



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 19, 2020 – 07:51 pm BST

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 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 following versions of software and data (see [references ⓘ](#)) 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	:	2.11
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)	:	2.11

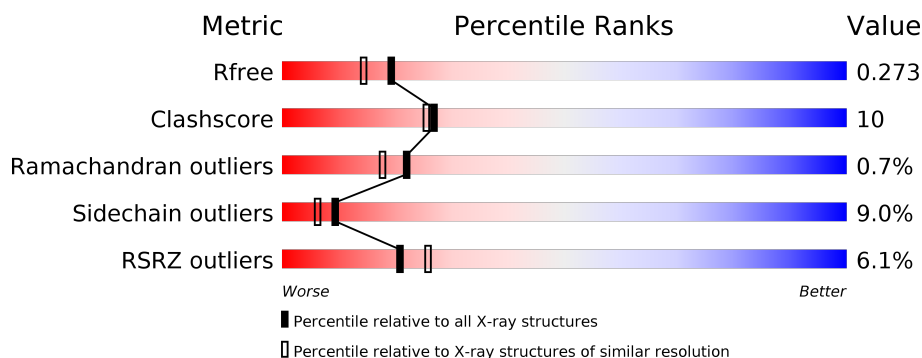
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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 on 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	440	<div> <div>3%</div> <div> <div></div> <div>70%</div> <div>22%</div> <div>• •</div> </div> </div>
1	B	440	<div> <div>5%</div> <div> <div></div> <div>73%</div> <div>19%</div> <div>• •</div> </div> </div>
1	C	440	<div> <div>5%</div> <div> <div></div> <div>75%</div> <div>18%</div> <div>• •</div> </div> </div>
1	D	440	<div> <div>8%</div> <div> <div></div> <div>72%</div> <div>22%</div> <div>• •</div> </div> </div>
1	E	440	<div> <div>5%</div> <div> <div></div> <div>71%</div> <div>21%</div> <div>• •</div> </div> </div>
1	F	440	<div> <div>10%</div> <div> <div></div> <div>75%</div> <div>19%</div> <div>• •</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	440	<div><div></div><div>3%</div><div>73%</div><div>19%</div><div></div><div></div></div>
1	H	440	<div><div></div><div>6%</div><div>73%</div><div>19%</div><div>5%</div><div></div></div>
1	I	440	<div><div></div><div>4%</div><div>73%</div><div>20%</div><div></div><div></div></div>
1	J	440	<div><div></div><div>4%</div><div>72%</div><div>20%</div><div></div><div></div></div>
1	K	440	<div><div></div><div>12%</div><div>71%</div><div>20%</div><div></div><div>5%</div></div>
1	L	440	<div><div></div><div>5%</div><div>73%</div><div>20%</div><div></div><div></div></div>

2 Entry composition

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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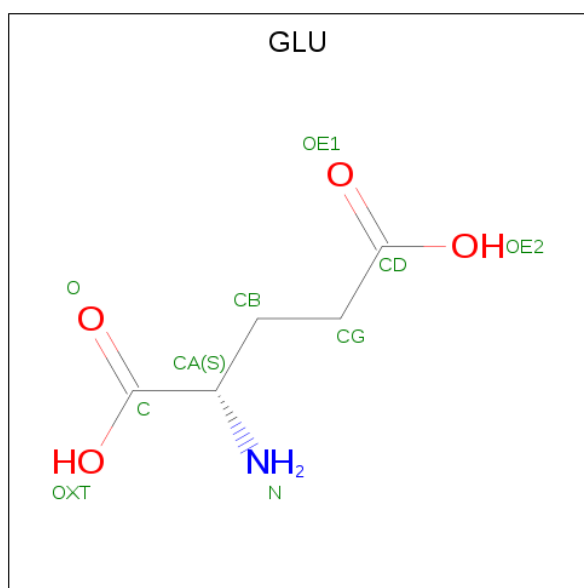
Chain	Residue	Modelled	Actual	Comment	Reference
I	-12	SER	-	EXPRESSION TAG	UNP Q72IC1
I	-11	HIS	-	EXPRESSION TAG	UNP Q72IC1
I	-10	HIS	-	EXPRESSION TAG	UNP Q72IC1
I	-9	HIS	-	EXPRESSION TAG	UNP Q72IC1
I	-8	HIS	-	EXPRESSION TAG	UNP Q72IC1
I	-7	HIS	-	EXPRESSION TAG	UNP Q72IC1
I	-6	HIS	-	EXPRESSION TAG	UNP 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: C₅H₉NO₄).



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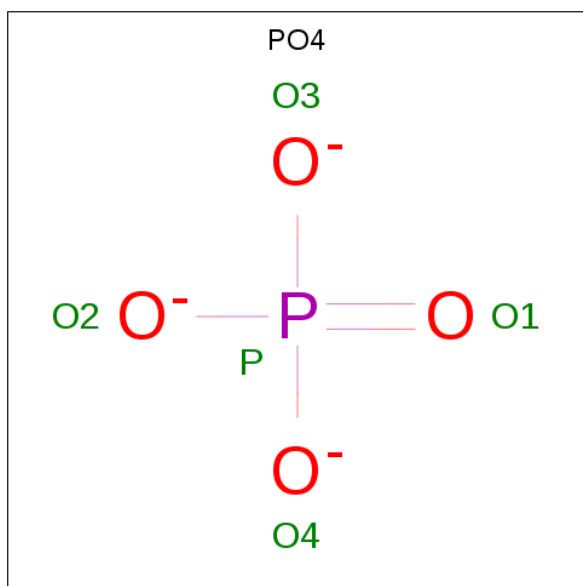
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			10	5	1	4		
2	B	1	Total	C	N	O	0	0
			10	5	1	4		
2	C	1	Total	C	N	O	0	0
			10	5	1	4		
2	C	1	Total	C	N	O	0	0
			10	5	1	4		
2	D	1	Total	C	N	O	0	0
			10	5	1	4		
2	D	1	Total	C	N	O	0	0
			10	5	1	4		
2	E	1	Total	C	N	O	0	0
			10	5	1	4		
2	E	1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

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

- Molecule 4 is AMMONIUM ION (three-letter code: NH4) (formula: H₄N).



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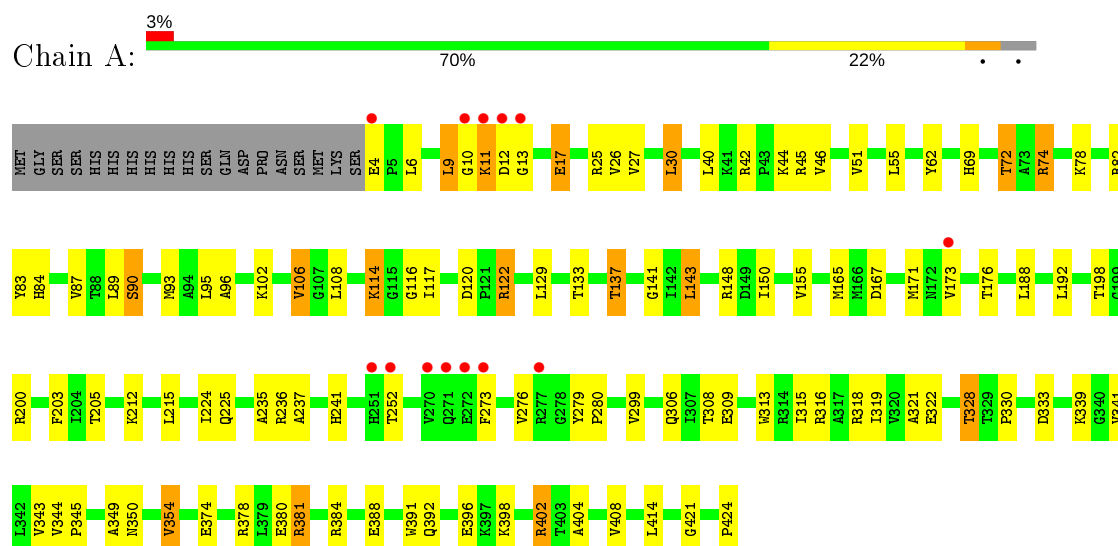
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	187	Total 187	O 187	0	0
5	H	125	Total 125	O 125	0	0
5	I	178	Total 178	O 178	0	0
5	J	157	Total 157	O 157	0	0
5	K	121	Total 121	O 121	0	0
5	L	106	Total 106	O 106	0	0

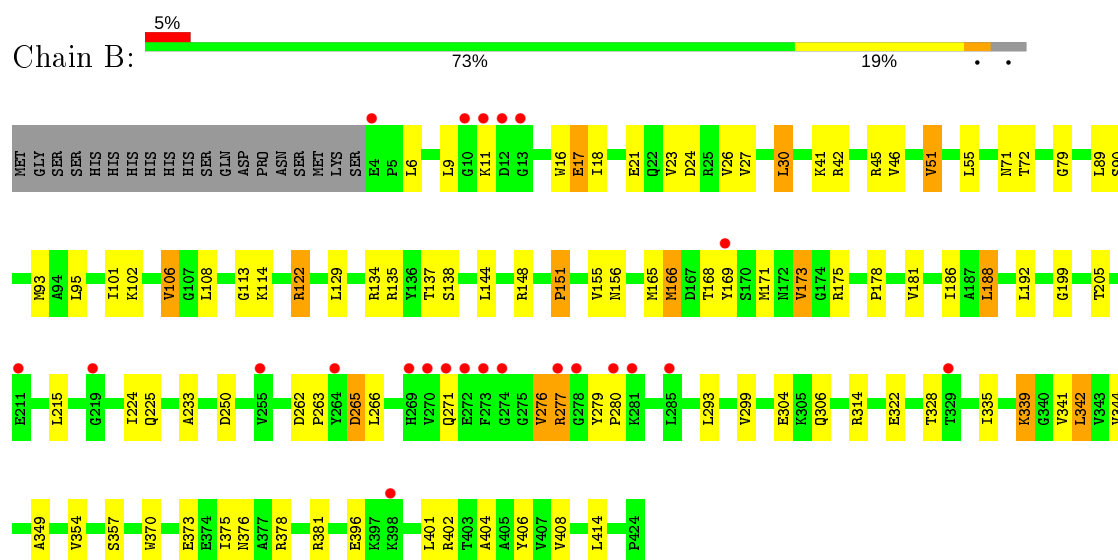
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

