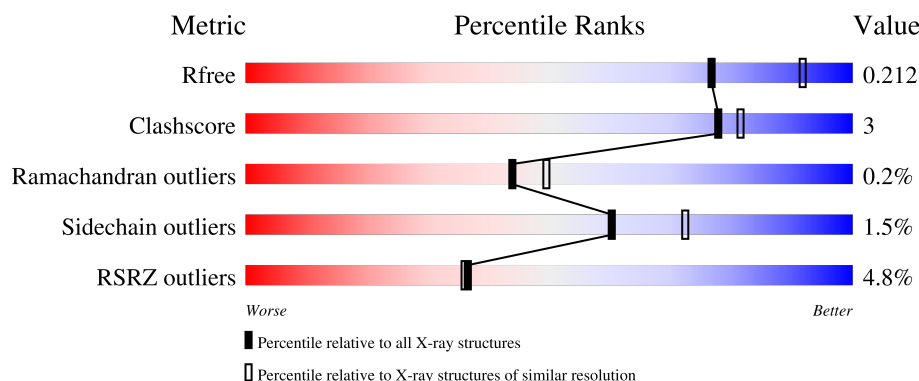
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.18 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}	164625	8336 (2.20-2.16)
Clashscore	180529	9404 (2.20-2.16)
Ramachandran outliers	177936	9297 (2.20-2.16)
Sidechain outliers	177891	9297 (2.20-2.16)
RSRZ outliers	164620	8337 (2.20-2.16)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	487	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> % </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 90% 6% . </div> </div>
1	B	487	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> 5% </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 89% 6% . . </div> </div>
1	C	487	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> 8% </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 89% 6% . . </div> </div>
1	D	487	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> 8% </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 89% 7% . </div> </div>
1	E	487	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> 4% </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 88% 7% . . </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	487	<div><div></div><div>2%</div><div>90%</div><div>6%</div><div></div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22270 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	467	Total	C	N	O	S	0	0	0
			3591	2278	611	683	19			
1	B	466	Total	C	N	O	S	0	0	0
			3569	2264	607	679	19			
1	C	466	Total	C	N	O	S	0	0	0
			3573	2266	607	681	19			
1	D	467	Total	C	N	O	S	0	0	0
			3573	2268	607	679	19			
1	E	467	Total	C	N	O	S	0	0	0
			3591	2278	611	683	19			
1	F	467	Total	C	N	O	S	0	0	0
			3591	2278	611	683	19			

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A0A0K3AUK4
A	-18	ALA	-	expression tag	UNP A0A0K3AUK4
A	-17	HIS	-	expression tag	UNP A0A0K3AUK4
A	-16	HIS	-	expression tag	UNP A0A0K3AUK4
A	-15	HIS	-	expression tag	UNP A0A0K3AUK4
A	-14	HIS	-	expression tag	UNP A0A0K3AUK4
A	-13	HIS	-	expression tag	UNP A0A0K3AUK4
A	-12	HIS	-	expression tag	UNP A0A0K3AUK4
A	-11	MET	-	expression tag	UNP A0A0K3AUK4
A	-10	GLY	-	expression tag	UNP A0A0K3AUK4
A	-9	THR	-	expression tag	UNP A0A0K3AUK4
A	-8	LEU	-	expression tag	UNP A0A0K3AUK4
A	-7	GLU	-	expression tag	UNP A0A0K3AUK4
A	-6	ALA	-	expression tag	UNP A0A0K3AUK4
A	-5	GLN	-	expression tag	UNP A0A0K3AUK4
A	-4	THR	-	expression tag	UNP A0A0K3AUK4
A	-3	GLN	-	expression tag	UNP A0A0K3AUK4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP A0A0K3AUK4
A	-1	PRO	-	expression tag	UNP A0A0K3AUK4
A	0	GLY	-	expression tag	UNP A0A0K3AUK4
A	1	SER	-	expression tag	UNP A0A0K3AUK4
B	-19	MET	-	initiating methionine	UNP A0A0K3AUK4
B	-18	ALA	-	expression tag	UNP A0A0K3AUK4
B	-17	HIS	-	expression tag	UNP A0A0K3AUK4
B	-16	HIS	-	expression tag	UNP A0A0K3AUK4
B	-15	HIS	-	expression tag	UNP A0A0K3AUK4
B	-14	HIS	-	expression tag	UNP A0A0K3AUK4
B	-13	HIS	-	expression tag	UNP A0A0K3AUK4
B	-12	HIS	-	expression tag	UNP A0A0K3AUK4
B	-11	MET	-	expression tag	UNP A0A0K3AUK4
B	-10	GLY	-	expression tag	UNP A0A0K3AUK4
B	-9	THR	-	expression tag	UNP A0A0K3AUK4
B	-8	LEU	-	expression tag	UNP A0A0K3AUK4
B	-7	GLU	-	expression tag	UNP A0A0K3AUK4
B	-6	ALA	-	expression tag	UNP A0A0K3AUK4
B	-5	GLN	-	expression tag	UNP A0A0K3AUK4
B	-4	THR	-	expression tag	UNP A0A0K3AUK4
B	-3	GLN	-	expression tag	UNP A0A0K3AUK4
B	-2	GLY	-	expression tag	UNP A0A0K3AUK4
B	-1	PRO	-	expression tag	UNP A0A0K3AUK4
B	0	GLY	-	expression tag	UNP A0A0K3AUK4
B	1	SER	-	expression tag	UNP A0A0K3AUK4
C	-19	MET	-	initiating methionine	UNP A0A0K3AUK4
C	-18	ALA	-	expression tag	UNP A0A0K3AUK4
C	-17	HIS	-	expression tag	UNP A0A0K3AUK4
C	-16	HIS	-	expression tag	UNP A0A0K3AUK4
C	-15	HIS	-	expression tag	UNP A0A0K3AUK4
C	-14	HIS	-	expression tag	UNP A0A0K3AUK4
C	-13	HIS	-	expression tag	UNP A0A0K3AUK4
C	-12	HIS	-	expression tag	UNP A0A0K3AUK4
C	-11	MET	-	expression tag	UNP A0A0K3AUK4
C	-10	GLY	-	expression tag	UNP A0A0K3AUK4
C	-9	THR	-	expression tag	UNP A0A0K3AUK4
C	-8	LEU	-	expression tag	UNP A0A0K3AUK4
C	-7	GLU	-	expression tag	UNP A0A0K3AUK4
C	-6	ALA	-	expression tag	UNP A0A0K3AUK4
C	-5	GLN	-	expression tag	UNP A0A0K3AUK4
C	-4	THR	-	expression tag	UNP A0A0K3AUK4
C	-3	GLN	-	expression tag	UNP A0A0K3AUK4

