wwPDB X-ray Structure Validation Summary Report (i)

Mar 5, 2024 – 06:38 PM EST

PDB ID	:	3AOG
Title	:	Crystal structure of glutamate dehydrogenase (GdhB) from Thermus thermophilus (Glu bound form)
Authors	:	Tomita, T.; Kuzuyama, T.; Nishiyama, M.
Deposited on	:	2010-09-28
Resolution	:	2.10 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

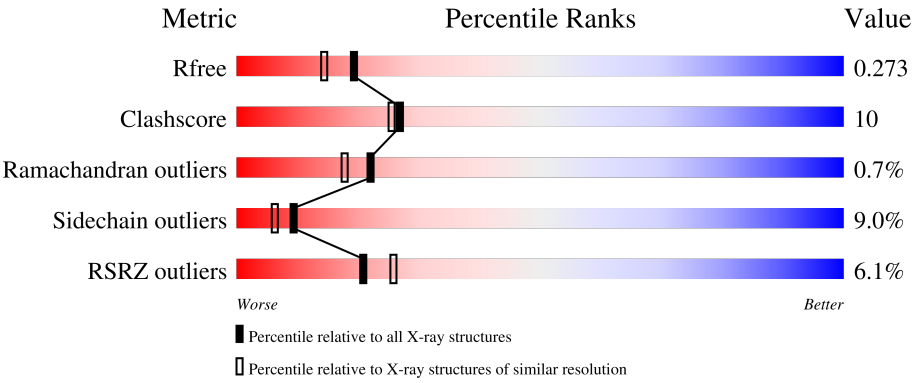
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 <=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	440	3% 70% 22%
1	B	440	5% 73% 19%
1	C	440	5% 75% 18%
1	D	440	8% 72% 22%
1	E	440	5% 71% 21%

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Mol	Chain	Length	Quality of chain
1	F	440	10% 75% 19%
1	G	440	3% 73% 19%
1	H	440	6% 72% 19% 5%
1	I	440	4% 73% 20%
1	J	440	4% 72% 20%
1	K	440	12% 71% 20% 5%
1	L	440	5% 72% 20%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 40944 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	421	Total	C	N	O	S	0	0	0
			3236	2057	582	591	6			
1	B	421	Total	C	N	O	S	0	0	0
			3236	2057	582	591	6			
1	C	421	Total	C	N	O	S	0	2	0
			3248	2065	583	594	6			
1	D	421	Total	C	N	O	S	0	0	0
			3236	2057	582	591	6			
1	E	421	Total	C	N	O	S	0	0	0
			3236	2057	582	591	6			
1	F	421	Total	C	N	O	S	8	1	0
			3244	2062	585	591	6			
1	G	421	Total	C	N	O	S	0	1	0
			3244	2062	585	591	6			
1	H	421	Total	C	N	O	S	0	2	0
			3252	2067	588	591	6			
1	I	421	Total	C	N	O	S	0	1	0
			3244	2062	585	591	6			
1	J	421	Total	C	N	O	S	0	1	0
			3244	2062	585	591	6			
1	K	416	Total	C	N	O	S	0	0	0
			3187	2025	570	586	6			
1	L	421	Total	C	N	O	S	0	0	0
			3236	2057	582	591	6			

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	expression tag	UNP Q72IC1
A	-14	GLY	-	expression tag	UNP Q72IC1
A	-13	SER	-	expression tag	UNP Q72IC1
A	-12	SER	-	expression tag	UNP Q72IC1
A	-11	HIS	-	expression tag	UNP Q72IC1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	HIS	-	expression tag	UNP Q72IC1
A	-9	HIS	-	expression tag	UNP Q72IC1
A	-8	HIS	-	expression tag	UNP Q72IC1
A	-7	HIS	-	expression tag	UNP Q72IC1
A	-6	HIS	-	expression tag	UNP Q72IC1
A	-5	SER	-	expression tag	UNP Q72IC1
A	-4	GLN	-	expression tag	UNP Q72IC1
A	-3	ASP	-	expression tag	UNP Q72IC1
A	-2	PRO	-	expression tag	UNP Q72IC1
A	-1	ASN	-	expression tag	UNP Q72IC1
A	0	SER	-	expression tag	UNP Q72IC1
B	-15	MET	-	expression tag	UNP Q72IC1
B	-14	GLY	-	expression tag	UNP Q72IC1
B	-13	SER	-	expression tag	UNP Q72IC1
B	-12	SER	-	expression tag	UNP Q72IC1
B	-11	HIS	-	expression tag	UNP Q72IC1
B	-10	HIS	-	expression tag	UNP Q72IC1
B	-9	HIS	-	expression tag	UNP Q72IC1
B	-8	HIS	-	expression tag	UNP Q72IC1
B	-7	HIS	-	expression tag	UNP Q72IC1
B	-6	HIS	-	expression tag	UNP Q72IC1
B	-5	SER	-	expression tag	UNP Q72IC1
B	-4	GLN	-	expression tag	UNP Q72IC1
B	-3	ASP	-	expression tag	UNP Q72IC1
B	-2	PRO	-	expression tag	UNP Q72IC1
B	-1	ASN	-	expression tag	UNP Q72IC1
B	0	SER	-	expression tag	UNP Q72IC1
C	-15	MET	-	expression tag	UNP Q72IC1
C	-14	GLY	-	expression tag	UNP Q72IC1
C	-13	SER	-	expression tag	UNP Q72IC1
C	-12	SER	-	expression tag	UNP Q72IC1
C	-11	HIS	-	expression tag	UNP Q72IC1
C	-10	HIS	-	expression tag	UNP Q72IC1
C	-9	HIS	-	expression tag	UNP Q72IC1
C	-8	HIS	-	expression tag	UNP Q72IC1
C	-7	HIS	-	expression tag	UNP Q72IC1
C	-6	HIS	-	expression tag	UNP Q72IC1
C	-5	SER	-	expression tag	UNP Q72IC1
C	-4	GLN	-	expression tag	UNP Q72IC1
C	-3	ASP	-	expression tag	UNP Q72IC1
C	-2	PRO	-	expression tag	UNP Q72IC1
C	-1	ASN	-	expression tag	UNP Q72IC1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	SER	-	expression tag	UNP Q72IC1
D	-15	MET	-	expression tag	UNP Q72IC1
D	-14	GLY	-	expression tag	UNP Q72IC1
D	-13	SER	-	expression tag	UNP Q72IC1
D	-12	SER	-	expression tag	UNP Q72IC1
D	-11	HIS	-	expression tag	UNP Q72IC1
D	-10	HIS	-	expression tag	UNP Q72IC1
D	-9	HIS	-	expression tag	UNP Q72IC1
D	-8	HIS	-	expression tag	UNP Q72IC1
D	-7	HIS	-	expression tag	UNP Q72IC1
D	-6	HIS	-	expression tag	UNP Q72IC1
D	-5	SER	-	expression tag	UNP Q72IC1
D	-4	GLN	-	expression tag	UNP Q72IC1
D	-3	ASP	-	expression tag	UNP Q72IC1
D	-2	PRO	-	expression tag	UNP Q72IC1
D	-1	ASN	-	expression tag	UNP Q72IC1
D	0	SER	-	expression tag	UNP Q72IC1
E	-15	MET	-	expression tag	UNP Q72IC1
E	-14	GLY	-	expression tag	UNP Q72IC1
E	-13	SER	-	expression tag	UNP Q72IC1
E	-12	SER	-	expression tag	UNP Q72IC1
E	-11	HIS	-	expression tag	UNP Q72IC1
E	-10	HIS	-	expression tag	UNP Q72IC1
E	-9	HIS	-	expression tag	UNP Q72IC1
E	-8	HIS	-	expression tag	UNP Q72IC1
E	-7	HIS	-	expression tag	UNP Q72IC1
E	-6	HIS	-	expression tag	UNP Q72IC1
E	-5	SER	-	expression tag	UNP Q72IC1
E	-4	GLN	-	expression tag	UNP Q72IC1
E	-3	ASP	-	expression tag	UNP Q72IC1
E	-2	PRO	-	expression tag	UNP Q72IC1
E	-1	ASN	-	expression tag	UNP Q72IC1
E	0	SER	-	expression tag	UNP Q72IC1
F	-15	MET	-	expression tag	UNP Q72IC1
F	-14	GLY	-	expression tag	UNP Q72IC1
F	-13	SER	-	expression tag	UNP Q72IC1
F	-12	SER	-	expression tag	UNP Q72IC1
F	-11	HIS	-	expression tag	UNP Q72IC1
F	-10	HIS	-	expression tag	UNP Q72IC1
F	-9	HIS	-	expression tag	UNP Q72IC1
F	-8	HIS	-	expression tag	UNP Q72IC1
F	-7	HIS	-	expression tag	UNP Q72IC1