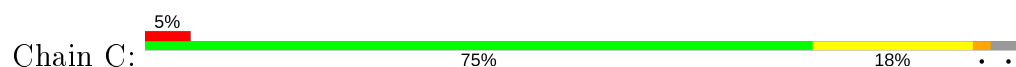
• Molecule 1: Glutamate dehydrogenase

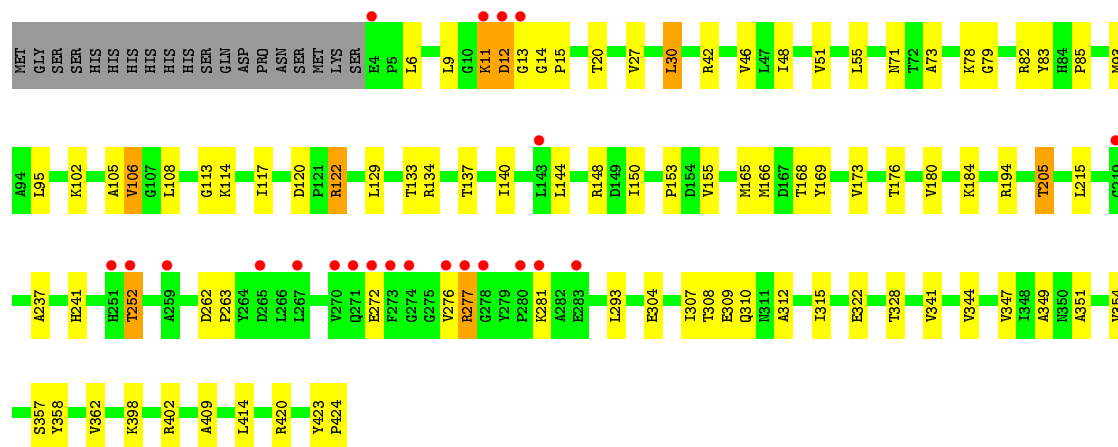


• Molecule 1: Glutamate dehydrogenase

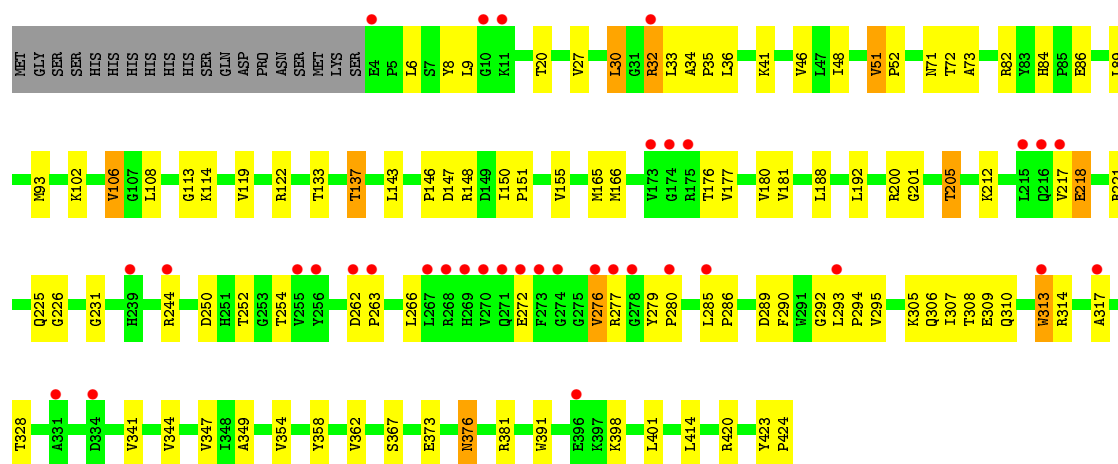


• Molecule 1: Glutamate dehydrogenase

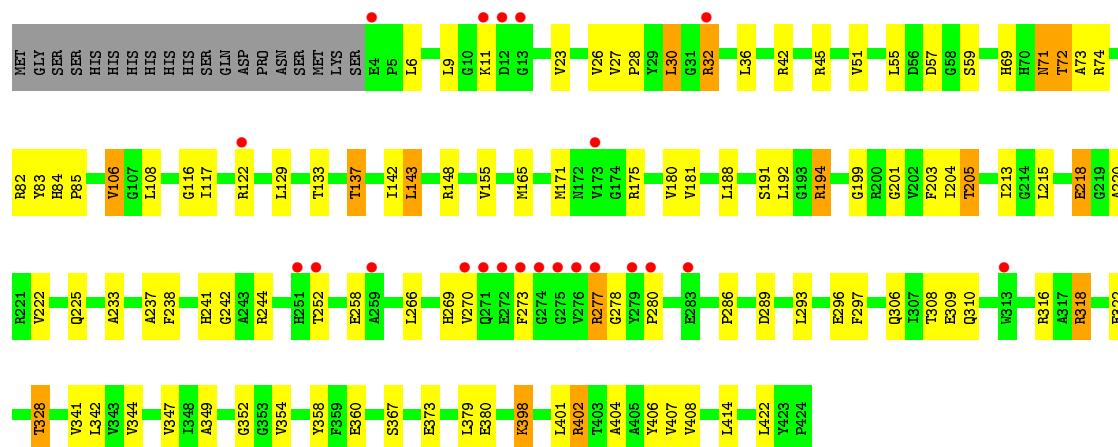




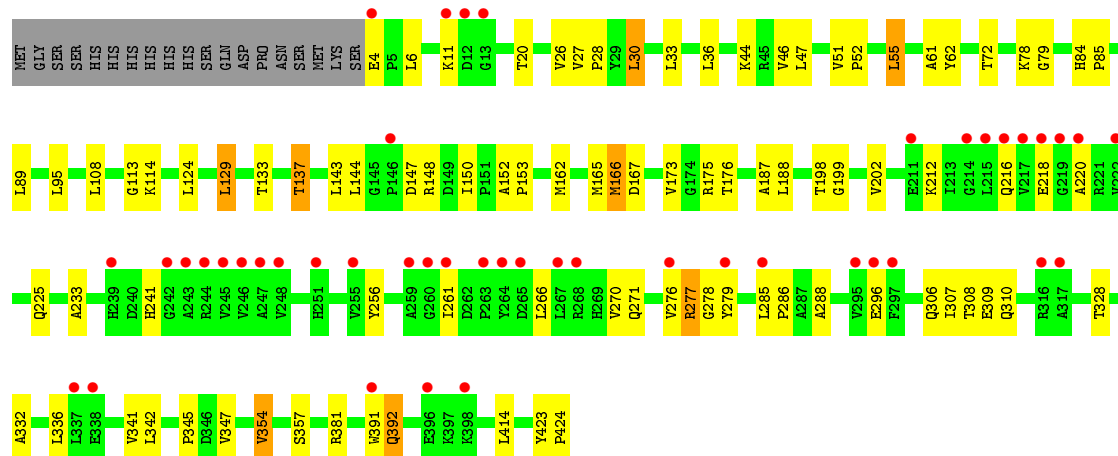
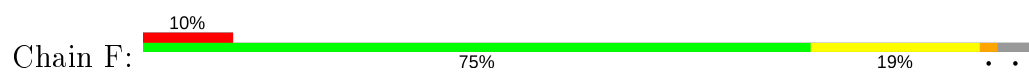
• Molecule 1: Glutamate dehydrogenase



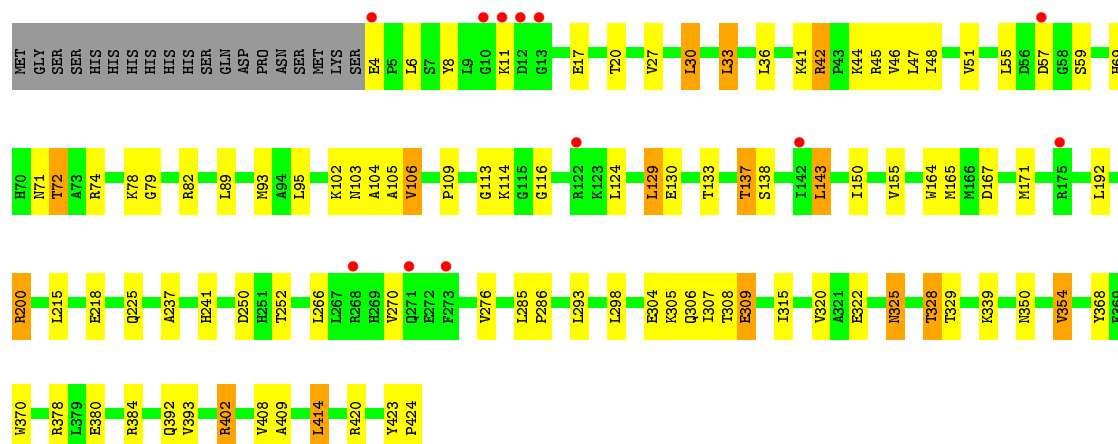
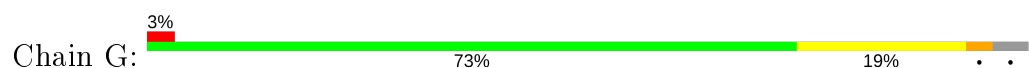
• Molecule 1: Glutamate dehydrogenase