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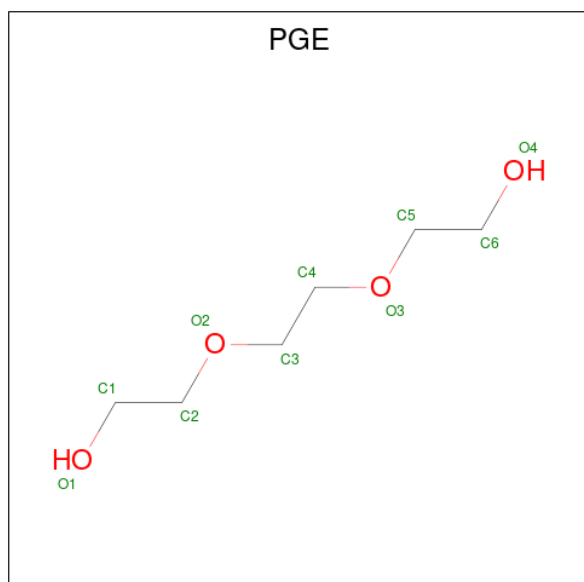
Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP A0A0K3AUK4
C	-1	PRO	-	expression tag	UNP A0A0K3AUK4
C	0	GLY	-	expression tag	UNP A0A0K3AUK4
C	1	SER	-	expression tag	UNP A0A0K3AUK4
D	-19	MET	-	initiating methionine	UNP A0A0K3AUK4
D	-18	ALA	-	expression tag	UNP A0A0K3AUK4
D	-17	HIS	-	expression tag	UNP A0A0K3AUK4
D	-16	HIS	-	expression tag	UNP A0A0K3AUK4
D	-15	HIS	-	expression tag	UNP A0A0K3AUK4
D	-14	HIS	-	expression tag	UNP A0A0K3AUK4
D	-13	HIS	-	expression tag	UNP A0A0K3AUK4
D	-12	HIS	-	expression tag	UNP A0A0K3AUK4
D	-11	MET	-	expression tag	UNP A0A0K3AUK4
D	-10	GLY	-	expression tag	UNP A0A0K3AUK4
D	-9	THR	-	expression tag	UNP A0A0K3AUK4
D	-8	LEU	-	expression tag	UNP A0A0K3AUK4
D	-7	GLU	-	expression tag	UNP A0A0K3AUK4
D	-6	ALA	-	expression tag	UNP A0A0K3AUK4
D	-5	GLN	-	expression tag	UNP A0A0K3AUK4
D	-4	THR	-	expression tag	UNP A0A0K3AUK4
D	-3	GLN	-	expression tag	UNP A0A0K3AUK4
D	-2	GLY	-	expression tag	UNP A0A0K3AUK4
D	-1	PRO	-	expression tag	UNP A0A0K3AUK4
D	0	GLY	-	expression tag	UNP A0A0K3AUK4
D	1	SER	-	expression tag	UNP A0A0K3AUK4
E	-19	MET	-	initiating methionine	UNP A0A0K3AUK4
E	-18	ALA	-	expression tag	UNP A0A0K3AUK4
E	-17	HIS	-	expression tag	UNP A0A0K3AUK4
E	-16	HIS	-	expression tag	UNP A0A0K3AUK4
E	-15	HIS	-	expression tag	UNP A0A0K3AUK4
E	-14	HIS	-	expression tag	UNP A0A0K3AUK4
E	-13	HIS	-	expression tag	UNP A0A0K3AUK4
E	-12	HIS	-	expression tag	UNP A0A0K3AUK4
E	-11	MET	-	expression tag	UNP A0A0K3AUK4
E	-10	GLY	-	expression tag	UNP A0A0K3AUK4
E	-9	THR	-	expression tag	UNP A0A0K3AUK4
E	-8	LEU	-	expression tag	UNP A0A0K3AUK4
E	-7	GLU	-	expression tag	UNP A0A0K3AUK4
E	-6	ALA	-	expression tag	UNP A0A0K3AUK4
E	-5	GLN	-	expression tag	UNP A0A0K3AUK4
E	-4	THR	-	expression tag	UNP A0A0K3AUK4
E	-3	GLN	-	expression tag	UNP A0A0K3AUK4