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-6	HIS	-	expression tag	UNP Q72IC1
F	-5	SER	-	expression tag	UNP Q72IC1
F	-4	GLN	-	expression tag	UNP Q72IC1
F	-3	ASP	-	expression tag	UNP Q72IC1
F	-2	PRO	-	expression tag	UNP Q72IC1
F	-1	ASN	-	expression tag	UNP Q72IC1
F	0	SER	-	expression tag	UNP Q72IC1
G	-15	MET	-	expression tag	UNP Q72IC1
G	-14	GLY	-	expression tag	UNP Q72IC1
G	-13	SER	-	expression tag	UNP Q72IC1
G	-12	SER	-	expression tag	UNP Q72IC1
G	-11	HIS	-	expression tag	UNP Q72IC1
G	-10	HIS	-	expression tag	UNP Q72IC1
G	-9	HIS	-	expression tag	UNP Q72IC1
G	-8	HIS	-	expression tag	UNP Q72IC1
G	-7	HIS	-	expression tag	UNP Q72IC1
G	-6	HIS	-	expression tag	UNP Q72IC1
G	-5	SER	-	expression tag	UNP Q72IC1
G	-4	GLN	-	expression tag	UNP Q72IC1
G	-3	ASP	-	expression tag	UNP Q72IC1
G	-2	PRO	-	expression tag	UNP Q72IC1
G	-1	ASN	-	expression tag	UNP Q72IC1
G	0	SER	-	expression tag	UNP Q72IC1
H	-15	MET	-	expression tag	UNP Q72IC1
H	-14	GLY	-	expression tag	UNP Q72IC1
H	-13	SER	-	expression tag	UNP Q72IC1
H	-12	SER	-	expression tag	UNP Q72IC1
H	-11	HIS	-	expression tag	UNP Q72IC1
H	-10	HIS	-	expression tag	UNP Q72IC1
H	-9	HIS	-	expression tag	UNP Q72IC1
H	-8	HIS	-	expression tag	UNP Q72IC1
H	-7	HIS	-	expression tag	UNP Q72IC1
H	-6	HIS	-	expression tag	UNP Q72IC1
H	-5	SER	-	expression tag	UNP Q72IC1
H	-4	GLN	-	expression tag	UNP Q72IC1
H	-3	ASP	-	expression tag	UNP Q72IC1
H	-2	PRO	-	expression tag	UNP Q72IC1
H	-1	ASN	-	expression tag	UNP Q72IC1
H	0	SER	-	expression tag	UNP Q72IC1
I	-15	MET	-	expression tag	UNP Q72IC1
I	-14	GLY	-	expression tag	UNP Q72IC1
I	-13	SER	-	expression tag	UNP Q72IC1

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-12	SER	-	expression tag	UNP Q72IC1
I	-11	HIS	-	expression tag	UNP Q72IC1
I	-10	HIS	-	expression tag	UNP Q72IC1
I	-9	HIS	-	expression tag	UNP Q72IC1
I	-8	HIS	-	expression tag	UNP Q72IC1
I	-7	HIS	-	expression tag	UNP Q72IC1
I	-6	HIS	-	expression tag	UNP Q72IC1
I	-5	SER	-	expression tag	UNP Q72IC1
I	-4	GLN	-	expression tag	UNP Q72IC1
I	-3	ASP	-	expression tag	UNP Q72IC1
I	-2	PRO	-	expression tag	UNP Q72IC1
I	-1	ASN	-	expression tag	UNP Q72IC1
I	0	SER	-	expression tag	UNP Q72IC1
J	-15	MET	-	expression tag	UNP Q72IC1
J	-14	GLY	-	expression tag	UNP Q72IC1
J	-13	SER	-	expression tag	UNP Q72IC1
J	-12	SER	-	expression tag	UNP Q72IC1
J	-11	HIS	-	expression tag	UNP Q72IC1
J	-10	HIS	-	expression tag	UNP Q72IC1
J	-9	HIS	-	expression tag	UNP Q72IC1
J	-8	HIS	-	expression tag	UNP Q72IC1
J	-7	HIS	-	expression tag	UNP Q72IC1
J	-6	HIS	-	expression tag	UNP Q72IC1
J	-5	SER	-	expression tag	UNP Q72IC1
J	-4	GLN	-	expression tag	UNP Q72IC1
J	-3	ASP	-	expression tag	UNP Q72IC1
J	-2	PRO	-	expression tag	UNP Q72IC1
J	-1	ASN	-	expression tag	UNP Q72IC1
J	0	SER	-	expression tag	UNP Q72IC1
K	-15	MET	-	expression tag	UNP Q72IC1
K	-14	GLY	-	expression tag	UNP Q72IC1
K	-13	SER	-	expression tag	UNP Q72IC1
K	-12	SER	-	expression tag	UNP Q72IC1
K	-11	HIS	-	expression tag	UNP Q72IC1
K	-10	HIS	-	expression tag	UNP Q72IC1
K	-9	HIS	-	expression tag	UNP Q72IC1
K	-8	HIS	-	expression tag	UNP Q72IC1
K	-7	HIS	-	expression tag	UNP Q72IC1
K	-6	HIS	-	expression tag	UNP Q72IC1
K	-5	SER	-	expression tag	UNP Q72IC1
K	-4	GLN	-	expression tag	UNP Q72IC1
K	-3	ASP	-	expression tag	UNP Q72IC1

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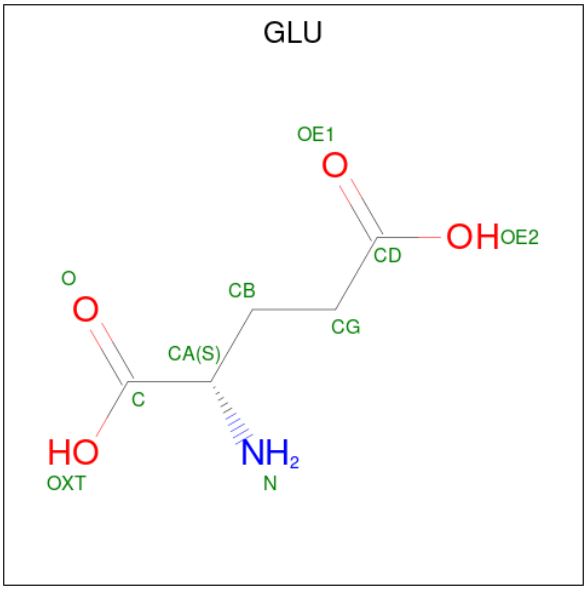
Chain	Residue	Modelled	Actual	Comment	Reference
K	-2	PRO	-	expression tag	UNP Q72IC1
K	-1	ASN	-	expression tag	UNP Q72IC1
K	0	SER	-	expression tag	UNP Q72IC1
L	-15	MET	-	expression tag	UNP Q72IC1
L	-14	GLY	-	expression tag	UNP Q72IC1
L	-13	SER	-	expression tag	UNP Q72IC1
L	-12	SER	-	expression tag	UNP Q72IC1
L	-11	HIS	-	expression tag	UNP Q72IC1
L	-10	HIS	-	expression tag	UNP Q72IC1
L	-9	HIS	-	expression tag	UNP Q72IC1
L	-8	HIS	-	expression tag	UNP Q72IC1
L	-7	HIS	-	expression tag	UNP Q72IC1
L	-6	HIS	-	expression tag	UNP Q72IC1
L	-5	SER	-	expression tag	UNP Q72IC1
L	-4	GLN	-	expression tag	UNP Q72IC1
L	-3	ASP	-	expression tag	UNP Q72IC1
L	-2	PRO	-	expression tag	UNP Q72IC1
L	-1	ASN	-	expression tag	UNP Q72IC1
L	0	SER	-	expression tag	UNP Q72IC1