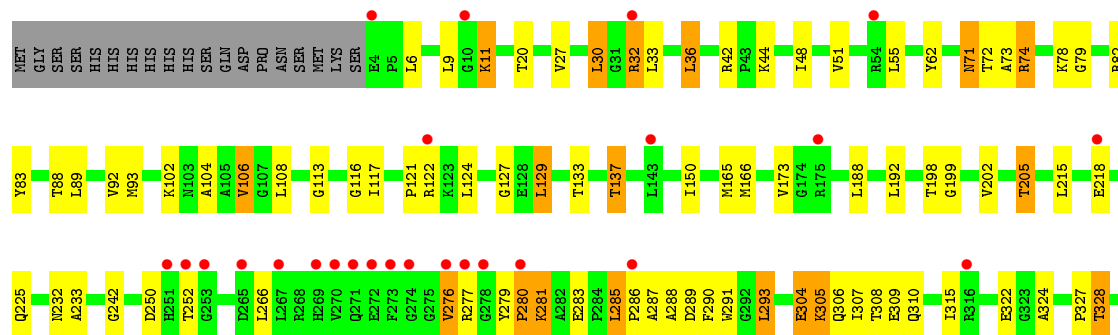
• Molecule 1: Glutamate dehydrogenase



• Molecule 1: Glutamate dehydrogenase

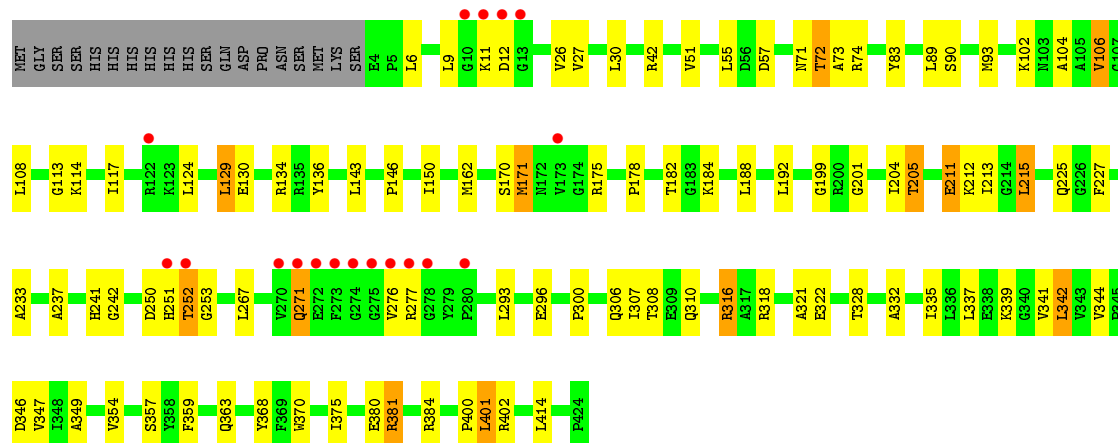


• Molecule 1: Glutamate dehydrogenase

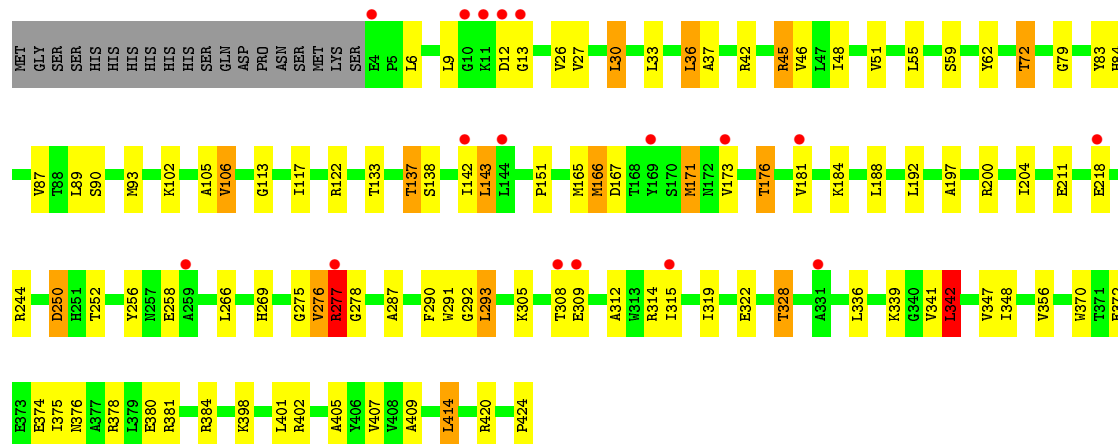




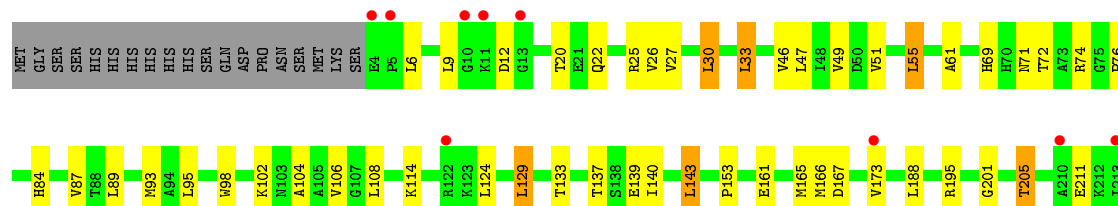
• Molecule 1: Glutamate dehydrogenase

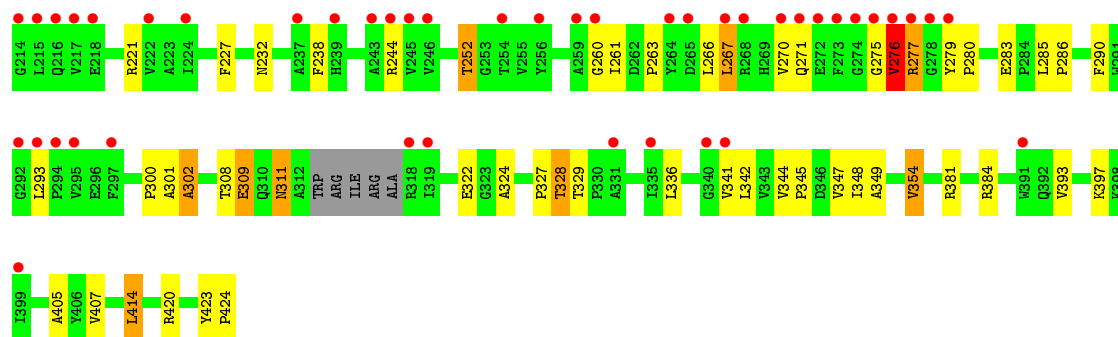


• Molecule 1: Glutamate dehydrogenase

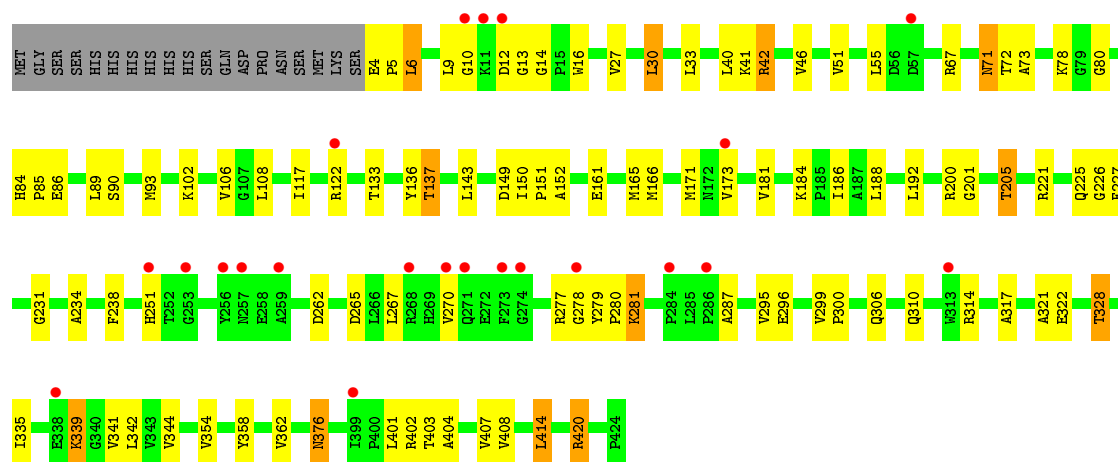
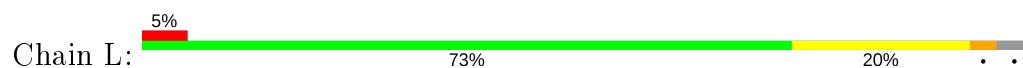


• Molecule 1: Glutamate dehydrogenase





- Molecule 1: Glutamate dehydrogenase



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NH4, PO4

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

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
1	E	402	ARG	NE-CZ-NH1	-6.00	117.30	120.30
1	B	342	LEU	CA-CB-CG	5.90	128.88	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	402	ARG	NE-CZ-NH2	5.67	123.13	120.30
1	A	381	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	H	36	LEU	CA-CB-CG	5.44	127.81	115.30
1	F	166	MET	CG-SD-CE	5.07	108.31	100.20
1	J	342	LEU	CA-CB-CG	5.06	126.93	115.30
1	E	74	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	G	354	VAL	CB-CA-C	5.04	120.97	111.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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.