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	expression tag	UNP A0A0K3AUK4
E	-1	PRO	-	expression tag	UNP A0A0K3AUK4
E	0	GLY	-	expression tag	UNP A0A0K3AUK4
E	1	SER	-	expression tag	UNP A0A0K3AUK4
F	-19	MET	-	initiating methionine	UNP A0A0K3AUK4
F	-18	ALA	-	expression tag	UNP A0A0K3AUK4
F	-17	HIS	-	expression tag	UNP A0A0K3AUK4
F	-16	HIS	-	expression tag	UNP A0A0K3AUK4
F	-15	HIS	-	expression tag	UNP A0A0K3AUK4
F	-14	HIS	-	expression tag	UNP A0A0K3AUK4
F	-13	HIS	-	expression tag	UNP A0A0K3AUK4
F	-12	HIS	-	expression tag	UNP A0A0K3AUK4
F	-11	MET	-	expression tag	UNP A0A0K3AUK4
F	-10	GLY	-	expression tag	UNP A0A0K3AUK4
F	-9	THR	-	expression tag	UNP A0A0K3AUK4
F	-8	LEU	-	expression tag	UNP A0A0K3AUK4
F	-7	GLU	-	expression tag	UNP A0A0K3AUK4
F	-6	ALA	-	expression tag	UNP A0A0K3AUK4
F	-5	GLN	-	expression tag	UNP A0A0K3AUK4
F	-4	THR	-	expression tag	UNP A0A0K3AUK4
F	-3	GLN	-	expression tag	UNP A0A0K3AUK4
F	-2	GLY	-	expression tag	UNP A0A0K3AUK4
F	-1	PRO	-	expression tag	UNP A0A0K3AUK4
F	0	GLY	-	expression tag	UNP A0A0K3AUK4
F	1	SER	-	expression tag	UNP A0A0K3AUK4

- Molecule 2 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).

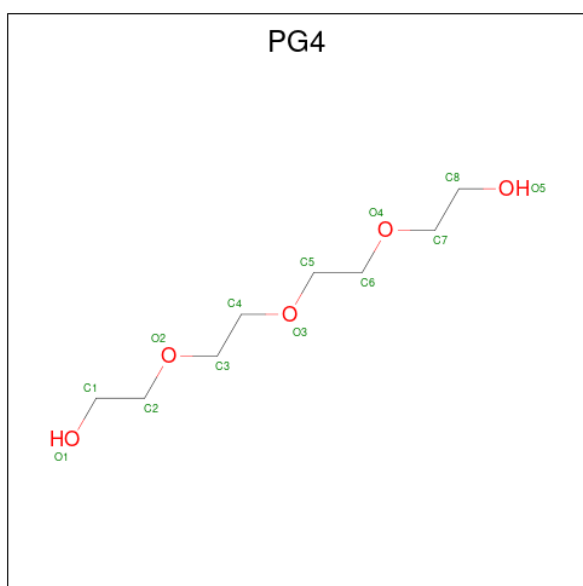


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	6	4		
2	B	1	Total	C	O	0	0
			10	6	4		
2	C	1	Total	C	O	0	0
			10	6	4		
2	D	1	Total	C	O	0	0
			10	6	4		
2	E	1	Total	C	O	0	0
			10	6	4		
2	F	1	Total	C	O	0	0
			10	6	4		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	D	1	Total	Na	0	0
			1	1		

- Molecule 4 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			13	8	5		
4	D	1	Total	C	O	0	0
			13	8	5		

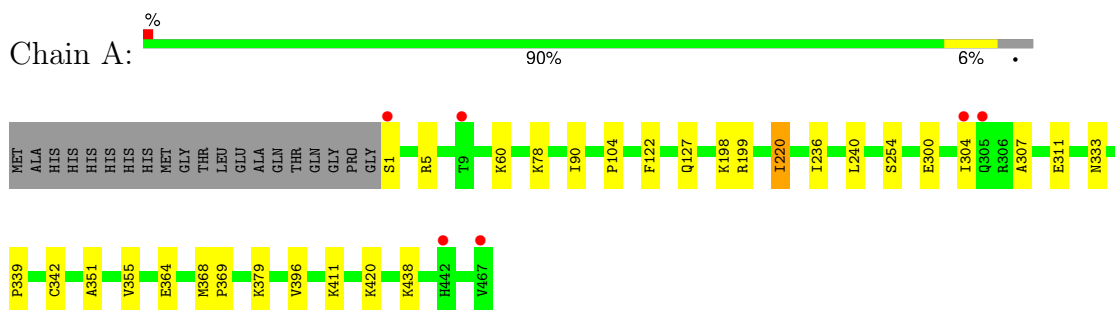
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	143	Total 143	O 143	0	0
5	B	94	Total 94	O 94	0	0
5	C	105	Total 105	O 105	0	0
5	D	103	Total 103	O 103	0	0
5	E	104	Total 104	O 104	0	0
5	F	145	Total 145	O 145	0	0