- Molecule 2 is GLUTAMIC ACID (three-letter code: GLU) (formula: $C_5H_9NO_4$).



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	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	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	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	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		
2	F	1	Total	C	N	O	0	0
			10	5	1	4		
2	G	1	Total	C	N	O	0	0
			10	5	1	4		
2	G	1	Total	C	N	O	0	0
			10	5	1	4		
2	H	1	Total	C	N	O	0	0
			10	5	1	4		
2	H	1	Total	C	N	O	0	0
			10	5	1	4		
2	I	1	Total	C	N	O	0	0
			10	5	1	4		
2	I	1	Total	C	N	O	0	0
			10	5	1	4		
2	J	1	Total	C	N	O	0	0
			10	5	1	4		
2	J	1	Total	C	N	O	0	0
			10	5	1	4		
2	K	1	Total	C	N	O	0	0
			10	5	1	4		
2	K	1	Total	C	N	O	0	0
			10	5	1	4		
2	L	1	Total	C	N	O	0	0
			10	5	1	4		

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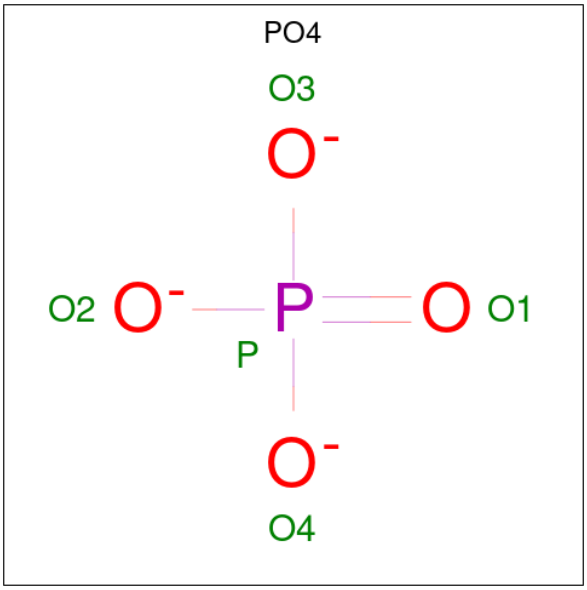
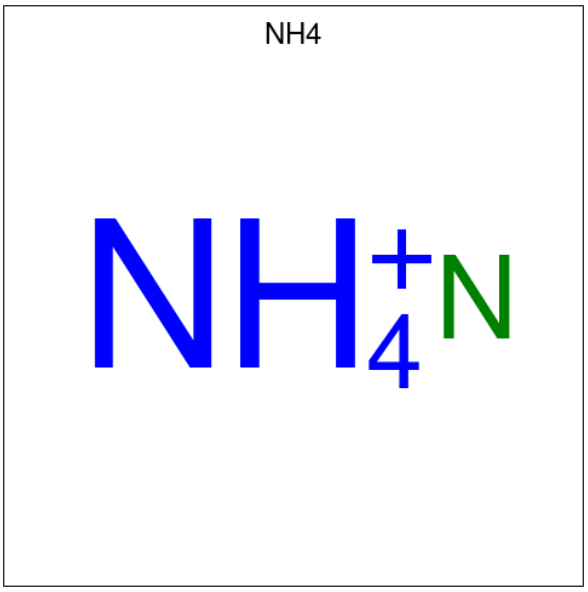
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	L	1	Total C N O 10 5 1 4	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	C	1	Total O P 5 4 1	0	0
3	D	1	Total O P 5 4 1	0	0
3	F	1	Total O P 4 3 1	0	0
3	G	1	Total O P 5 4 1	0	0
3	I	1	Total O P 5 4 1	0	0
3	I	1	Total O P 5 4 1	0	0
3	J	1	Total O P 5 4 1	0	0
3	K	1	Total O P 5 4 1	0	0

- Molecule 4 is AMMONIUM ION (three-letter code: NH4) (formula: H_4N).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total N 1 1	0	0
4	B	1	Total N 1 1	0	0
4	F	1	Total N 1 1	0	0
4	H	1	Total N 1 1	0	0
4	J	1	Total N 1 1	0	0
4	L	1	Total N 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	209	Total O 209 209	0	0
5	B	161	Total O 161 161	0	0
5	C	159	Total O 159 159	0	0
5	D	118	Total O 118 118	0	0
5	E	157	Total O 157 157	0	0
5	F	133	Total O 133 133	0	0

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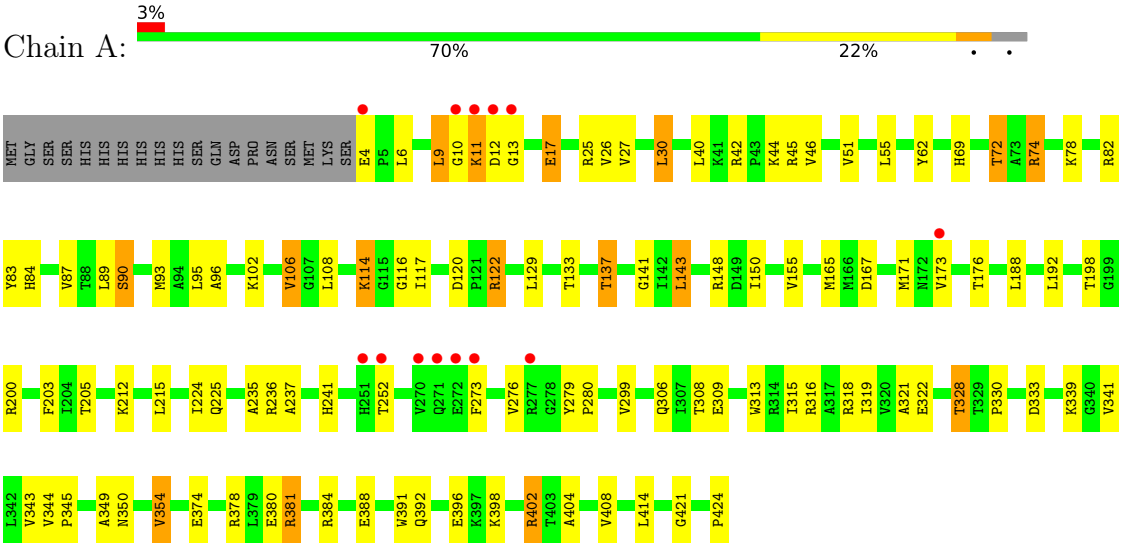
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	187	Total O 187 187	0	0
5	H	125	Total O 125 125	0	0
5	I	178	Total O 178 178	0	0
5	J	157	Total O 157 157	0	0
5	K	121	Total O 121 121	0	0
5	L	106	Total O 106 106	0	0

3 Residue-property plots (i)

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.