All (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:HH11	1:K:277:ARG:HG3	1.24	1.02
1:K:301:ALA:N	1:K:302:ALA:HB2	1.73	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:277:ARG:HH11	1:F:277:ARG:HG2	1.25	1.02
1:A:205:THR:HG22	1:A:344:VAL:HG11	1.44	0.98
1:F:162:MET:CE	1:F:165:MET:HE2	1.92	0.98
1:G:89:LEU:HG	1:G:93:MET:HE3	1.46	0.98
1:A:381:ARG:HD3	5:A:453:HOH:O	1.63	0.97
1:L:420:ARG:HH11	1:L:420:ARG:HG2	1.27	0.97
1:F:162:MET:CE	1:F:165:MET:CE	2.41	0.97
1:J:374:GLU:O	1:J:378:ARG:HG3	1.65	0.97
1:H:9:LEU:HD21	1:H:93:MET:HE3	1.44	0.97
1:K:201:GLY:O	1:K:205:THR:HG22	1.63	0.96
1:F:162:MET:HE2	1:F:165:MET:HE2	1.44	0.96
1:C:308:THR:HG22	1:C:310:GLN:H	1.29	0.95
1:B:277:ARG:HG3	1:B:277:ARG:HH11	1.28	0.95
1:H:308:THR:HG22	1:H:310:GLN:H	1.33	0.92
1:J:89:LEU:HG	1:J:93:MET:CE	2.00	0.91
1:E:322:GLU:OE2	1:E:402:ARG:NH1	2.04	0.90
1:L:200:ARG:HD3	1:L:376:ASN:HD21	1.34	0.90
1:J:171:MET:HA	1:J:171:MET:HE2	1.53	0.90
1:K:308:THR:HG22	1:K:309:GLU:H	1.36	0.90
1:A:205:THR:CG2	1:A:344:VAL:HG11	2.03	0.88
1:A:225:GLN:HE22	1:A:306:GLN:HE21	1.22	0.87
1:J:256:TYR:OH	1:J:258:GLU:HG2	1.75	0.87
1:J:45:ARG:NH2	5:J:548:HOH:O	2.07	0.87
1:D:20:THR:HG22	5:D:1540:HOH:O	1.75	0.85
1:J:89:LEU:HG	1:J:93:MET:HE1	1.58	0.85
1:F:216:GLN:HE21	1:F:218:GLU:HB2	1.39	0.85
1:B:205:THR:HG21	1:B:349:ALA:HA	1.59	0.85
1:G:322:GLU:OE1	1:G:328:THR:HG23	1.77	0.85
1:A:25:ARG:HD3	5:A:1372:HOH:O	1.74	0.84
1:E:308:THR:HG22	1:E:310:GLN:H	1.42	0.84
1:A:167:ASP:OD1	1:C:420:ARG:NH1	2.09	0.84
1:H:89:LEU:HG	1:H:93:MET:CE	2.07	0.84
1:I:124:LEU:HD12	1:I:129:LEU:HD13	1.60	0.83
1:L:133:THR:O	1:L:137:THR:HG23	1.77	0.83
1:F:266:LEU:HD21	1:F:276:VAL:HG23	1.60	0.82
1:H:287:ALA:O	1:H:289:ASP:N	2.11	0.82
1:K:275:GLY:O	1:K:276:VAL:HB	1.77	0.82
1:A:380:GLU:OE2	1:G:218:GLU:HG3	1.80	0.81
1:A:90:SER:HA	1:A:93:MET:CE	2.10	0.81
1:B:90:SER:HA	1:B:93:MET:CE	2.10	0.81
1:I:9:LEU:HD21	1:I:93:MET:HE1	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:162:MET:SD	1:F:165:MET:CE	2.69	0.81
1:A:96:ALA:HB2	1:A:114:LYS:HB2	1.63	0.80
1:G:322:GLU:OE2	1:G:402:ARG:NH1	2.12	0.80
1:G:89:LEU:HG	1:G:93:MET:CE	2.10	0.80
1:A:9:LEU:HD11	1:A:93:MET:CE	2.11	0.79
1:D:205:THR:HG23	1:D:344:VAL:HG11	1.63	0.79
1:I:171:MET:CE	1:I:171:MET:HA	2.11	0.79
5:A:1218:HOH:O	1:B:45:ARG:HD3	1.82	0.79
1:I:205:THR:HG21	1:I:349:ALA:HA	1.65	0.78
1:A:392:GLN:O	1:A:396:GLU:HG3	1.84	0.78
1:J:381:ARG:HD3	5:J:661:HOH:O	1.82	0.78
1:B:186:ILE:HD12	1:B:186:ILE:H	1.49	0.78
1:I:225:GLN:HE22	1:I:306:GLN:HE21	1.31	0.78
1:A:380:GLU:OE1	1:A:384:ARG:NH1	2.17	0.78
1:F:225:GLN:HE22	1:F:306:GLN:HE21	1.27	0.77
1:H:137:THR:HG21	1:H:165:MET:HG2	1.66	0.77
1:J:90:SER:HA	1:J:93:MET:HE3	1.66	0.77
1:H:89:LEU:HG	1:H:93:MET:HE2	1.66	0.77
1:H:280:PRO:O	1:H:281:LYS:HB2	1.84	0.76
1:L:322:GLU:OE1	1:L:328:THR:HG23	1.84	0.76
1:D:250:ASP:HB3	5:D:1163:HOH:O	1.85	0.76
1:H:133:THR:O	1:H:137:THR:HG23	1.86	0.74
1:K:9:LEU:HD21	1:K:93:MET:HE3	1.69	0.74
1:K:9:LEU:HD21	1:K:93:MET:CE	2.17	0.74
1:D:176:THR:HA	5:D:1354:HOH:O	1.87	0.74
1:C:11:LYS:O	1:C:12:ASP:HB2	1.88	0.74
1:E:322:GLU:CD	1:E:402:ARG:HH12	1.89	0.74
1:I:9:LEU:HD21	1:I:93:MET:CE	2.17	0.74
1:L:72:THR:HG21	5:L:440:HOH:O	1.87	0.74
1:B:90:SER:HA	1:B:93:MET:HE2	1.67	0.73
1:C:205:THR:HG21	1:C:349:ALA:HA	1.69	0.73
1:E:218:GLU:O	1:E:242:GLY:O	2.06	0.73
1:B:27:VAL:HA	1:B:30:LEU:HD22	1.70	0.73
1:G:250:ASP:HB3	1:G:252:THR:H	1.52	0.73
1:H:11:LYS:C	1:H:11:LYS:HD3	2.09	0.73
1:F:308:THR:HG22	1:F:309:GLU:H	1.54	0.72
1:A:9:LEU:HD11	1:A:93:MET:HE3	1.69	0.72
1:D:89:LEU:HG	1:D:93:MET:HE2	1.71	0.72
1:D:276:VAL:HG22	5:D:1163:HOH:O	1.89	0.72
1:F:277:ARG:HH11	1:F:277:ARG:CG	2.00	0.72
1:G:89:LEU:CG	1:G:93:MET:HE3	2.18	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:225:GLN:HE22	1:H:306:GLN:HE21	1.38	0.72
1:A:90:SER:HA	1:A:93:MET:HE3	1.72	0.71
1:K:244:ARG:HD2	1:K:260:GLY:HA3	1.72	0.71
1:F:162:MET:HE1	1:F:165:MET:CE	2.20	0.71
1:K:89:LEU:HG	1:K:93:MET:CE	2.20	0.71
1:G:325:ASN:ND2	1:G:350:ASN:HD21	1.89	0.71
1:J:89:LEU:HG	1:J:93:MET:HE2	1.72	0.71
1:F:133:THR:O	1:F:137:THR:HG23	1.90	0.71
1:I:322:GLU:OE2	1:I:402:ARG:NH1	2.22	0.71
1:D:89:LEU:HG	1:D:93:MET:CE	2.21	0.70
1:K:221:ARG:NH2	5:K:1185:HOH:O	2.23	0.70
1:D:205:THR:HG21	1:D:349:ALA:HA	1.74	0.70
1:I:171:MET:HE2	1:I:171:MET:HA	1.72	0.70
1:L:420:ARG:NH1	1:L:420:ARG:HG2	2.04	0.70
1:F:162:MET:HE1	1:F:165:MET:HE1	1.72	0.70
1:L:9:LEU:HD21	1:L:93:MET:HE1	1.72	0.70
1:B:89:LEU:HG	1:B:93:MET:HE1	1.74	0.70
1:H:9:LEU:HD21	1:H:93:MET:CE	2.19	0.70
1:K:95:LEU:HB3	1:K:114:LYS:HG3	1.73	0.70
1:H:83:TYR:CE2	1:H:117:ILE:HD12	2.26	0.70
1:L:205:THR:CG2	1:L:344:VAL:HG11	2.21	0.69
1:A:198:THR:HG23	1:A:350:ASN:O	1.93	0.69
1:G:225:GLN:HE22	1:G:306:GLN:HE21	1.39	0.69
1:H:71:ASN:ND2	1:H:73:ALA:H	1.90	0.69
1:K:302:ALA:HB3	1:K:324:ALA:HB2	1.74	0.69
1:I:113:GLY:O	1:I:114:LYS:HG2	1.92	0.69
1:K:205:THR:OG1	1:K:344:VAL:HG11	1.93	0.69
1:J:176:THR:HG21	1:K:76:PRO:HD3	1.73	0.69
1:D:244:ARG:HH11	1:D:244:ARG:HB2	1.58	0.68
1:K:89:LEU:HG	1:K:93:MET:HE1	1.74	0.68
1:G:133:THR:O	1:G:137:THR:HG23	1.93	0.68
1:G:102:LYS:O	1:G:106:VAL:HG12	1.93	0.68
1:I:71:ASN:ND2	1:I:73:ALA:H	1.92	0.68
1:K:205:THR:HG21	1:K:349:ALA:HA	1.74	0.68
1:L:27:VAL:HA	1:L:30:LEU:HD22	1.76	0.68
1:A:90:SER:HA	1:A:93:MET:HE2	1.75	0.67
1:A:322:GLU:OE2	1:A:402:ARG:NH1	2.25	0.67
1:K:102:LYS:O	1:K:106:VAL:HG12	1.94	0.67
1:I:27:VAL:HA	1:I:30:LEU:HD22	1.76	0.67
1:J:133:THR:O	1:J:137:THR:CG2	2.43	0.67
1:L:102:LYS:O	1:L:106:VAL:HG13	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:42:ARG:HD2	1:J:62:TYR:HB3	1.77	0.67
1:J:171:MET:CE	1:J:171:MET:HA	2.23	0.67
1:A:133:THR:O	1:A:137:THR:HG23	1.94	0.67
1:C:153:PRO:HG2	1:C:194:ARG:HH12	1.59	0.67
1:F:162:MET:CE	1:F:165:MET:HE1	2.21	0.67
1:B:277:ARG:HG3	1:B:277:ARG:NH1	2.04	0.66
1:H:89:LEU:HG	1:H:93:MET:HE1	1.77	0.66
1:B:108:LEU:HD11	1:B:354:VAL:HG12	1.77	0.66
1:D:290:PHE:HA	1:D:293:LEU:HD23	1.76	0.66
1:H:285:LEU:HD22	1:H:286:PRO:HD2	1.77	0.66