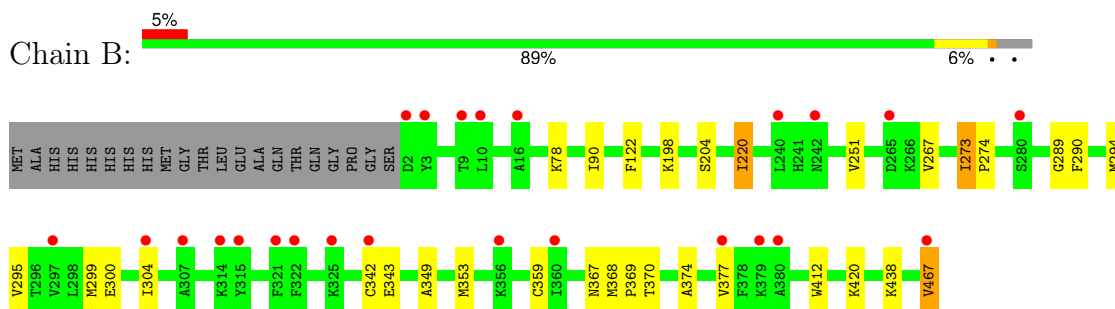
3 Residue-property plots

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

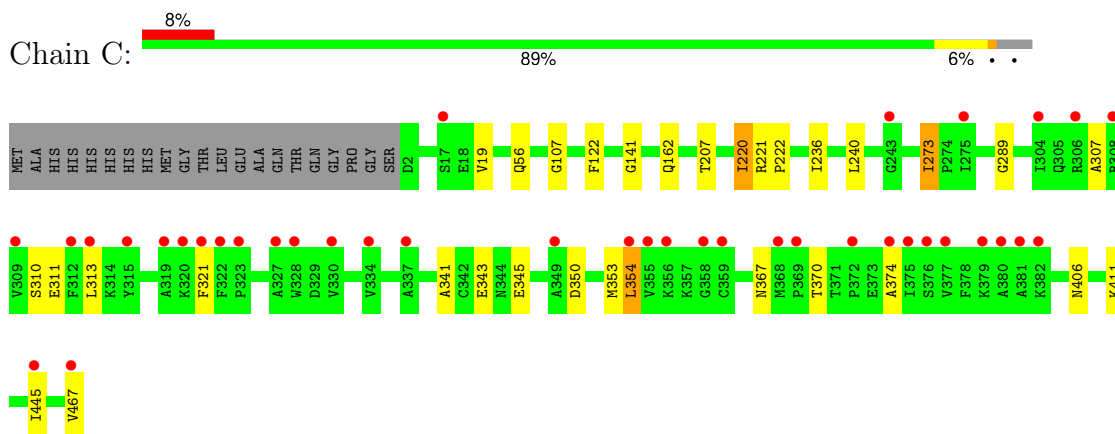
- Molecule 1: Glutamate dehydrogenase




- Molecule 1: Glutamate dehydrogenase

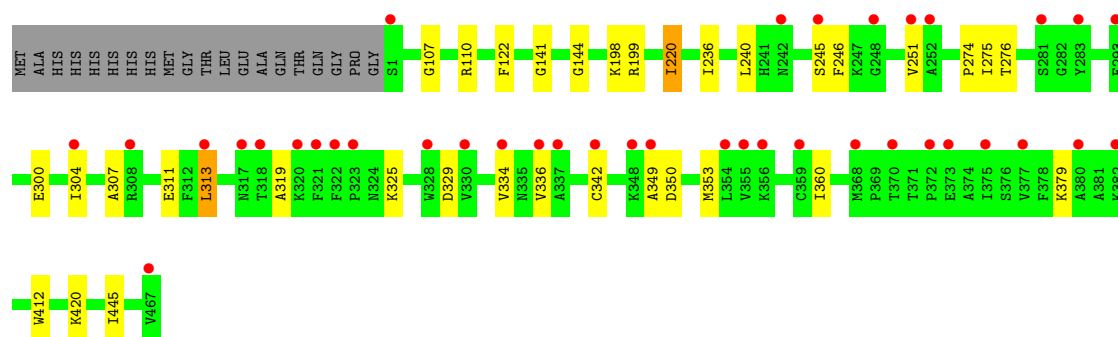


- Molecule 1: Glutamate dehydrogenase




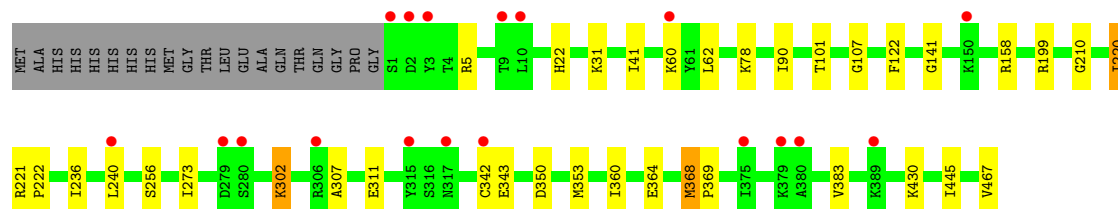
- Molecule 1: Glutamate dehydrogenase

Chain D: 




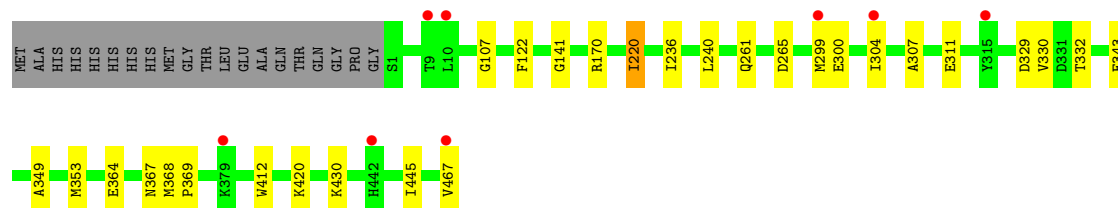
• Molecule 1: Glutamate dehydrogenase

Chain E: 



• Molecule 1: Glutamate dehydrogenase

Chain F: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	154.07Å 197.30Å 229.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.58 – 2.18 48.58 – 2.18	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.58-2.18) 100.0 (48.58-2.18)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.18Å)	Xtrriage
Refinement program	PHENIX (dev_5438: ???)	Depositor
R, R_{free}	0.183 , 0.209 0.189 , 0.212	Depositor DCC
R_{free} test set	9005 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	34.0	Xtrriage
Anisotropy	0.536	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 32.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	22270	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.17 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.9193e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: NA, PG4, PGE

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	0.22	0/3665	0.42	0/4944
1	B	0.22	0/3643	0.42	0/4919
1	C	0.21	0/3647	0.38	0/4924
1	D	0.21	0/3647	0.41	0/4923
1	E	0.21	0/3665	0.40	0/4944
1	F	0.22	0/3665	0.42	0/4944
All	All	0.21	0/21932	0.41	0/29598

There are no bond length outliers.