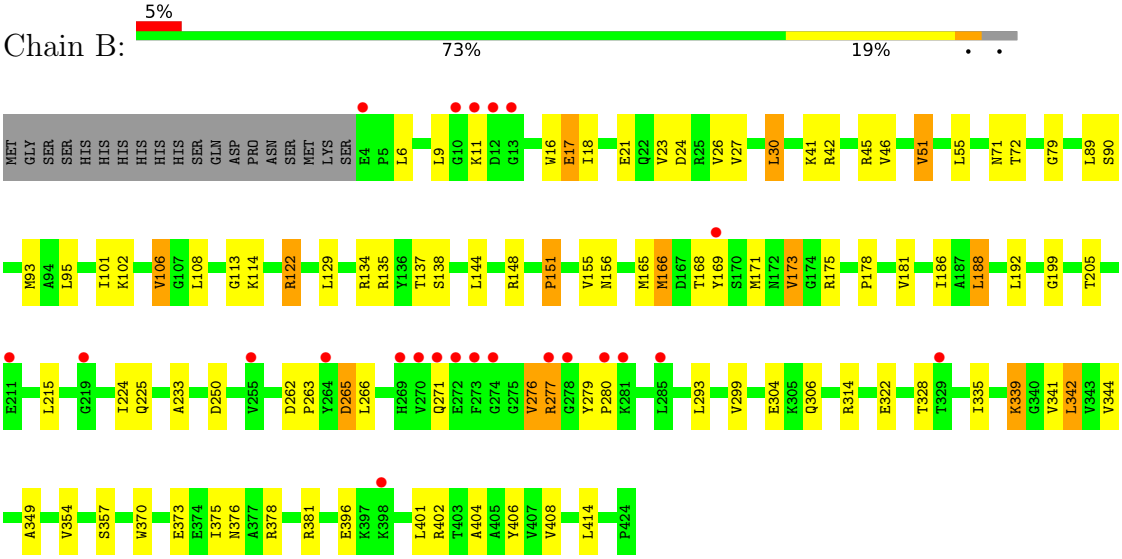
• Molecule 1: Glutamate dehydrogenase

Chain A:



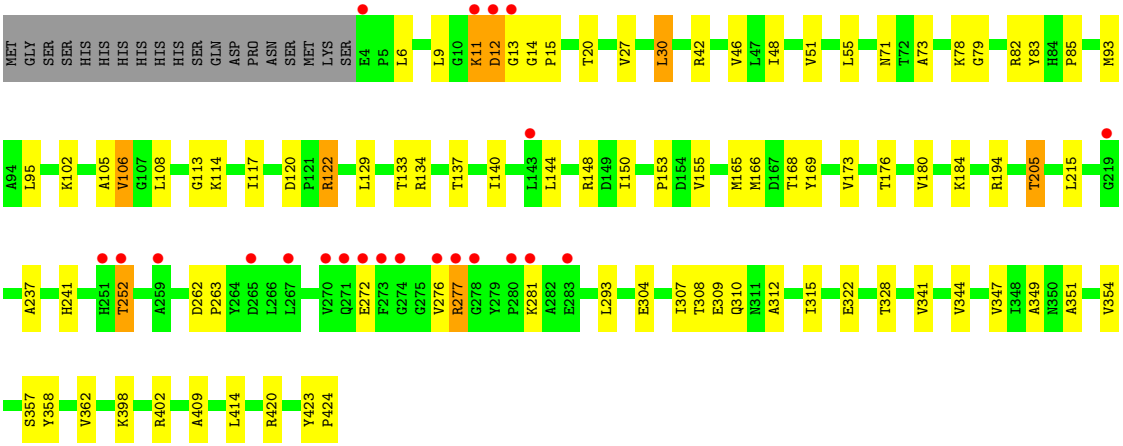
• Molecule 1: Glutamate dehydrogenase

Chain B:



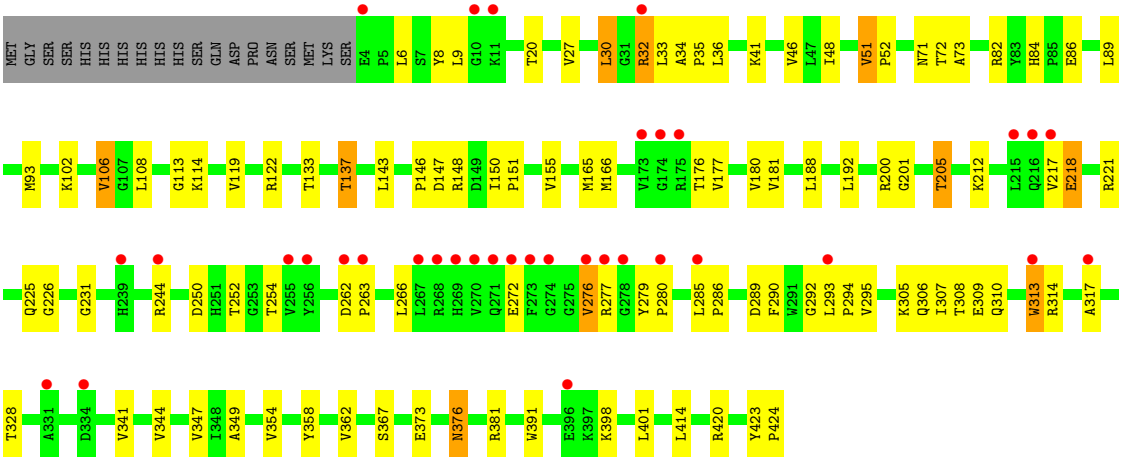
• Molecule 1: Glutamate dehydrogenase

Chain C:



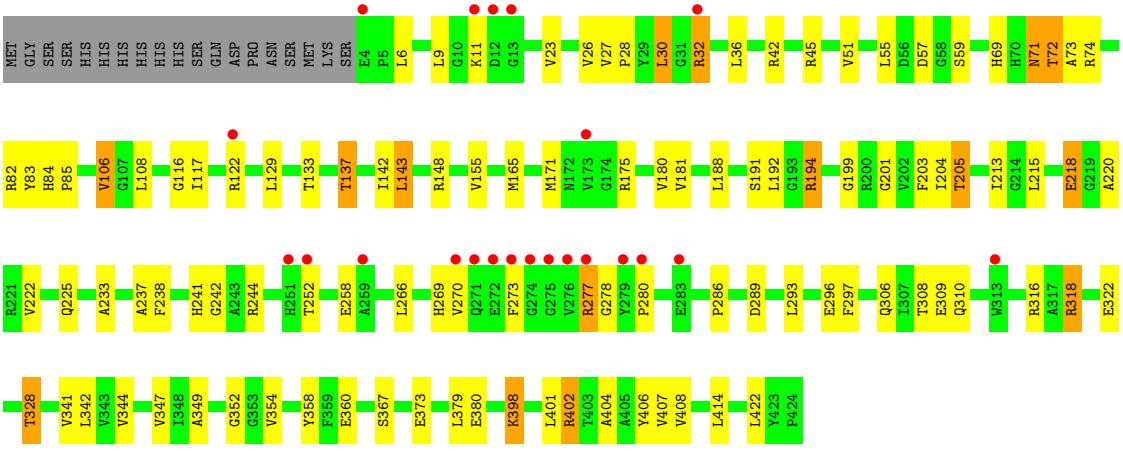
• Molecule 1: Glutamate dehydrogenase

Chain D:



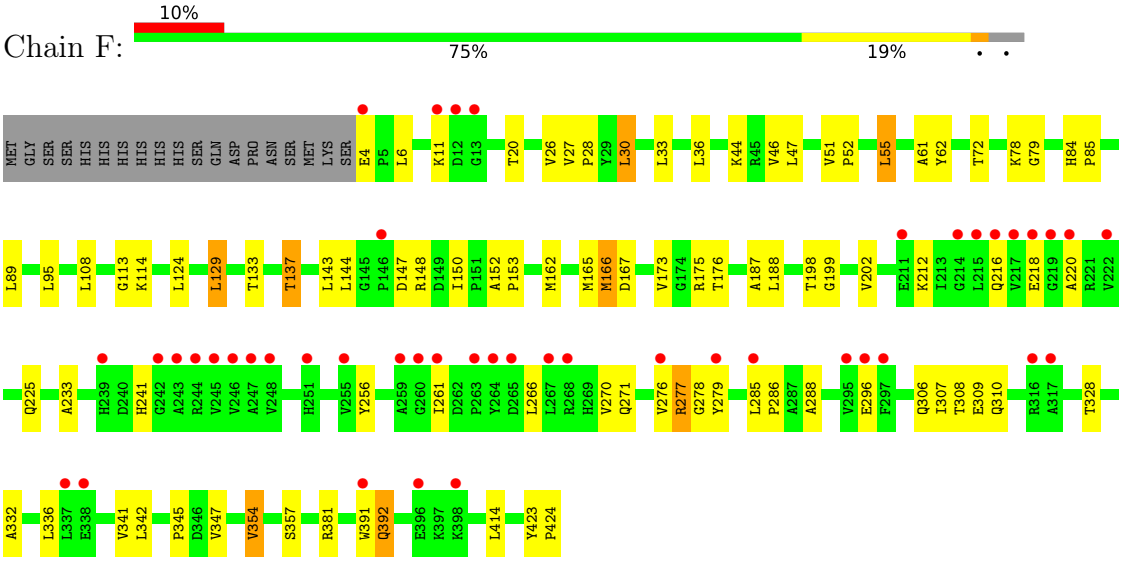
• Molecule 1: Glutamate dehydrogenase

Chain E:



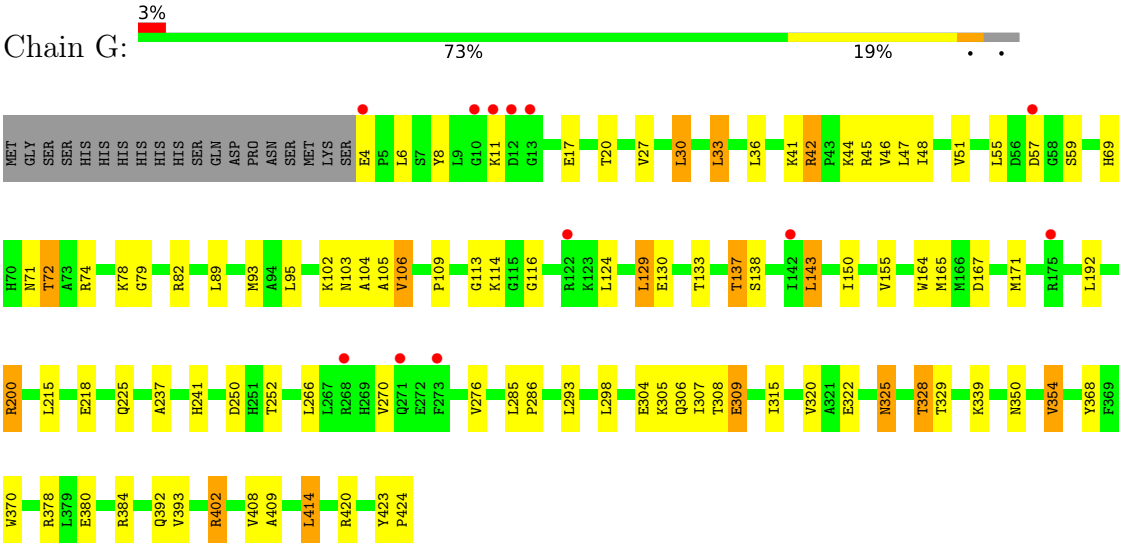
• Molecule 1: Glutamate dehydrogenase

Chain F:



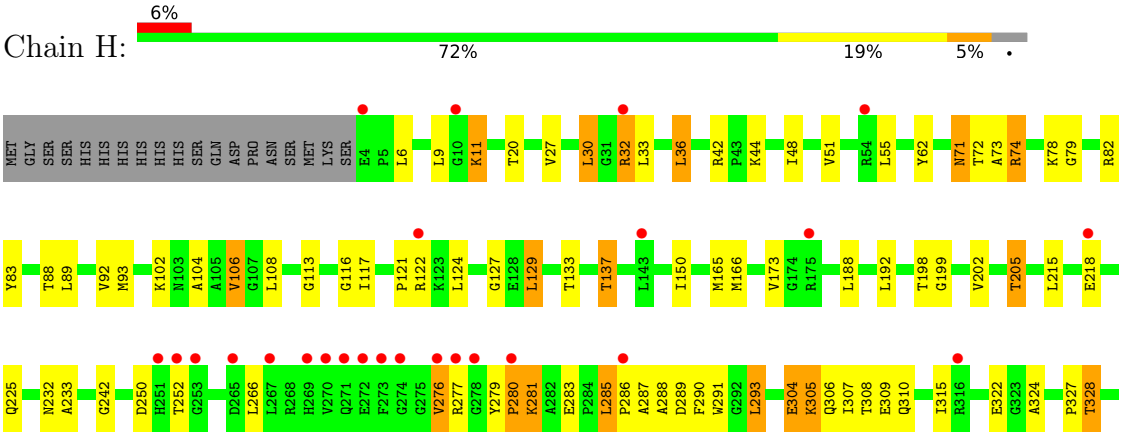
• Molecule 1: Glutamate dehydrogenase

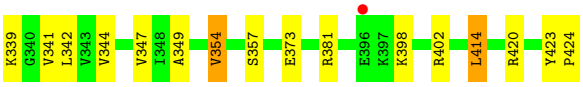
Chain G:



• Molecule 1: Glutamate dehydrogenase

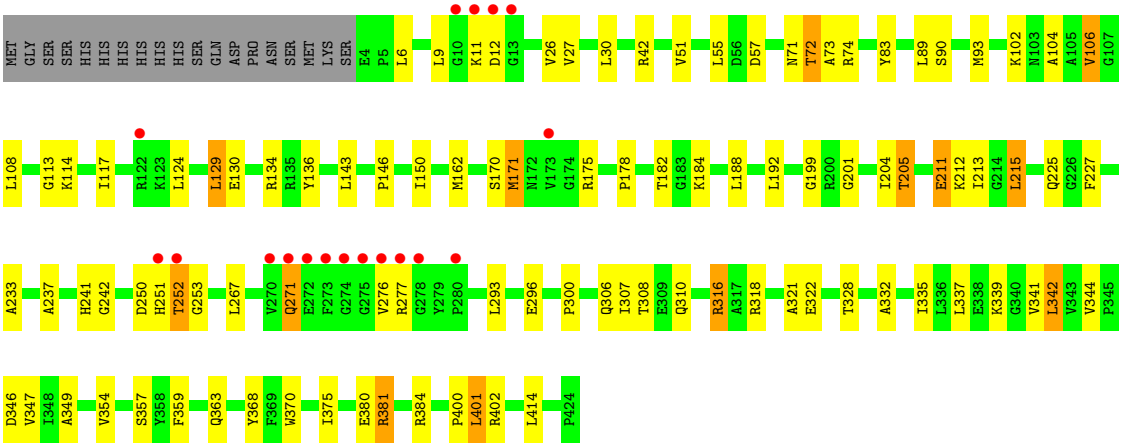
Chain H:





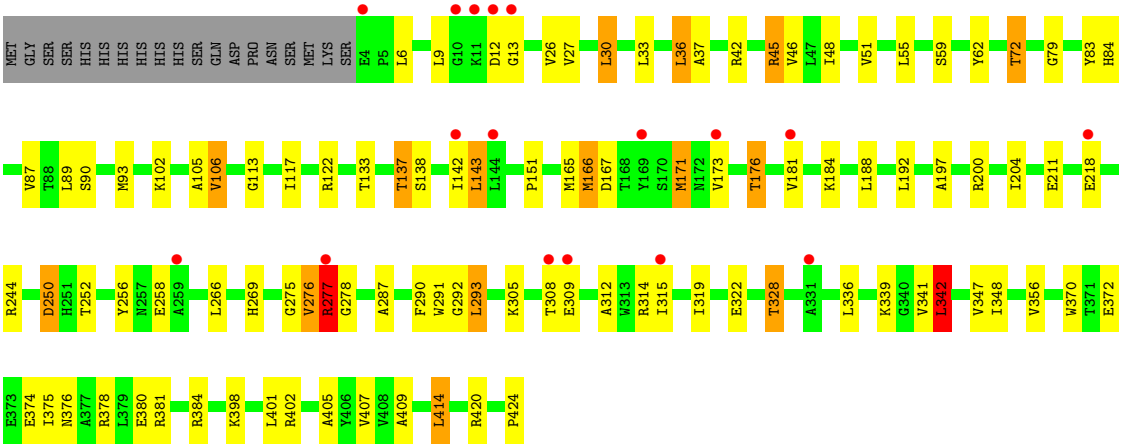
• Molecule 1: Glutamate dehydrogenase

Chain I:



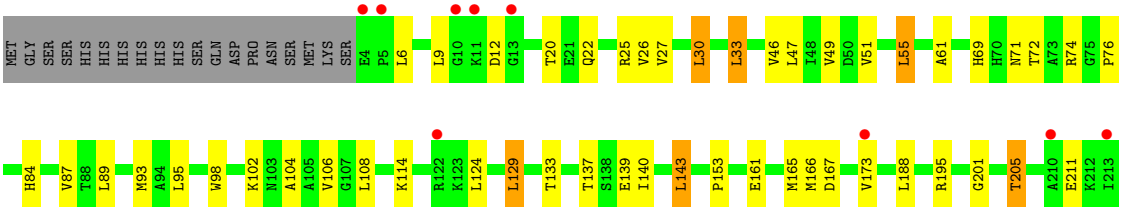
• Molecule 1: Glutamate dehydrogenase

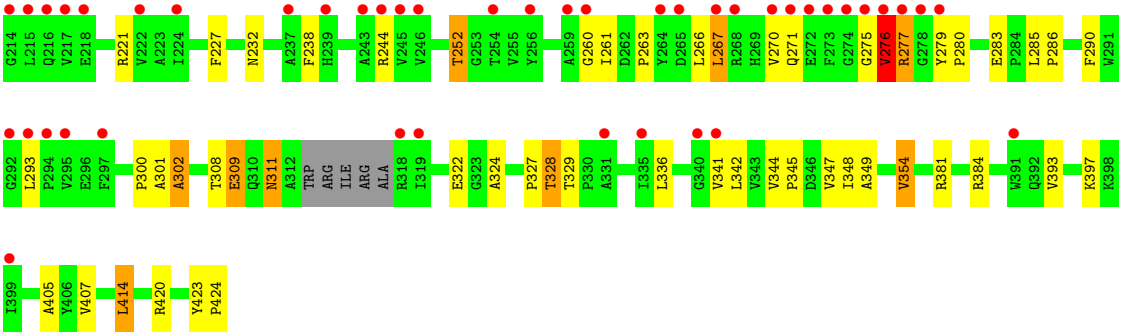
Chain J:



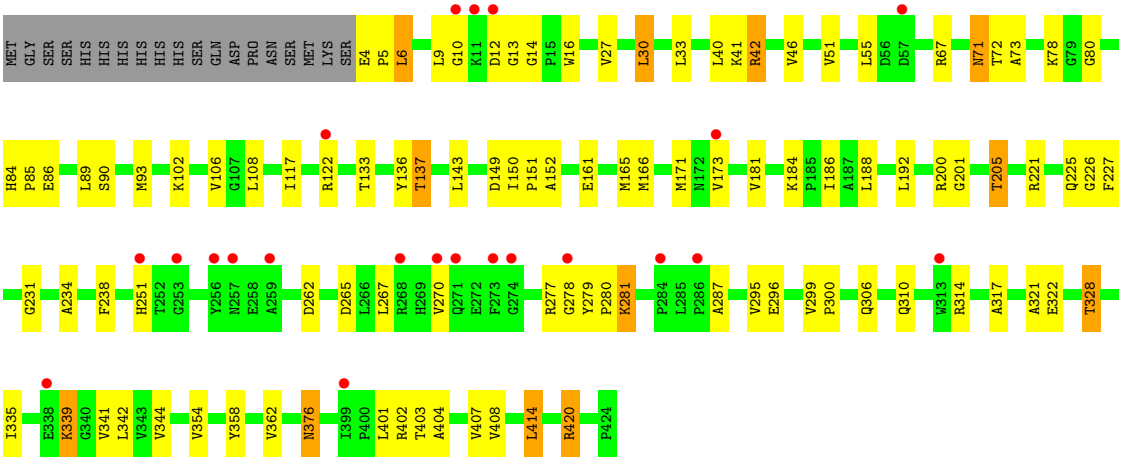
• Molecule 1: Glutamate dehydrogenase

Chain K:





• Molecule 1: Glutamate dehydrogenase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	99.73Å 106.55Å 166.81Å 82.83° 87.18° 70.60°	Depositor
Resolution (Å)	49.77 – 2.10 49.77 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.6 (49.77-2.10) 95.6 (49.77-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.41 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.226 , 0.277 0.224 , 0.273	Depositor DCC
R_{free} test set	17984 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	37.5	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 43.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	40944	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.95% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: PO4, NH4

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	0.73	0/3312	0.83	4/4508 (0.1%)
1	B	0.61	0/3312	0.70	1/4508 (0.0%)
1	C	0.54	0/3330	0.69	0/4532
1	D	0.53	0/3312	0.64	0/4508
1	E	0.64	2/3312 (0.1%)	0.75	2/4508 (0.0%)
1	F	0.53	0/3323	0.68	1/4522 (0.0%)
1	G	0.65	0/3323	0.76	3/4522 (0.1%)
1	H	0.50	0/3334	0.65	2/4536 (0.0%)
1	I	0.57	0/3323	0.69	0/4522
1	J	0.57	0/3323	0.71	1/4522 (0.0%)
1	K	0.51	0/3260	0.65	0/4436
1	L	0.47	0/3312	0.62	0/4508
All	All	0.58	2/39776 (0.0%)	0.70	14/54132 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	358	TYR	CD1-CE1	6.51	1.49	1.39
1	E	360	GLU	CG-CD	5.41	1.60	1.51

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	74	ARG	NE-CZ-NH2	-8.15	116.23	120.30
1	A	402	ARG	NE-CZ-NH1	-7.62	116.49	120.30
1	H	74	ARG	NE-CZ-NH2	-7.01	116.80	120.30
1	G	402	ARG	NE-CZ-NH1	-6.87	116.87	120.30
1	A	74	ARG	NE-CZ-NH1	6.63	123.61	120.30