1:G:42:ARG:HD2	1:J:62:TYR:CB	2.25	0.66
1:C:276:VAL:O	1:C:277:ARG:HB2	1.96	0.66
1:A:322:GLU:CD	1:A:402:ARG:HH12	1.99	0.65
1:L:106:VAL:HG22	1:L:108:LEU:HG	1.76	0.65
1:E:106:VAL:HG22	1:E:108:LEU:HG	1.78	0.65
1:D:106:VAL:HG22	1:D:108:LEU:HG	1.78	0.65
1:E:205:THR:HG21	1:E:349:ALA:HA	1.78	0.65
1:E:352:GLY:HA2	1:E:379:LEU:HD11	1.79	0.65
1:I:114:LYS:HE3	5:I:1053:HOH:O	1.97	0.65
1:I:102:LYS:O	1:I:106:VAL:HG13	1.96	0.65
1:B:335:ILE:O	1:B:339:LYS:HG3	1.97	0.65
1:I:42:ARG:NH1	5:I:1000:HOH:O	2.29	0.65
1:H:205:THR:HG21	1:H:344:VAL:HG11	1.78	0.64
1:A:318:ARG:HD2	5:A:1759:HOH:O	1.96	0.64
1:K:153:PRO:O	2:K:500:GLU:HB2	1.96	0.64
1:F:137:THR:HG21	1:F:165:MET:HA	1.80	0.64
1:G:325:ASN:HD22	1:G:350:ASN:HD21	1.45	0.64
1:E:225:GLN:HE22	1:E:306:GLN:HE21	1.46	0.64
1:J:72:THR:HG22	5:J:1420:HOH:O	1.98	0.64
1:B:9:LEU:HD21	1:B:93:MET:HE1	1.78	0.64
1:E:222:VAL:HG22	1:E:297:PHE:HB2	1.81	0.63
1:A:176:THR:HB	5:C:1478:HOH:O	1.97	0.63
1:H:79:GLY:HA3	1:H:113:GLY:O	1.97	0.63
1:H:102:LYS:O	1:H:106:VAL:HG13	1.99	0.63
1:I:370:TRP:HE3	1:I:375:ILE:HD13	1.64	0.63
1:E:72:THR:HG21	5:E:1813:HOH:O	2.00	0.62
1:E:322:GLU:OE1	1:E:328:THR:HG23	1.99	0.62
1:B:186:ILE:N	1:B:186:ILE:HD12	2.14	0.62
1:E:71:ASN:ND2	1:E:73:ALA:H	1.97	0.62
1:H:218:GLU:O	1:H:242:GLY:O	2.18	0.62
1:J:151:PRO:HB2	1:J:181:VAL:HG12	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:ALA:O	1:C:241:HIS:HD2	1.83	0.61
1:B:186:ILE:CD1	1:B:186:ILE:H	2.12	0.61
1:A:9:LEU:HD11	1:A:93:MET:HE1	1.80	0.61
1:F:392:GLN:HA	1:F:392:GLN:HE21	1.65	0.61
1:J:308:THR:HG22	1:J:309:GLU:H	1.66	0.61
1:K:301:ALA:N	1:K:302:ALA:CB	2.56	0.61
1:C:106:VAL:HG22	1:C:108:LEU:HG	1.82	0.61
1:A:10:GLY:O	1:A:12:ASP:N	2.33	0.61
1:A:225:GLN:NE2	1:A:306:GLN:HE21	1.98	0.61
1:B:16:TRP:HZ2	1:B:41:LYS:O	1.83	0.61
1:G:89:LEU:CD1	1:G:93:MET:HE3	2.31	0.61
1:K:322:GLU:OE1	1:K:328:THR:HG23	2.00	0.61
1:C:133:THR:O	1:C:137:THR:HG23	2.01	0.60
1:K:271:GLN:O	1:K:271:GLN:HG3	2.01	0.60
1:D:221:ARG:HH21	1:D:294:PRO:HB2	1.66	0.60
1:B:9:LEU:HD21	1:B:93:MET:CE	2.30	0.60
1:D:9:LEU:HD21	1:D:93:MET:CE	2.32	0.60
1:L:200:ARG:HD3	1:L:376:ASN:ND2	2.12	0.60
1:F:308:THR:HG22	1:F:309:GLU:N	2.15	0.60
1:J:244:ARG:HD2	1:J:258:GLU:O	2.01	0.60
1:E:45:ARG:HG2	1:F:47:LEU:HD11	1.81	0.60
1:G:27:VAL:HA	1:G:30:LEU:HD22	1.84	0.60
1:A:72:THR:HA	5:A:1313:HOH:O	2.02	0.60
1:G:322:GLU:CD	1:G:402:ARG:HH12	2.04	0.60
1:K:285:LEU:HG	1:K:286:PRO:HD2	1.84	0.60
1:A:89:LEU:HG	1:A:93:MET:HE1	1.84	0.60
1:K:133:THR:O	1:K:137:THR:HG23	2.02	0.60
1:K:271:GLN:O	1:K:271:GLN:CG	2.49	0.59
1:C:137:THR:HG21	1:C:165:MET:HA	1.83	0.59
1:D:84:HIS:CE1	1:D:86:GLU:HG2	2.37	0.59
1:E:308:THR:CG2	1:E:309:GLU:N	2.65	0.59
1:A:89:LEU:HG	1:A:93:MET:CE	2.32	0.59
1:C:322:GLU:OE2	1:C:402:ARG:NH1	2.34	0.59
1:I:90:SER:HA	1:I:93:MET:CE	2.32	0.59
1:L:221:ARG:H	1:L:296:GLU:HG2	1.67	0.59
1:I:211:GLU:HG2	5:I:1301:HOH:O	2.02	0.59
1:K:277:ARG:NH1	1:K:277:ARG:HG3	1.99	0.59
5:J:1545:HOH:O	1:L:171:MET:HE2	2.02	0.59
1:G:47:LEU:HD11	1:J:45:ARG:HG2	1.84	0.59
1:I:89:LEU:HG	1:I:93:MET:HE1	1.85	0.59
1:D:276:VAL:CG2	5:D:1163:HOH:O	2.47	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:LYS:O	1:B:106:VAL:HG13	2.02	0.58
1:H:324:ALA:HB3	1:H:327:PRO:HB3	1.86	0.58
1:E:269:HIS:CE1	1:E:278:GLY:HA3	2.38	0.58
1:I:308:THR:HG23	1:I:310:GLN:H	1.68	0.58
4:A:427:NH4:N	5:A:1369:HOH:O	2.32	0.58
1:H:106:VAL:HG22	1:H:108:LEU:HG	1.84	0.58
1:K:137:THR:HG21	1:K:165:MET:HG2	1.84	0.58
1:F:124:LEU:HD12	1:F:129:LEU:HD13	1.85	0.58
1:F:78:LYS:HD2	1:F:150:ILE:HB	1.85	0.58
1:K:290:PHE:HA	1:K:293:LEU:HD13	1.85	0.58
1:C:11:LYS:O	1:C:12:ASP:CB	2.52	0.58
1:H:266:LEU:HD11	1:H:276:VAL:HG22	1.85	0.58
1:J:420:ARG:HH12	1:L:171:MET:CE	2.16	0.58
1:G:315:ILE:O	1:G:339:LYS:NZ	2.28	0.57
1:E:133:THR:O	1:E:137:THR:CG2	2.53	0.57
1:C:169:TYR:CD1	1:C:180:VAL:HG21	2.39	0.57
1:J:133:THR:O	1:J:137:THR:HG23	2.04	0.57
1:J:322:GLU:OE2	1:J:402:ARG:NH1	2.37	0.57
1:C:79:GLY:HA3	1:C:113:GLY:O	2.04	0.57
1:H:137:THR:CG2	1:H:165:MET:HG2	2.32	0.57
1:L:403:THR:O	1:L:407:VAL:HG23	2.04	0.57
1:H:315:ILE:O	1:H:339:LYS:NZ	2.33	0.57
1:G:46:VAL:HB	1:J:48:ILE:HB	1.86	0.57
1:I:237:ALA:O	1:I:241:HIS:HD2	1.87	0.57
1:B:166:MET:HE2	1:B:178:PRO:HA	1.86	0.57
1:G:307:ILE:HB	1:G:328:THR:HB	1.87	0.57
1:A:374:GLU:O	1:A:378:ARG:HG3	2.05	0.56
1:C:153:PRO:HG2	1:C:194:ARG:NH1	2.20	0.56
1:A:27:VAL:HA	1:A:30:LEU:HD22	1.87	0.56
1:B:144:LEU:O	1:B:148:ARG:NH2	2.38	0.56
1:J:138:SER:HB3	5:J:1014:HOH:O	2.05	0.56
1:G:325:ASN:ND2	5:G:1107:HOH:O	2.38	0.56
1:H:127:GLY:HA3	5:H:1158:HOH:O	2.05	0.56
1:K:55:LEU:HD21	1:K:61:ALA:HB2	1.87	0.56
1:B:21:GLU:O	1:B:24:ASP:HB2	2.05	0.56
1:D:217:VAL:O	1:D:218:GLU:HB2	2.05	0.56
1:D:151:PRO:HD2	1:D:181:VAL:HG12	1.87	0.56
1:F:261:ILE:HG21	1:F:266:LEU:HD12	1.87	0.56
1:H:307:ILE:HB	1:H:328:THR:HB	1.86	0.56
1:E:205:THR:HG23	1:E:344:VAL:HG11	1.87	0.56
1:E:42:ARG:HD2	1:F:62:TYR:CD1	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:300:PRO:C	1:K:302:ALA:HB2	2.24	0.56
1:I:211:GLU:HG3	1:I:212:LYS:N	2.17	0.56
1:J:166:MET:HG3	1:J:184:LYS:HD3	1.87	0.56
1:J:9:LEU:HD21	1:J:93:MET:CE	2.35	0.56
1:J:292:GLY:HA2	1:J:314:ARG:O	2.06	0.55
1:K:74:ARG:NH2	1:K:108:LEU:O	2.38	0.55
1:C:9:LEU:HD11	1:C:93:MET:HE1	1.89	0.55
1:J:133:THR:O	1:J:137:THR:HG22	2.05	0.55
1:G:89:LEU:CG	1:G:93:MET:CE	2.82	0.55
1:D:252:THR:HB	1:D:277:ARG:HB2	1.89	0.55
1:I:26:VAL:O	1:I:30:LEU:HD13	2.06	0.55
1:A:74:ARG:NH2	1:A:108:LEU:O	2.34	0.55
1:C:205:THR:HG23	1:C:344:VAL:HG11	1.89	0.55
1:I:89:LEU:HG	1:I:93:MET:CE	2.37	0.55
1:D:354:VAL:CG2	5:D:1175:HOH:O	2.54	0.55
1:F:4:GLU:HB2	5:F:830:HOH:O	2.07	0.55
1:F:152:ALA:HB1	1:F:153:PRO:HD2	1.87	0.55
1:F:162:MET:SD	1:F:165:MET:HE3	2.46	0.55
1:K:302:ALA:HB3	1:K:324:ALA:CB	2.36	0.55
1:F:162:MET:SD	1:F:165:MET:HE1	2.46	0.55
1:H:322:GLU:OE1	1:H:328:THR:HG23	2.07	0.55
1:I:205:THR:HG23	1:I:344:VAL:HG11	1.89	0.55
1:I:322:GLU:CD	1:I:402:ARG:HH12	2.11	0.55
1:J:102:LYS:O	1:J:106:VAL:CG1	2.54	0.55
1:C:312:ALA:HA	1:C:315:ILE:HD12	1.88	0.54