There are no bond angle outliers.

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	3591	0	3559	13	0
1	B	3569	0	3514	23	0
1	C	3573	0	3518	21	0
1	D	3573	0	3529	20	0
1	E	3591	0	3559	23	0
1	F	3591	0	3559	18	0
2	A	10	0	14	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	10	0	14	1	0
2	C	10	0	14	2	0
2	D	10	0	14	0	0
2	E	10	0	14	0	0
2	F	10	0	14	0	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
4	C	13	0	18	0	0
4	D	13	0	18	0	0
5	A	143	0	0	0	0
5	B	94	0	0	1	0
5	C	105	0	0	2	0
5	D	103	0	0	0	0
5	E	104	0	0	1	0
5	F	145	0	0	2	0
All	All	22270	0	21358	114	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 3.

All (114) 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:329:ASP:OD1	1:F:353:MET:HE1	1.86	0.76
1:B:251:VAL:CG2	1:B:274:PRO:HA	2.16	0.75
1:F:240:LEU:HD11	1:F:445:ILE:HD11	1.70	0.73
1:F:300:GLU:HG3	1:F:304:ILE:HD12	1.70	0.72
1:D:251:VAL:HG12	1:D:336:VAL:HB	1.73	0.71
1:D:307:ALA:HB1	1:D:311:GLU:HG3	1.72	0.71
1:F:236:ILE:HG23	1:F:240:LEU:HD12	1.74	0.68
1:A:300:GLU:HG2	1:A:304:ILE:HD12	1.78	0.66
1:C:310:SER:O	1:C:313:LEU:HD13	1.95	0.66
1:B:290:PHE:HA	1:B:294:MET:HE2	1.77	0.65
1:B:251:VAL:HG22	1:B:274:PRO:HA	1.80	0.62
1:B:251:VAL:HG23	1:B:274:PRO:HA	1.81	0.61
1:E:467:VAL:O	1:E:467:VAL:HG13	2.01	0.60
1:D:240:LEU:HD11	1:D:445:ILE:HD11	1.85	0.58
1:E:360:ILE:C	1:E:383:VAL:HG13	2.28	0.58
1:E:236:ILE:HG23	1:E:240:LEU:HD12	1.86	0.57
1:E:5:ARG:NH1	1:E:60:LYS:HD3	2.20	0.57
1:C:313:LEU:HD11	1:C:321:PHE:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:240:LEU:HD11	1:E:445:ILE:HD11	1.87	0.57
1:F:261:GLN:HB3	1:F:299:MET:HE3	1.86	0.56
1:E:78:LYS:HG3	1:E:90:ILE:HG23	1.88	0.55
1:A:307:ALA:HB1	1:A:311:GLU:HG3	1.87	0.55
1:B:78:LYS:HG3	1:B:90:ILE:HG23	1.89	0.53
1:B:251:VAL:HG21	1:B:267:VAL:HG11	1.90	0.53
1:B:220:ILE:HG22	1:B:220:ILE:O	2.07	0.53
1:D:236:ILE:HG23	1:D:240:LEU:HD12	1.90	0.53
1:B:412:TRP:CZ3	1:B:420:LYS:HD2	2.44	0.53
1:E:221:ARG:HB3	1:E:222:PRO:HD3	1.91	0.52
1:C:350:ASP:O	1:C:354:LEU:HD22	2.10	0.51
1:D:350:ASP:HA	1:D:353:MET:HE2	1.91	0.51
1:F:364:GLU:CD	1:F:369:PRO:HD2	2.35	0.51
1:B:251:VAL:CG2	1:B:274:PRO:CA	2.89	0.50
1:E:220:ILE:HG22	1:E:220:ILE:O	2.11	0.50
1:C:273:ILE:HG23	1:C:289:GLY:HA3	1.94	0.50
1:A:78:LYS:HG3	1:A:90:ILE:HG23	1.94	0.50
1:C:240:LEU:HD11	1:C:445:ILE:HD11	1.94	0.49
1:A:364:GLU:CD	1:A:369:PRO:HD2	2.37	0.49
1:B:251:VAL:HG22	1:B:274:PRO:CA	2.41	0.49
1:A:198:LYS:NZ	5:C:602:HOH:O	2.44	0.49
2:B:501:PGE:H22	5:B:601:HOH:O	2.13	0.49
1:C:236:ILE:HG23	1:C:240:LEU:HD12	1.95	0.49
1:B:251:VAL:HG22	1:B:273:ILE:C	2.38	0.48
1:A:220:ILE:HG22	1:A:220:ILE:O	2.13	0.48
1:B:251:VAL:HG23	1:B:251:VAL:O	2.13	0.48
1:C:406:ASN:HA	2:C:502:PGE:H3	1.96	0.48
1:D:334:VAL:O	1:D:334:VAL:HG23	2.14	0.47
1:B:300:GLU:HG3	1:B:304:ILE:HG13	1.94	0.47
1:C:341:ALA:HB3	1:C:345:GLU:OE1	2.14	0.47
1:F:220:ILE:HG22	1:F:220:ILE:O	2.14	0.47