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	3236	0	3229	85	0
1	B	3236	0	3229	65	0
1	C	3248	0	3243	54	0
1	D	3236	0	3229	70	0
1	E	3236	0	3229	62	0
1	F	3244	0	3242	66	0
1	G	3244	0	3242	81	0
1	H	3252	0	3255	59	0
1	I	3244	0	3242	72	0
1	J	3244	0	3242	78	0
1	K	3187	0	3176	73	0
1	L	3236	0	3229	67	0
2	A	20	0	10	2	0
2	B	20	0	10	0	0
2	C	20	0	10	1	0
2	D	20	0	10	0	0
2	E	20	0	10	0	0
2	F	20	0	10	3	0
2	G	20	0	10	1	0
2	H	20	0	10	1	0
2	I	20	0	10	0	0
2	J	20	0	10	1	0
2	K	20	0	10	1	0
2	L	20	0	10	0	0
3	A	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	1	0
3	F	4	0	0	0	0
3	G	5	0	0	1	0
3	I	10	0	0	0	0
3	J	5	0	0	0	0
3	K	5	0	0	0	0
4	A	1	0	0	1	0
4	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	1	0	0	0	0
4	H	1	0	0	0	0
4	J	1	0	0	0	0
4	L	1	0	0	0	0
5	A	209	0	0	13	0
5	B	161	0	0	4	0
5	C	159	0	0	3	0
5	D	118	0	0	9	0
5	E	157	0	0	4	0
5	F	133	0	0	4	0
5	G	187	0	0	12	0
5	H	125	0	0	3	0
5	I	178	0	0	5	0
5	J	157	0	0	5	0
5	K	121	0	0	2	0
5	L	106	0	0	2	0
All	All	40944	0	38907	793	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 10.

The worst 5 of 793 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:L:205:THR:HG23	1:L:344:VAL:HG11	1.37	1.06
1:H:205:THR:HG23	1:H:344:VAL:HG11	1.40	1.03
1:H:205:THR:CG2	1:H:344:VAL:HG11	1.88	1.03
1:K:277:ARG:HG3	1:K:277:ARG:HH11	1.24	1.02
1:K:301:ALA:N	1:K:302:ALA:HB2	1.73	1.02

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	419/440 (95%)	400 (96%)	17 (4%)	2 (0%)	29 26
1	B	419/440 (95%)	405 (97%)	14 (3%)	0	100 100
1	C	421/440 (96%)	407 (97%)	11 (3%)	3 (1%)	22 18
1	D	419/440 (95%)	397 (95%)	20 (5%)	2 (0%)	29 26
1	E	419/440 (95%)	397 (95%)	19 (4%)	3 (1%)	22 18
1	F	420/440 (96%)	398 (95%)	20 (5%)	2 (0%)	29 26
1	G	420/440 (96%)	409 (97%)	11 (3%)	0	100 100
1	H	421/440 (96%)	403 (96%)	15 (4%)	3 (1%)	22 18
1	I	420/440 (96%)	401 (96%)	17 (4%)	2 (0%)	29 26
1	J	420/440 (96%)	398 (95%)	17 (4%)	5 (1%)	13 8
1	K	412/440 (94%)	386 (94%)	21 (5%)	5 (1%)	13 8
1	L	419/440 (95%)	396 (94%)	16 (4%)	7 (2%)	9 4
All	All	5029/5280 (95%)	4797 (95%)	198 (4%)	34 (1%)	22 18

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	277	ARG
1	D	218	GLU
1	F	220	ALA
1	H	281	LYS
1	H	288	ALA

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	325/343 (95%)	293 (90%)	32 (10%)	8 5
1	B	325/343 (95%)	292 (90%)	33 (10%)	7 4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	327/343 (95%)	304 (93%)	23 (7%)	15 12
1	D	325/343 (95%)	297 (91%)	28 (9%)	10 7
1	E	325/343 (95%)	291 (90%)	34 (10%)	7 4
1	F	326/343 (95%)	298 (91%)	28 (9%)	10 7
1	G	326/343 (95%)	301 (92%)	25 (8%)	13 9
1	H	327/343 (95%)	289 (88%)	38 (12%)	5 3
1	I	326/343 (95%)	300 (92%)	26 (8%)	12 8
1	J	326/343 (95%)	293 (90%)	33 (10%)	7 4
1	K	321/343 (94%)	290 (90%)	31 (10%)	8 5
1	L	325/343 (95%)	302 (93%)	23 (7%)	14 11
All	All	3904/4116 (95%)	3550 (91%)	354 (9%)	9 6

5 of 354 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	309	GLU
1	J	188	LEU
1	H	381	ARG
1	I	316	ARG
1	K	6	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	269	HIS
1	H	306	GLN
1	L	71	ASN
1	G	306	GLN
1	H	71	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 39 ligands modelled in this entry, 6 are modelled with single atom - leaving 33 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	D	500	-	8,9,9	1.21	1 (12%)	10,11,11	1.38	1 (10%)
2	GLU	G	425	-	8,9,9	1.07	0	10,11,11	1.11	0
2	GLU	F	425	-	8,9,9	1.02	0	10,11,11	1.23	1 (10%)
3	PO4	C	426	-	4,4,4	0.83	0	6,6,6	0.48	0
2	GLU	L	425	-	8,9,9	1.02	0	10,11,11	1.77	2 (20%)
2	GLU	K	425	-	8,9,9	1.02	0	10,11,11	1.18	1 (10%)
2	GLU	A	425	-	8,9,9	0.92	0	10,11,11	1.49	2 (20%)
2	GLU	I	500	-	8,9,9	1.15	1 (12%)	10,11,11	1.58	2 (20%)
3	PO4	I	427	-	4,4,4	0.90	0	6,6,6	0.74	0
2	GLU	C	500	-	8,9,9	1.08	1 (12%)	10,11,11	0.99	0
3	PO4	D	426	-	4,4,4	0.91	0	6,6,6	0.64	0
3	PO4	K	426	-	4,4,4	0.82	0	6,6,6	0.66	0
2	GLU	E	500	-	8,9,9	1.09	1 (12%)	10,11,11	1.59	2 (20%)
2	GLU	B	500	-	8,9,9	1.05	1 (12%)	10,11,11	1.60	2 (20%)
2	GLU	I	425	-	8,9,9	1.25	1 (12%)	10,11,11	0.86	0
2	GLU	H	425	-	8,9,9	1.25	1 (12%)	10,11,11	1.29	2 (20%)
2	GLU	G	500	-	8,9,9	1.00	1 (12%)	10,11,11	1.13	0
3	PO4	J	426	-	4,4,4	0.85	0	6,6,6	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GLU	D	425	-	8,9,9	1.13	1 (12%)	10,11,11	1.66	2 (20%)
3	PO4	A	426	-	4,4,4	0.91	0	6,6,6	0.87	0
2	GLU	H	500	-	8,9,9	1.08	1 (12%)	10,11,11	1.05	1 (10%)
2	GLU	L	500	-	8,9,9	1.07	1 (12%)	10,11,11	1.24	1 (10%)
2	GLU	F	500	-	8,9,9	1.00	0	10,11,11	0.93	0
2	GLU	C	425	-	8,9,9	1.03	1 (12%)	10,11,11	1.39	1 (10%)
2	GLU	J	500	-	8,9,9	1.18	1 (12%)	10,11,11	1.31	2 (20%)
2	GLU	A	500	-	8,9,9	1.18	1 (12%)	10,11,11	1.44	1 (10%)
2	GLU	K	500	-	8,9,9	0.91	0	10,11,11	1.32	2 (20%)
3	PO4	G	426	-	4,4,4	0.75	0	6,6,6	0.85	0
3	PO4	I	426	-	4,4,4	0.97	0	6,6,6	0.51	0
2	GLU	J	425	-	8,9,9	1.07	0	10,11,11	1.26	2 (20%)
2	GLU	E	425	-	8,9,9	1.10	1 (12%)	10,11,11	1.35	2 (20%)
3	PO4	F	426	-	0,3,4	-	-	0,3,6	-	-
2	GLU	B	425	-	8,9,9	1.02	0	10,11,11	1.30	2 (20%)