1:A:316:ARG:NH2	1:I:384:ARG:HH12	2.05	0.54
1:L:151:PRO:HD2	1:L:181:VAL:HG12	1.88	0.54
1:B:314:ARG:HD3	5:B:744:HOH:O	2.07	0.54
1:G:105:ALA:HB2	1:G:409:ALA:HB2	1.89	0.54
1:H:420:ARG:HD2	2:H:425:GLU:HB2	1.88	0.54
1:I:89:LEU:O	1:I:93:MET:HE2	2.07	0.54
1:K:46:VAL:HG11	1:K:89:LEU:HD11	1.89	0.54
1:C:78:LYS:HD2	1:C:150:ILE:HB	1.88	0.54
1:E:84:HIS:ND1	1:E:85:PRO:HD2	2.22	0.54
1:A:12:ASP:HA	5:A:699:HOH:O	2.07	0.54
1:D:137:THR:HG21	1:D:165:MET:HA	1.88	0.54
1:D:9:LEU:HD21	1:D:93:MET:HE1	1.89	0.54
1:A:83:TYR:CE2	1:A:117:ILE:HD12	2.43	0.54
1:F:95:LEU:HB3	1:F:114:LYS:HG3	1.88	0.54
1:A:322:GLU:OE1	1:A:328:THR:HG23	2.07	0.54
1:D:358:TYR:O	1:D:362:VAL:HG23	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:167:ASP:OD1	1:K:420:ARG:NH1	2.40	0.54
1:F:55:LEU:HD21	1:F:61:ALA:HB2	1.89	0.54
1:G:20:THR:HG23	1:G:41:LYS:HE3	1.90	0.54
1:I:90:SER:HA	1:I:93:MET:HE3	1.90	0.54
1:K:345:PRO:HB2	1:K:347:VAL:HG22	1.89	0.54
1:D:285:LEU:N	1:D:286:PRO:HD3	2.23	0.54
1:F:423:TYR:O	2:F:425:GLU:N	2.41	0.54
1:H:423:TYR:CD1	1:H:424:PRO:HA	2.43	0.54
1:A:137:THR:HG21	1:A:165:MET:HA	1.89	0.54
1:A:82:ARG:HG3	1:A:155:VAL:HB	1.90	0.54
1:K:22:GLN:HG2	1:K:98:TRP:HH2	1.73	0.54
1:E:213:ILE:HD12	1:E:318:ARG:NH2	2.23	0.53
1:G:420:ARG:HD2	2:G:425:GLU:HB2	1.90	0.53
1:A:316:ARG:HH22	1:I:384:ARG:HH12	1.56	0.53
1:E:82:ARG:HG3	1:E:155:VAL:HB	1.89	0.53
1:K:336:LEU:HD22	1:K:341:VAL:HG11	1.88	0.53
1:E:71:ASN:HD21	1:E:73:ALA:CB	2.21	0.53
1:F:133:THR:O	1:F:137:THR:CG2	2.55	0.53
1:H:27:VAL:HA	1:H:30:LEU:HD22	1.90	0.53
1:L:9:LEU:HD21	1:L:93:MET:CE	2.37	0.53
1:B:71:ASN:ND2	5:B:464:HOH:O	2.42	0.53
1:A:44:LYS:NZ	5:A:457:HOH:O	2.41	0.53
1:B:17:GLU:HG2	1:B:18:ILE:N	2.24	0.53
1:J:420:ARG:HD3	2:J:425:GLU:HB2	1.91	0.53
1:E:201:GLY:O	1:E:205:THR:HB	2.08	0.53
1:I:380:GLU:OE1	1:I:384:ARG:NH1	2.42	0.53
1:K:9:LEU:HD21	1:K:93:MET:HE1	1.90	0.53
1:E:171:MET:CE	5:E:1708:HOH:O	2.57	0.53
1:E:199:GLY:HA3	1:E:233:ALA:HB3	1.90	0.53
1:L:89:LEU:HG	1:L:93:MET:HE1	1.91	0.53
1:G:130:GLU:HG3	1:G:164:TRP:CE2	2.44	0.53
1:J:308:THR:O	1:J:312:ALA:HB2	2.09	0.53
1:B:166:MET:CE	1:B:178:PRO:HA	2.39	0.53
1:C:83:TYR:CE2	1:C:117:ILE:HD12	2.43	0.53
1:D:221:ARG:HG3	1:D:295:VAL:HA	1.90	0.52
1:G:167:ASP:HB2	1:H:420:ARG:HD3	1.91	0.52
1:H:62:TYR:HB3	1:L:42:ARG:HD2	1.91	0.52
1:J:27:VAL:HA	1:J:30:LEU:HD22	1.91	0.52
1:G:378:ARG:NH2	5:G:1343:HOH:O	2.41	0.52
1:L:71:ASN:ND2	1:L:73:ALA:H	2.07	0.52
1:E:28:PRO:O	5:E:480:HOH:O	2.19	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:277:ARG:NH1	1:F:277:ARG:HG2	2.04	0.52
1:J:308:THR:HG22	1:J:309:GLU:N	2.24	0.52
1:K:267:LEU:O	1:K:271:GLN:HG2	2.10	0.52
1:B:322:GLU:OE2	1:B:402:ARG:NH1	2.42	0.52
1:D:46:VAL:HG11	1:D:89:LEU:HD11	1.90	0.52
1:K:167:ASP:HA	1:L:420:ARG:HH12	1.74	0.52
1:G:137:THR:HG21	1:G:165:MET:HG2	1.91	0.52
1:J:197:ALA:HB2	1:J:356:VAL:HG21	1.92	0.52
1:A:205:THR:CG2	1:A:344:VAL:CG1	2.84	0.51
1:D:147:ASP:OD1	1:F:175:ARG:HD2	2.10	0.51
1:K:95:LEU:HB3	1:K:114:LYS:HE2	1.91	0.51
1:C:9:LEU:HD11	1:C:93:MET:CE	2.40	0.51
1:F:241:HIS:HE1	5:F:493:HOH:O	1.92	0.51
1:I:170:SER:HB3	1:I:175:ARG:O	2.10	0.51
1:A:46:VAL:HG11	1:A:89:LEU:HD11	1.93	0.51
1:B:381:ARG:HD3	5:B:733:HOH:O	2.09	0.51
1:G:200:ARG:HG3	5:G:1072:HOH:O	2.09	0.51
1:J:137:THR:HG21	1:J:165:MET:HA	1.91	0.51
1:L:295:VAL:O	1:L:317:ALA:HA	2.10	0.51
1:C:423:TYR:CD1	1:C:424:PRO:HA	2.45	0.51
1:L:262:ASP:HB3	1:L:265:ASP:HB3	1.93	0.51
1:L:4:GLU:N	1:L:5:PRO:HD3	2.25	0.51
1:A:237:ALA:O	1:A:241:HIS:HD2	1.94	0.51
1:I:337:LEU:HD13	1:I:400:PRO:HB3	1.93	0.51
1:L:67:ARG:NH2	1:L:149:ASP:OD2	2.38	0.51
1:G:138:SER:OG	1:J:424:PRO:HG2	2.11	0.51
1:J:256:TYR:CZ	1:J:258:GLU:HG2	2.45	0.51
1:J:322:GLU:CD	1:J:402:ARG:HH12	2.13	0.51
1:J:176:THR:HG21	1:K:76:PRO:CD	2.39	0.51
1:G:74:ARG:NE	5:G:910:HOH:O	2.10	0.51
1:H:199:GLY:HA3	1:H:233:ALA:HB3	1.93	0.51
1:I:250:ASP:HB2	1:I:276:VAL:HG22	1.92	0.51
1:G:44:LYS:HE3	5:G:474:HOH:O	2.11	0.50
1:I:201:GLY:O	1:I:205:THR:HB	2.11	0.50
1:L:358:TYR:O	1:L:362:VAL:HG23	2.11	0.50
1:H:78:LYS:HD2	1:H:150:ILE:HB	1.92	0.50
1:J:347:VAL:HG23	1:J:348:ILE:HG23	1.92	0.50
1:E:27:VAL:HA	1:E:30:LEU:HD22	1.93	0.50
1:L:137:THR:HG21	1:L:165:MET:HG2	1.91	0.50
1:I:146:PRO:O	1:I:150:ILE:HD11	2.11	0.50
1:H:304:GLU:HB2	1:H:305:LYS:HD2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:384:ARG:NH1	5:I:1271:HOH:O	2.44	0.50
1:D:148:ARG:HD2	1:F:175:ARG:HG2	1.92	0.50
1:L:280:PRO:O	1:L:281:LYS:CB	2.60	0.50
1:A:318:ARG:NH1	5:A:446:HOH:O	2.39	0.50
1:E:191:SER:H	1:E:194:ARG:NH2	2.09	0.50
1:E:225:GLN:HE22	1:E:306:GLN:NE2	2.09	0.50
1:J:83:TYR:CE2	1:J:117:ILE:HD12	2.47	0.50
1:E:133:THR:O	1:E:137:THR:HG22	2.12	0.50
1:G:250:ASP:HB3	1:G:252:THR:N	2.24	0.50
1:J:266:LEU:HD11	1:J:276:VAL:HG12	1.93	0.50
1:K:89:LEU:HG	1:K:93:MET:HE2	1.93	0.50
1:J:420:ARG:HH12	1:L:171:MET:HE1	1.76	0.50
1:B:89:LEU:HG	1:B:93:MET:CE	2.42	0.50
1:G:305:LYS:HG3	1:G:329:THR:HG22	1.93	0.50
1:B:262:ASP:HB3	1:B:265:ASP:HB2	1.94	0.49
1:F:285:LEU:HD23	1:F:286:PRO:HD2	1.94	0.49
1:G:325:ASN:HD22	1:G:350:ASN:ND2	2.09	0.49
1:B:122:ARG:HE	1:B:122:ARG:HA	1.76	0.49
1:C:71:ASN:ND2	1:C:73:ALA:H	2.10	0.49
1:C:46:VAL:HB	1:D:48:ILE:HB	1.95	0.49
1:E:83:TYR:CE2	1:E:117:ILE:HD12	2.47	0.49
1:J:250:ASP:HB2	1:J:276:VAL:HG22	1.93	0.49
1:A:78:LYS:HD2	1:A:150:ILE:HB	1.94	0.49
1:D:84:HIS:HE1	1:D:86:GLU:HG2	1.77	0.49
1:I:225:GLN:HE22	1:I:306:GLN:NE2	2.05	0.49
1:E:220:ALA:HB1	1:E:296:GLU:HB2	1.93	0.49
1:F:137:THR:HG21	1:F:165:MET:HG2	1.95	0.49
1:G:4:GLU:O	1:G:42:ARG:NH2	2.46	0.49
1:G:200:ARG:HD2	5:G:1072:HOH:O	2.12	0.49
1:H:11:LYS:O	1:H:11:LYS:HD3	2.13	0.49
1:G:171:MET:HE1	5:H:450:HOH:O	2.13	0.49
1:J:380:GLU:O	1:J:384:ARG:HB2	2.11	0.49
1:H:373:GLU:H	1:H:373:GLU:CD	2.16	0.49
1:I:106:VAL:HG22	1:I:108:LEU:HG	1.94	0.49
1:J:102:LYS:O	1:J:106:VAL:HG12	2.11	0.49
1:J:37:ALA:HA	1:J:414:LEU:HD21	1.93	0.49
1:K:347:VAL:HG23	1:K:348:ILE:N	2.28	0.49
1:K:423:TYR:CD1	1:K:424:PRO:HA	2.48	0.49
1:A:424:PRO:HG2	1:B:138:SER:OG	2.13	0.49
1:D:133:THR:O	1:D:137:THR:HG22	2.12	0.49