1:D:251:VAL:CG2	1:D:274:PRO:HA	2.44	0.47
2:C:502:PGE:H22	5:C:644:HOH:O	2.15	0.47
1:F:261:GLN:HB3	1:F:299:MET:CE	2.45	0.47
1:B:251:VAL:HG22	1:B:273:ILE:O	2.14	0.46
1:D:199:ARG:HD2	1:E:467:VAL:HG22	1.97	0.46
1:D:300:GLU:HG2	1:D:304:ILE:HD12	1.96	0.46
1:B:343:GLU:HG3	1:B:367:ASN:O	2.15	0.46
1:C:350:ASP:HA	1:C:353:MET:HE2	1.98	0.46
1:E:256:SER:HB2	1:E:302:LYS:HG3	1.98	0.45
1:E:307:ALA:HB1	1:E:311:GLU:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:307:ALA:HB1	1:C:311:GLU:HG3	1.99	0.45
1:E:342:CYS:SG	1:E:343:GLU:N	2.90	0.45
1:B:349:ALA:O	1:B:353:MET:HG3	2.17	0.45
1:A:127:GLN:OE1	1:A:396:VAL:HG11	2.17	0.45
1:A:351:ALA:O	1:A:355:VAL:HG23	2.16	0.45
1:B:273:ILE:HG22	1:B:289:GLY:HA3	1.98	0.44
1:E:368:MET:N	1:E:369:PRO:HD3	2.32	0.44
1:F:307:ALA:HB1	1:F:311:GLU:HG3	1.98	0.44
1:C:220:ILE:O	1:C:220:ILE:HG22	2.18	0.44
1:D:275:ILE:HG13	1:D:276:THR:HG23	2.00	0.44
1:C:343:GLU:HG3	1:C:367:ASN:O	2.18	0.44
1:D:313:LEU:HD22	1:D:319:ALA:CB	2.48	0.44
1:E:31:LYS:HG2	1:E:41:ILE:HD13	2.00	0.44
1:E:364:GLU:CD	1:E:369:PRO:HD2	2.43	0.44
1:C:19:VAL:HG21	1:C:56:GLN:HG2	1.99	0.43
1:D:220:ILE:O	1:D:220:ILE:HG22	2.17	0.43
1:A:199:ARG:HD2	1:C:467:VAL:HG22	2.00	0.43
1:E:210:GLY:HA2	1:E:221:ARG:CD	2.49	0.43
1:A:236:ILE:HG23	1:A:240:LEU:HD12	1.99	0.43
1:F:368:MET:N	1:F:369:PRO:HD3	2.34	0.43
1:C:207:THR:O	1:C:207:THR:HG22	2.18	0.43
1:B:251:VAL:HG11	1:B:267:VAL:HG11	2.00	0.43
1:F:349:ALA:O	1:F:353:MET:HG3	2.19	0.42
1:B:295:VAL:O	1:B:299:MET:HG3	2.20	0.42
1:A:104:PRO:HD3	1:B:204:SER:HB2	2.01	0.42
1:D:349:ALA:O	1:D:353:MET:HG3	2.19	0.42
1:E:199:ARG:HD2	1:F:467:VAL:CG2	2.49	0.42
1:D:412:TRP:CZ3	1:D:420:LYS:HD2	2.55	0.42
1:F:353:MET:HE2	5:F:694:HOH:O	2.19	0.42
1:C:370:THR:HG22	1:C:374:ALA:HB3	2.01	0.42
1:C:107:GLY:HA3	1:C:141:GLY:O	2.20	0.41
1:B:467:VAL:HG11	1:C:162:GLN:OE1	2.21	0.41
1:C:221:ARG:HB3	1:C:222:PRO:HD3	2.01	0.41
1:F:343:GLU:HG3	1:F:367:ASN:O	2.20	0.41
1:D:198:LYS:NZ	1:E:101:THR:HA	2.35	0.41
1:D:325:LYS:NZ	1:D:329:ASP:OD2	2.48	0.41
1:F:330:VAL:HG22	1:F:332:THR:HG22	2.03	0.41
1:F:412:TRP:CZ3	1:F:420:LYS:HD2	2.56	0.41
1:F:265:ASP:HB3	5:F:671:HOH:O	2.20	0.41
1:E:107:GLY:HA3	1:E:141:GLY:O	2.21	0.41
1:E:210:GLY:HA2	1:E:221:ARG:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:107:GLY:HA3	1:F:141:GLY:O	2.21	0.41
1:D:110:ARG:O	1:D:144:GLY:HA3	2.21	0.41
1:B:370:THR:HG22	1:B:374:ALA:HB3	2.02	0.41
1:C:313:LEU:HD12	1:C:313:LEU:H	1.86	0.41
1:A:5:ARG:NH1	1:A:60:LYS:HD3	2.35	0.41
1:B:368:MET:N	1:B:369:PRO:HD3	2.36	0.41
1:E:158:ARG:NE	5:E:602:HOH:O	2.46	0.41
1:E:350:ASP:HA	1:E:353:MET:HE2	2.02	0.41
1:D:107:GLY:HA3	1:D:141:GLY:O	2.21	0.40
1:D:251:VAL:HG22	1:D:274:PRO:HA	2.03	0.40
1:E:22:HIS:HB3	1:E:62:LEU:CD2	2.52	0.40
1:A:254:SER:OG	1:A:339:PRO:HA	2.21	0.40
1:C:313:LEU:HD12	1:C:313:LEU:N	2.36	0.40
1:D:245:SER:OG	1:D:246:PHE:N	2.54	0.40