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	D	500	-	-	2/9/9/9	-
2	GLU	G	425	-	-	0/9/9/9	-
2	GLU	F	425	-	-	0/9/9/9	-
2	GLU	L	425	-	-	2/9/9/9	-
2	GLU	K	425	-	-	0/9/9/9	-
2	GLU	A	425	-	-	0/9/9/9	-
2	GLU	I	500	-	-	4/9/9/9	-
2	GLU	C	500	-	-	1/9/9/9	-
2	GLU	E	500	-	-	4/9/9/9	-
2	GLU	B	500	-	-	2/9/9/9	-
2	GLU	I	425	-	-	4/9/9/9	-
2	GLU	H	425	-	-	0/9/9/9	-
2	GLU	G	500	-	-	4/9/9/9	-
2	GLU	D	425	-	-	0/9/9/9	-
2	GLU	H	500	-	-	2/9/9/9	-
2	GLU	L	500	-	-	1/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLU	F	500	-	-	7/9/9/9	-
2	GLU	C	425	-	-	1/9/9/9	-
2	GLU	J	500	-	-	0/9/9/9	-
2	GLU	A	500	-	-	2/9/9/9	-
2	GLU	K	500	-	-	3/9/9/9	-
2	GLU	J	425	-	-	0/9/9/9	-
2	GLU	E	425	-	-	2/9/9/9	-
2	GLU	B	425	-	-	4/9/9/9	-

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	GLU	OXT-C	-2.53	1.22	1.30
2	H	425	GLU	OXT-C	-2.47	1.22	1.30
2	J	500	GLU	OXT-C	-2.45	1.22	1.30
2	L	500	GLU	OXT-C	-2.35	1.22	1.30
2	I	425	GLU	OXT-C	-2.33	1.22	1.30

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	425	GLU	OXT-C-O	-3.98	115.06	124.09
2	B	500	GLU	OXT-C-O	-3.75	115.58	124.09
2	L	425	GLU	OXT-C-O	-3.55	116.02	124.09
2	I	500	GLU	OXT-C-O	-3.39	116.38	124.09
2	A	425	GLU	OXT-C-CA	3.31	124.66	113.38

There are no chirality outliers.

5 of 45 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	425	GLU	N-CA-CB-CG
2	B	425	GLU	C-CA-CB-CG
2	F	500	GLU	O-C-CA-N
2	G	500	GLU	C-CA-CB-CG
2	I	425	GLU	C-CA-CB-CG

There are no ring outliers.

11 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	425	GLU	1	0
2	F	425	GLU	1	0
2	A	425	GLU	1	0
3	D	426	PO4	1	0
2	H	425	GLU	1	0
2	F	500	GLU	2	0
2	C	425	GLU	1	0
2	A	500	GLU	1	0
2	K	500	GLU	1	0
3	G	426	PO4	1	0
2	J	425	GLU	1	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, 95^{th} 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	421/440 (95%)	0.18	13 (3%) 49 55	18, 35, 62, 75	1 (0%)
1	B	421/440 (95%)	0.41	23 (5%) 25 31	20, 42, 75, 93	0
1	C	421/440 (95%)	0.37	22 (5%) 27 32	27, 44, 70, 85	1 (0%)
1	D	421/440 (95%)	0.57	35 (8%) 11 14	27, 51, 87, 94	1 (0%)
1	E	421/440 (95%)	0.26	22 (5%) 27 32	16, 41, 75, 91	2 (0%)
1	F	421/440 (95%)	0.49	45 (10%) 6 7	29, 46, 79, 84	2 (0%)
1	G	421/440 (95%)	0.23	12 (2%) 51 57	20, 37, 59, 71	1 (0%)
1	H	421/440 (95%)	0.34	26 (6%) 20 25	29, 47, 75, 89	2 (0%)
1	I	421/440 (95%)	0.31	18 (4%) 35 41	23, 41, 70, 86	1 (0%)
1	J	421/440 (95%)	0.37	17 (4%) 38 44	26, 41, 63, 76	2 (0%)
1	K	416/440 (94%)	0.68	53 (12%) 3 5	29, 52, 81, 89	1 (0%)
1	L	421/440 (95%)	0.47	22 (5%) 27 32	32, 54, 87, 96	1 (0%)
All	All	5047/5280 (95%)	0.39	308 (6%) 21 26	16, 43, 78, 96	15 (0%)

The worst 5 of 308 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	273	PHE	8.0
1	D	273	PHE	6.6
1	D	267	LEU	6.4
1	B	11	LYS	6.4
1	I	273	PHE	6.3

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 (i)

There are no monosaccharides 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, 95^{th} 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
4	NH4	L	426	1/1	0.70	0.17	44,44,44,44	0
4	NH4	B	426	1/1	0.80	0.24	51,51,51,51	0
2	GLU	D	425	10/10	0.85	0.14	36,38,39,42	0
2	GLU	K	500	10/10	0.87	0.15	56,57,58,60	0
3	PO4	A	426	5/5	0.89	0.20	75,76,77,77	0
2	GLU	F	500	10/10	0.89	0.20	62,63,65,66	0
2	GLU	C	425	10/10	0.89	0.17	42,43,46,49	0
2	GLU	K	425	10/10	0.90	0.16	40,40,46,48	0
4	NH4	J	427	1/1	0.90	0.14	40,40,40,40	0
4	NH4	A	427	1/1	0.90	0.46	17,17,17,17	0
2	GLU	B	425	10/10	0.91	0.16	35,36,49,51	0
2	GLU	G	500	10/10	0.91	0.15	42,42,46,50	0
2	GLU	L	425	10/10	0.91	0.14	49,49,52,53	0
2	GLU	I	425	10/10	0.91	0.13	38,39,41,44	0
3	PO4	G	426	5/5	0.92	0.14	62,63,64,64	0
2	GLU	A	500	10/10	0.92	0.15	43,45,46,46	0
2	GLU	C	500	10/10	0.92	0.13	42,43,46,48	0
2	GLU	I	500	10/10	0.92	0.14	50,51,55,55	0
2	GLU	E	425	10/10	0.92	0.16	37,38,43,45	0
3	PO4	K	426	5/5	0.93	0.11	67,68,69,69	0
2	GLU	L	500	10/10	0.93	0.15	52,53,53,54	0
2	GLU	J	500	10/10	0.93	0.17	47,48,54,55	0
4	NH4	H	426	1/1	0.93	0.28	34,34,34,34	0
2	GLU	F	425	10/10	0.93	0.15	31,34,44,45	0
2	GLU	E	500	10/10	0.93	0.12	39,42,47,49	0
2	GLU	A	425	10/10	0.94	0.13	28,29,32,34	0
2	GLU	G	425	10/10	0.94	0.13	28,30,33,33	0
2	GLU	H	500	10/10	0.94	0.14	50,53,53,54	0
3	PO4	D	426	5/5	0.94	0.14	79,80,80,80	0
2	GLU	B	500	10/10	0.94	0.10	35,37,38,39	0
3	PO4	J	426	5/5	0.94	0.19	62,62,63,64	0
2	GLU	D	500	10/10	0.95	0.12	43,46,46,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PO4	I	427	5/5	0.95	0.14	61,62,62,62	0
2	GLU	J	425	10/10	0.95	0.11	36,37,43,43	0
3	PO4	F	426	4/5	0.96	0.11	71,71,72,72	0
2	GLU	H	425	10/10	0.96	0.10	34,36,41,42	0
3	PO4	C	426	5/5	0.97	0.10	57,58,58,58	0
4	NH4	F	427	1/1	0.98	0.18	41,41,41,41	0
3	PO4	I	426	5/5	0.98	0.15	56,56,57,58	0

6.5 Other polymers (i)

There are no such residues in this entry.