1:G:57:ASP:OD2	1:G:59:SER:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:102:LYS:O	1:H:106:VAL:CG1	2.59	0.49
1:K:301:ALA:H	1:K:302:ALA:HB2	1.69	0.49
1:D:292:GLY:HA2	1:D:314:ARG:O	2.13	0.48
1:E:422:LEU:HD11	1:F:52:PRO:HB2	1.94	0.48
1:K:124:LEU:HD12	1:K:129:LEU:HD13	1.95	0.48
1:D:146:PRO:O	1:D:150:ILE:HD11	2.13	0.48
1:D:177:VAL:O	1:D:180:VAL:HG12	2.12	0.48
1:D:420:ARG:NH1	1:F:167:ASP:OD1	2.46	0.48
1:H:290:PHE:HA	1:H:293:LEU:HD22	1.95	0.48
1:H:291:TRP:O	1:H:315:ILE:HA	2.14	0.48
1:C:95:LEU:CB	1:C:114:LYS:HG3	2.43	0.48
1:D:217:VAL:O	1:D:218:GLU:CB	2.61	0.48
1:J:256:TYR:OH	1:J:258:GLU:CG	2.54	0.48
1:K:25:ARG:HD2	5:K:1389:HOH:O	2.14	0.48
1:L:90:SER:HA	1:L:93:MET:CE	2.43	0.48
1:D:201:GLY:O	1:D:205:THR:HB	2.13	0.48
1:I:171:MET:HE3	1:I:171:MET:HA	1.90	0.48
1:L:90:SER:HA	1:L:93:MET:HE2	1.95	0.48
1:B:266:LEU:HD11	1:B:276:VAL:CG2	2.44	0.48
1:D:113:GLY:O	1:D:114:LYS:HG2	2.12	0.48
1:D:82:ARG:HG3	1:D:155:VAL:HB	1.96	0.48
1:H:48:ILE:HB	1:L:46:VAL:HB	1.95	0.48
1:J:171:MET:CE	1:J:171:MET:CA	2.91	0.48
1:B:108:LEU:CD1	1:B:354:VAL:HG12	2.44	0.48
1:B:322:GLU:CD	1:B:402:ARG:HH12	2.16	0.48
1:C:48:ILE:HB	1:D:46:VAL:HB	1.96	0.48
1:E:213:ILE:HD12	1:E:318:ARG:HH22	1.78	0.48
1:H:252:THR:HB	1:H:277:ARG:HB2	1.94	0.48
1:A:72:THR:CA	5:A:1313:HOH:O	2.62	0.48
1:E:308:THR:HG22	1:E:310:GLN:N	2.20	0.48
1:F:108:LEU:HD11	1:F:354:VAL:HG13	1.96	0.48
1:J:26:VAL:HG13	1:J:407:VAL:HG22	1.95	0.48
1:K:308:THR:HG22	1:K:309:GLU:N	2.16	0.48
1:F:308:THR:CG2	1:F:309:GLU:H	2.25	0.47
1:G:48:ILE:HB	1:J:46:VAL:HB	1.94	0.47
1:B:225:GLN:HE22	1:B:306:GLN:NE2	2.11	0.47
1:G:266:LEU:O	1:G:270:VAL:HG23	2.14	0.47
1:G:308:THR:HG22	1:G:309:GLU:N	2.29	0.47
1:A:72:THR:CB	5:A:1313:HOH:O	2.52	0.47
1:F:277:ARG:NH1	1:F:277:ARG:CG	2.69	0.47
1:G:69:HIS:CE1	1:G:143:LEU:HG	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:89:LEU:CD1	1:G:93:MET:CE	2.92	0.47
1:D:252:THR:OG1	1:D:276:VAL:HG23	2.14	0.47
1:D:254:THR:HG21	1:D:290:PHE:HB2	1.95	0.47
1:I:199:GLY:HA3	1:I:233:ALA:HB3	1.96	0.47
1:C:134:ARG:O	1:C:168:THR:HG21	2.15	0.47
1:D:20:THR:HG23	1:D:41:LYS:HE3	1.97	0.47
1:F:212:LYS:HD2	1:F:391:TRP:CE2	2.48	0.47
1:I:83:TYR:CE2	1:I:117:ILE:HD12	2.50	0.47
1:K:106:VAL:HG13	1:K:108:LEU:HG	1.95	0.47
1:C:102:LYS:O	1:C:106:VAL:HG13	2.14	0.47
1:C:27:VAL:HA	1:C:30:LEU:HD22	1.96	0.47
1:C:351:ALA:O	1:C:354:VAL:HG12	2.14	0.47
1:C:420:ARG:HD3	2:C:425:GLU:HB2	1.96	0.47
1:J:171:MET:HG3	1:K:423:TYR:O	2.15	0.47
1:A:224:ILE:HD12	1:A:235:ALA:HB2	1.96	0.47
1:H:198:THR:O	1:H:202:VAL:HG23	2.15	0.47
1:I:213:ILE:HD12	1:I:318:ARG:NH2	2.30	0.47
1:A:13:GLY:HA3	1:A:17:GLU:HB2	1.97	0.47
1:C:95:LEU:HB3	1:C:114:LYS:HG3	1.96	0.47
1:G:72:THR:HG21	5:G:768:HOH:O	2.14	0.47
1:J:9:LEU:HD21	1:J:93:MET:HE3	1.95	0.47
1:B:46:VAL:HG11	1:B:89:LEU:HD11	1.97	0.47
1:L:267:LEU:HA	1:L:270:VAL:HG12	1.97	0.47
1:F:44:LYS:HE2	5:F:445:HOH:O	2.14	0.47
1:G:124:LEU:HD12	1:G:129:LEU:HD13	1.97	0.47
1:G:42:ARG:CD	1:J:62:TYR:HB3	2.44	0.47
1:K:270:VAL:CG2	1:K:276:VAL:HG23	2.45	0.47
1:D:122:ARG:HA	1:D:122:ARG:NE	2.30	0.47
1:B:137:THR:OG1	1:B:165:MET:HG2	2.15	0.46
1:C:166:MET:HE3	1:C:184:LYS:HD2	1.98	0.46
1:F:152:ALA:HB1	1:F:153:PRO:CD	2.45	0.46
1:G:370:TRP:CD2	1:G:378:ARG:NH1	2.83	0.46
1:J:398:LYS:HE2	1:J:398:LYS:HB2	1.80	0.46
1:F:84:HIS:CG	1:F:85:PRO:HD2	2.50	0.46
1:G:322:GLU:OE1	1:G:328:THR:CG2	2.58	0.46
1:H:250:ASP:HB2	1:H:276:VAL:HB	1.96	0.46
1:A:203:PHE:CE1	1:A:241:HIS:CD2	3.04	0.46
1:D:27:VAL:HA	1:D:30:LEU:HD22	1.97	0.46
1:L:226:GLY:O	1:L:231:GLY:HA3	2.15	0.46
1:A:176:THR:O	1:A:176:THR:HG23	2.15	0.46
1:I:26:VAL:HG12	1:I:30:LEU:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:316:ARG:HB3	1:I:316:ARG:HH11	1.79	0.46
1:J:420:ARG:NH1	1:L:171:MET:HE1	2.31	0.46
1:A:308:THR:HG22	1:A:309:GLU:N	2.30	0.46
1:E:23:VAL:O	1:E:27:VAL:HG23	2.15	0.46
1:L:71:ASN:ND2	5:L:823:HOH:O	2.48	0.46
1:A:82:ARG:O	1:A:116:GLY:HA2	2.16	0.46
1:D:225:GLN:HE22	1:D:306:GLN:NE2	2.14	0.46
1:E:204:ILE:HD13	1:E:380:GLU:HA	1.98	0.46
1:K:308:THR:HG23	1:K:329:THR:HG21	1.96	0.46
1:D:226:GLY:O	1:D:231:GLY:HA3	2.16	0.46
1:D:71:ASN:ND2	1:D:73:ALA:H	2.14	0.46
1:A:148:ARG:HD2	1:E:175:ARG:HG2	1.96	0.46
1:A:308:THR:CG2	5:A:447:HOH:O	2.64	0.46
1:L:402:ARG:HB2	1:L:402:ARG:HH21	1.81	0.46
1:B:175:ARG:HD2	1:F:147:ASP:OD1	2.16	0.46
1:K:22:GLN:HG2	1:K:98:TRP:CH2	2.51	0.46
1:L:404:ALA:O	1:L:408:VAL:HG23	2.16	0.46
1:B:199:GLY:HA3	1:B:233:ALA:HB3	1.98	0.45
1:K:33:LEU:HG	1:K:414:LEU:HB3	1.98	0.45
1:B:113:GLY:O	1:B:114:LYS:HG2	2.16	0.45
1:H:44:LYS:HD2	1:H:72:THR:HG22	1.98	0.45
1:I:267:LEU:O	1:I:271:GLN:HG2	2.16	0.45
1:J:269:HIS:HE1	1:J:277:ARG:HB2	1.81	0.45
1:A:72:THR:HG22	5:A:469:HOH:O	2.15	0.45
1:E:222:VAL:HG21	1:E:238:PHE:CD1	2.51	0.45
1:G:250:ASP:HB2	1:G:276:VAL:HG22	1.97	0.45
1:I:308:THR:HA	1:I:332:ALA:HB2	1.98	0.45
1:A:120:ASP:OD2	1:A:122:ARG:HB2	2.16	0.45
1:B:250:ASP:OD1	1:B:276:VAL:HB	2.17	0.45
1:E:308:THR:HG23	1:E:309:GLU:H	1.82	0.45
1:F:198:THR:O	1:F:202:VAL:HG23	2.15	0.45
1:G:380:GLU:HG3	1:G:384:ARG:HD3	1.98	0.45
1:I:178:PRO:O	1:I:184:LYS:HE3	2.17	0.45
1:C:169:TYR:CG	1:C:180:VAL:HG21	2.52	0.45
1:K:252:THR:CG2	1:K:277:ARG:HB2	2.47	0.45
1:I:124:LEU:HD12	1:I:129:LEU:CD1	2.40	0.45
1:L:335:ILE:O	1:L:339:LYS:HG3	2.16	0.45
1:A:84:HIS:HB3	1:A:87:VAL:HG23	1.97	0.45
1:I:57:ASP:OD2	1:I:57:ASP:C	2.55	0.45
1:A:133:THR:O	1:A:137:THR:CG2	2.64	0.45
1:A:69:HIS:CE1	1:A:143:LEU:HG	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:72:THR:O	1:E:72:THR:HG23	2.16	0.45
1:G:171:MET:HA	1:G:171:MET:CE	2.47	0.45
1:G:392:GLN:HG2	5:G:687:HOH:O	2.17	0.45
1:K:279:TYR:HA	1:K:280:PRO:HD3	1.83	0.45
1:C:237:ALA:O	1:C:241:HIS:CD2	2.68	0.45
1:E:133:THR:O	1:E:137:THR:HG23	2.17	0.45
1:G:82:ARG:HG3	1:G:155:VAL:HB	1.98	0.45
1:I:178:PRO:O	1:I:184:LYS:CE	2.65	0.45
1:J:142:ILE:HG13	1:J:143:LEU:HD13	1.98	0.45
1:J:322:GLU:OE1	1:J:328:THR:HG23	2.17	0.45
1:K:108:LEU:HD11	1:K:354:VAL:HG13	1.98	0.45
1:K:393:VAL:HG13	1:K:397:LYS:HD2	1.99	0.45