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	465/487 (96%)	457 (98%)	7 (2%)	1 (0%)	44	49
1	B	464/487 (95%)	459 (99%)	4 (1%)	1 (0%)	44	49
1	C	464/487 (95%)	459 (99%)	4 (1%)	1 (0%)	44	49
1	D	465/487 (96%)	459 (99%)	5 (1%)	1 (0%)	44	49
1	E	465/487 (96%)	458 (98%)	6 (1%)	1 (0%)	44	49
1	F	465/487 (96%)	458 (98%)	6 (1%)	1 (0%)	44	49
All	All	2788/2922 (95%)	2750 (99%)	32 (1%)	6 (0%)	44	49

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	220	ILE
1	B	220	ILE
1	C	220	ILE
1	D	220	ILE
1	E	220	ILE
1	F	220	ILE

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	386/401 (96%)	377 (98%)	9 (2%)	45	56
1	B	381/401 (95%)	373 (98%)	8 (2%)	48	60
1	C	382/401 (95%)	378 (99%)	4 (1%)	73	82
1	D	382/401 (95%)	377 (99%)	5 (1%)	65	76
1	E	386/401 (96%)	381 (99%)	5 (1%)	65	76
1	F	386/401 (96%)	383 (99%)	3 (1%)	79	87
All	All	2303/2406 (96%)	2269 (98%)	34 (2%)	60	72

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	122	PHE
1	A	333	ASN
1	A	342	CYS
1	A	368	MET
1	A	379	LYS
1	A	411	LYS
1	A	420	LYS
1	A	438	LYS
1	B	122	PHE
1	B	198	LYS
1	B	273	ILE
1	B	342	CYS

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Mol	Chain	Res	Type
1	B	359	CYS
1	B	377	VAL
1	B	438	LYS
1	B	467	VAL
1	C	122	PHE
1	C	273	ILE
1	C	354	LEU
1	C	411	LYS
1	D	122	PHE
1	D	313	LEU
1	D	342	CYS
1	D	360	ILE
1	D	379	LYS
1	E	122	PHE
1	E	273	ILE
1	E	302	LYS
1	E	368	MET
1	E	430	LYS
1	F	122	PHE
1	F	170	ARG
1	F	430	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	344	ASN
1	B	422	GLN
1	B	440	ASN
1	C	127	GLN
1	C	162	GLN
1	C	344	ASN
1	C	440	ASN
1	D	440	ASN
1	E	155	ASN
1	E	344	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	PG4	C	501	-	12,12,12	0.32	0	11,11,11	0.30	0
2	PGE	E	501	-	9,9,9	0.32	0	8,8,8	0.66	0
4	PG4	D	501	-	12,12,12	0.31	0	11,11,11	0.27	0
2	PGE	F	501	-	9,9,9	0.34	0	8,8,8	0.73	0
2	PGE	A	501	-	9,9,9	0.35	0	8,8,8	0.53	0
2	PGE	D	502	-	9,9,9	0.30	0	8,8,8	0.46	0
2	PGE	B	501	-	9,9,9	0.35	0	8,8,8	0.66	0
2	PGE	C	502	-	9,9,9	0.34	0	8,8,8	0.78	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PG4	C	501	-	-	1/10/10/10	-
2	PGE	E	501	-	-	4/7/7/7	-
4	PG4	D	501	-	-	1/10/10/10	-
2	PGE	F	501	-	-	4/7/7/7	-
2	PGE	A	501	-	-	4/7/7/7	-
2	PGE	D	502	-	-	4/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PGE	B	501	-	-	5/7/7/7	-
2	PGE	C	502	-	-	4/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	502	PGE	O1-C1-C2-O2
2	E	501	PGE	O1-C1-C2-O2
2	F	501	PGE	O1-C1-C2-O2
2	A	501	PGE	O3-C5-C6-O4
2	E	501	PGE	O3-C5-C6-O4
2	A	501	PGE	O1-C1-C2-O2
2	A	501	PGE	C1-C2-O2-C3
2	D	502	PGE	C4-C3-O2-C2
2	D	502	PGE	C1-C2-O2-C3
2	C	502	PGE	O3-C5-C6-O4
2	D	502	PGE	O1-C1-C2-O2
2	B	501	PGE	C1-C2-O2-C3
2	F	501	PGE	C4-C3-O2-C2
2	A	501	PGE	C4-C3-O2-C2
2	B	501	PGE	C4-C3-O2-C2
2	C	502	PGE	C4-C3-O2-C2
2	D	502	PGE	C3-C4-O3-C5
4	D	501	PG4	C1-C2-O2-C3
2	F	501	PGE	C1-C2-O2-C3
2	C	502	PGE	C1-C2-O2-C3
2	B	501	PGE	O1-C1-C2-O2
2	B	501	PGE	O2-C3-C4-O3
2	E	501	PGE	C1-C2-O2-C3
2	B	501	PGE	O3-C5-C6-O4
4	C	501	PG4	O2-C3-C4-O3
2	F	501	PGE	C3-C4-O3-C5
2	E	501	PGE	C4-C3-O2-C2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	PGE	1	0
2	C	502	PGE	2	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(Å ²)	Q<0.9
1	A	467/487 (95%)	-0.03	6 (1%) 74 73	29, 41, 63, 82	0
1	B	466/487 (95%)	0.34	24 (5%) 34 33	29, 54, 90, 112	0
1	C	466/487 (95%)	0.39	39 (8%) 18 18	31, 47, 103, 137	0
1	D	467/487 (95%)	0.40	39 (8%) 18 18	30, 47, 98, 122	0
1	E	467/487 (95%)	0.17	18 (3%) 44 43	28, 46, 80, 102	0
1	F	467/487 (95%)	-0.01	8 (1%) 69 67	30, 39, 63, 96	0
All	All	2800/2922 (95%)	0.21	134 (4%) 36 36	28, 45, 90, 137	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	304	ILE	4.9
1	D	334	VAL	4.3
1	C	368	MET	4.2
1	F	379	LYS	4.1
1	E	379	LYS	4.0
1	D	377	VAL	3.8
1	C	312	PHE	3.8
1	D	373	GLU	3.6
1	C	315	TYR	3.5
1	D	355	VAL	3.5
1	F	442	HIS	3.5
1	C	354	LEU	3.5
1	B	380	ALA	3.4
1	C	308	ARG	3.4
1	C	356	LYS	3.3
1	B	467	VAL	3.3
1	C	323	PRO	3.3
1	D	380	ALA	3.2
1	D	1	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	304	ILE	3.2
1	D	356	LYS	3.2
1	C	380	ALA	3.2
1	D	321	PHE	3.1
1	C	309	VAL	3.1
1	D	322	PHE	3.1
1	D	368	MET	3.1
1	E	342	CYS	3.1
1	B	10	LEU	3.0
1	C	328	TRP	3.0
1	B	315	TYR	3.0
1	D	304	ILE	3.0
1	E	317	ASN	3.0
1	B	377	VAL	2.9
1	C	321	PHE	2.9
1	F	299	MET	2.9
1	D	251	VAL	2.9
1	C	334	VAL	2.9
1	A	9	THR	2.9
1	B	342	CYS	2.9
1	B	2	ASP	2.8
1	A	442	HIS	2.8
1	B	16	ALA	2.8
1	C	377	VAL	2.8
1	D	281	SER	2.8
1	B	379	LYS	2.7
1	D	317	ASN	2.7
1	C	349	ALA	2.7
1	D	337	ALA	2.7
1	D	349	ALA	2.7
1	B	240	LEU	2.7
1	C	322	PHE	2.7
1	D	359	CYS	2.6
1	C	467	VAL	2.6
1	C	320	LYS	2.6
1	D	382	LYS	2.6
1	F	10	LEU	2.6
1	B	297	VAL	2.6
1	F	9	THR	2.6
1	D	248	GLY	2.5
1	C	374	ALA	2.5
1	D	320	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	279	ASP	2.5
1	B	242	ASN	2.5
1	C	359	CYS	2.5
1	C	327	ALA	2.5
1	E	380	ALA	2.5
1	D	348	LYS	2.5
1	C	313	LEU	2.5
1	C	355	VAL	2.5
1	D	467	VAL	2.5
1	F	467	VAL	2.5
1	C	369	PRO	2.4
1	C	372	PRO	2.4
1	C	304	ILE	2.4
1	C	445	ILE	2.4
1	D	375	ILE	2.4
1	C	379	LYS	2.4
1	E	389	LYS	2.4
1	B	3	TYR	2.4
1	C	319	ALA	2.4
1	E	240	LEU	2.4
1	D	328	TRP	2.4
1	D	323	PRO	2.4
1	B	265	ASP	2.4
1	C	358	GLY	2.4
1	C	375	ILE	2.4
1	E	375	ILE	2.4
1	B	356	LYS	2.3
1	A	1	SER	2.3
1	B	360	ILE	2.3
1	D	242	ASN	2.3
1	D	330	VAL	2.3
1	E	1	SER	2.3
1	E	150	LYS	2.2
1	B	307	ALA	2.2
1	B	321	PHE	2.2
1	D	283	TYR	2.2
1	F	315	TYR	2.2
1	B	314	LYS	2.2
1	E	60	LYS	2.2
1	C	330	VAL	2.2
1	C	275	ILE	2.2
1	D	354	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	370	THR	2.2
1	D	372	PRO	2.2
1	E	306	ARG	2.2
1	D	342	CYS	2.2
1	A	467	VAL	2.2
1	D	318	THR	2.1
1	C	337	ALA	2.1
1	C	381	ALA	2.1
1	D	252	ALA	2.1
1	D	308	ARG	2.1
1	E	280	SER	2.1
1	E	3	TYR	2.1
1	A	304	ILE	2.1
1	B	322	PHE	2.1
1	D	313	LEU	2.1
1	E	10	LEU	2.1
1	B	280	SER	2.1
1	C	376	SER	2.1
1	D	293	GLU	2.1
1	D	336	VAL	2.1
1	B	325	LYS	2.1
1	D	245	SER	2.1
1	B	9	THR	2.1
1	C	243	GLY	2.0
1	E	315	TYR	2.0
1	C	306	ARG	2.0
1	E	2	ASP	2.0
1	C	17	SER	2.0
1	A	305	GLN	2.0
1	E	9	THR	2.0
1	C	382	LYS	2.0

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 oligosaccharides 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. 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	B-factors(Å ²)	Q<0.9
2	PGE	B	501	10/10	0.84	0.14	38,39,49,51	0
2	PGE	D	502	10/10	0.84	0.13	35,41,44,53	0
2	PGE	E	501	10/10	0.85	0.15	34,38,45,51	0
2	PGE	F	501	10/10	0.86	0.13	33,39,48,49	0
4	PG4	C	501	13/13	0.86	0.13	49,51,59,60	0
2	PGE	A	501	10/10	0.88	0.13	31,39,47,49	0
2	PGE	C	502	10/10	0.88	0.12	36,43,50,50	0
4	PG4	D	501	13/13	0.90	0.12	42,49,53,53	0
3	NA	D	503	1/1	0.97	0.08	35,35,35,35	0
3	NA	A	502	1/1	0.98	0.04	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.