1:L:161:GLU:O	1:L:165:MET:HG3	2.15	0.45
1:C:308:THR:HG22	1:C:310:GLN:N	2.13	0.44
1:F:332:ALA:O	1:F:336:LEU:HG	2.16	0.44
1:G:285:LEU:HD12	1:G:286:PRO:HD2	1.98	0.44
1:J:72:THR:CG2	1:J:72:THR:O	2.64	0.44
1:A:330:PRO:O	1:A:333:ASP:HB2	2.17	0.44
1:A:344:VAL:HG12	1:A:349:ALA:HB2	1.99	0.44
1:A:354:VAL:HG23	2:A:500:GLU:HG3	1.98	0.44
1:F:345:PRO:HB2	1:F:347:VAL:HG22	1.99	0.44
1:A:102:LYS:O	1:A:106:VAL:HG13	2.18	0.44
1:B:51:VAL:HG23	1:B:135:ARG:HB3	1.99	0.44
1:D:89:LEU:HG	1:D:93:MET:HE1	1.95	0.44
1:F:256:TYR:HB2	1:F:285:LEU:HD12	1.98	0.44
1:J:84:HIS:HB3	1:J:87:VAL:HG23	1.99	0.44
1:A:10:GLY:C	1:A:12:ASP:N	2.71	0.44
1:A:13:GLY:HA3	1:A:17:GLU:HG3	1.99	0.44
1:G:44:LYS:HZ1	1:G:45:ARG:NH1	2.16	0.44
1:E:142:ILE:O	1:E:148:ARG:NH2	2.49	0.44
1:E:347:VAL:HG11	1:E:406:TYR:HE1	1.82	0.44
1:F:27:VAL:HA	1:F:30:LEU:HD22	1.98	0.44
1:J:347:VAL:HG21	1:J:405:ALA:HB1	2.00	0.44
1:J:105:ALA:HB2	1:J:409:ALA:HB2	2.00	0.44
1:J:36:LEU:HB3	1:J:414:LEU:HG	2.00	0.44
1:K:84:HIS:HB3	1:K:87:VAL:HG23	2.00	0.44
1:L:166:MET:CE	1:L:184:LYS:HD2	2.48	0.44
1:L:201:GLY:O	1:L:205:THR:HB	2.17	0.44
1:L:84:HIS:CG	1:L:85:PRO:HD2	2.53	0.44
1:B:224:ILE:HG12	1:B:299:VAL:HB	1.99	0.44
1:G:368:TYR:OH	3:G:426:PO4:O1	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:266:LEU:HD11	1:K:276:VAL:HG22	2.00	0.44
1:A:95:LEU:CB	1:A:114:LYS:HG3	2.47	0.44
1:H:280:PRO:O	1:H:281:LYS:CB	2.62	0.44
1:H:322:GLU:OE2	1:H:402:ARG:NH1	2.51	0.44
1:D:200:ARG:HD3	1:D:376:ASN:HD21	1.83	0.44
2:F:500:GLU:N	5:F:979:HOH:O	2.50	0.44
1:I:300:PRO:HD2	1:I:321:ALA:O	2.18	0.44
1:L:225:GLN:HE22	1:L:306:GLN:HE21	1.66	0.44
1:B:23:VAL:O	1:B:27:VAL:HG23	2.18	0.44
1:B:404:ALA:O	1:B:408:VAL:HG23	2.18	0.44
1:I:381:ARG:HD3	5:I:1809:HOH:O	2.18	0.44
1:K:324:ALA:HB3	1:K:327:PRO:HG3	2.00	0.44
5:D:852:HOH:O	1:F:187:ALA:HB1	2.18	0.43
1:F:423:TYR:CD1	1:F:424:PRO:HA	2.52	0.43
1:G:44:LYS:NZ	1:G:45:ARG:NH1	2.66	0.43
1:H:344:VAL:HG12	1:H:349:ALA:HB2	1.99	0.43
1:K:227:PHE:CE2	1:K:267:LEU:HD12	2.53	0.43
1:L:227:PHE:HD2	1:L:270:VAL:HG11	1.83	0.43
1:C:140:ILE:HD12	1:C:144:LEU:HD21	1.99	0.43
1:D:279:TYR:HA	1:D:280:PRO:HD2	1.91	0.43
1:E:404:ALA:O	1:E:408:VAL:HG23	2.18	0.43
1:E:69:HIS:CE1	1:E:143:LEU:HG	2.53	0.43
1:F:307:ILE:HG22	1:F:332:ALA:HB1	1.99	0.43
1:G:237:ALA:O	1:G:241:HIS:HD2	2.01	0.43
1:G:33:LEU:HG	1:G:414:LEU:HB3	2.01	0.43
1:A:308:THR:HG22	1:A:309:GLU:H	1.83	0.43
1:C:14:GLY:H	1:C:15:PRO:HD2	1.83	0.43
1:F:27:VAL:N	1:F:28:PRO:CD	2.81	0.43
1:L:40:LEU:HD11	1:L:414:LEU:HD21	2.01	0.43
1:A:9:LEU:CD1	1:A:93:MET:HE1	2.47	0.43
1:B:370:TRP:HE3	1:B:375:ILE:HD13	1.83	0.43
1:D:266:LEU:HD11	1:D:276:VAL:HG12	1.99	0.43
1:A:421:GLY:O	2:A:425:GLU:HB3	2.18	0.43
1:D:307:ILE:HB	1:D:328:THR:HG22	2.00	0.43
1:D:9:LEU:HD21	1:D:93:MET:HE3	2.00	0.43
1:F:278:GLY:O	1:F:279:TYR:C	2.57	0.43
1:H:83:TYR:HB3	1:H:121:PRO:HG3	2.01	0.43
1:H:124:LEU:HB2	1:H:129:LEU:HD13	2.01	0.43
1:E:237:ALA:O	1:E:241:HIS:HD2	2.02	0.43
1:G:82:ARG:O	1:G:116:GLY:HA2	2.19	0.43
1:G:420:ARG:NH2	5:G:1332:HOH:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:THR:HG21	1:A:344:VAL:HG11	1.94	0.43
1:A:212:LYS:NZ	1:A:388:GLU:OE1	2.43	0.43
1:E:398:LYS:HD2	5:E:745:HOH:O	2.18	0.43
1:G:304:GLU:H	1:G:304:GLU:HG2	1.72	0.43
1:I:130:GLU:O	1:I:134:ARG:HG3	2.19	0.43
1:I:89:LEU:C	1:I:93:MET:HE2	2.38	0.43
1:K:285:LEU:HG	1:K:286:PRO:CD	2.48	0.43
1:C:48:ILE:HG21	1:D:8:TYR:CE1	2.54	0.43
1:D:102:LYS:O	1:D:106:VAL:HG13	2.17	0.43
1:D:119:VAL:HA	5:D:1164:HOH:O	2.18	0.43
1:E:286:PRO:O	1:E:289:ASP:HB2	2.19	0.43
1:F:46:VAL:HG11	1:F:89:LEU:HD11	2.01	0.43
1:I:90:SER:HA	1:I:93:MET:HE2	2.01	0.43
1:A:299:VAL:HG13	1:A:321:ALA:O	2.18	0.43
1:B:114:LYS:HE3	5:B:441:HOH:O	2.17	0.43
1:C:148:ARG:NH1	5:C:1045:HOH:O	2.52	0.43
1:G:424:PRO:HG2	1:J:138:SER:OG	2.18	0.43
1:J:277:ARG:HB3	1:J:278:GLY:H	1.47	0.43
1:K:277:ARG:NH1	1:K:277:ARG:CG	2.74	0.43
1:K:347:VAL:HG21	1:K:405:ALA:HB1	2.01	0.43
1:E:71:ASN:HD21	1:E:73:ALA:HB3	1.83	0.42
1:E:9:LEU:HA	1:E:9:LEU:HD23	1.89	0.42
1:F:144:LEU:O	1:F:148:ARG:CZ	2.67	0.42
1:G:308:THR:HG22	1:G:309:GLU:H	1.84	0.42
1:I:359:PHE:O	1:I:363:GLN:HG3	2.19	0.42
1:I:204:ILE:HD13	1:I:380:GLU:HA	2.01	0.42
1:C:194:ARG:NE	5:C:1253:HOH:O	2.52	0.42
1:G:8:TYR:HE2	1:G:93:MET:CE	2.32	0.42
1:H:354:VAL:HG22	5:H:829:HOH:O	2.18	0.42
1:J:290:PHE:HA	1:J:293:LEU:HD22	2.01	0.42
1:J:79:GLY:HA3	1:J:113:GLY:O	2.19	0.42
1:L:133:THR:O	1:L:137:THR:CG2	2.58	0.42
1:A:205:THR:HG22	1:A:344:VAL:CG1	2.32	0.42
1:A:404:ALA:O	1:A:408:VAL:HG23	2.19	0.42
1:C:85:PRO:HD3	1:C:120:ASP:HA	2.00	0.42
1:E:180:VAL:HG13	1:E:181:VAL:HG13	2.01	0.42
1:J:420:ARG:HH12	1:L:171:MET:HE3	1.83	0.42
1:L:122:ARG:HA	1:L:122:ARG:CZ	2.49	0.42
1:A:315:ILE:O	1:A:339:LYS:NZ	2.38	0.42
1:C:308:THR:CG2	1:C:309:GLU:N	2.82	0.42
1:D:32:ARG:HH11	1:D:32:ARG:HB3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:266:LEU:O	1:F:270:VAL:HG23	2.18	0.42
1:G:89:LEU:HD11	1:G:93:MET:CE	2.49	0.42
1:I:182:THR:HG1	1:I:357:SER:HG	1.64	0.42
1:I:71:ASN:HD21	1:I:73:ALA:CB	2.32	0.42
1:L:221:ARG:H	1:L:296:GLU:CG	2.31	0.42
1:L:310:GLN:O	1:L:314:ARG:NH1	2.52	0.42
1:B:279:TYR:HA	1:B:280:PRO:HD3	1.81	0.42
1:B:101:ILE:HG21	1:B:406:TYR:CD1	2.55	0.42
1:B:171:MET:HG3	1:F:423:TYR:O	2.19	0.42
1:G:78:LYS:HD2	1:G:150:ILE:HB	2.02	0.42
1:H:88:THR:O	1:H:92:VAL:HG23	2.19	0.42
1:L:300:PRO:HD2	1:L:321:ALA:O	2.19	0.42
1:L:342:LEU:HD22	1:L:401:LEU:HD22	2.02	0.42
1:B:344:VAL:HG12	1:B:349:ALA:HB2	2.00	0.42
1:D:262:ASP:HA	1:D:263:PRO:HD3	1.85	0.42
1:E:203:PHE:C	1:E:203:PHE:CD1	2.93	0.42
1:G:378:ARG:CZ	5:G:1343:HOH:O	2.67	0.42
1:G:79:GLY:HA3	1:G:113:GLY:O	2.20	0.42
1:I:74[A]:ARG:NH1	1:I:104:ALA:HA	2.34	0.42
1:K:261:ILE:O	1:K:263:PRO:HD3	2.20	0.42
1:A:167:ASP:O	1:A:171:MET:HG2	2.19	0.42
1:E:244:ARG:NH2	1:E:258:GLU:O	2.51	0.42
1:E:27:VAL:N	1:E:28:PRO:CD	2.82	0.42
1:F:354:VAL:HG23	2:F:500:GLU:HG2	2.00	0.42
1:J:252:THR:O	1:J:252:THR:HG22	2.19	0.42
1:B:277:ARG:NH1	1:B:277:ARG:CG	2.76	0.42
1:C:358:TYR:O	1:C:362:VAL:HG23	2.20	0.42
1:F:199:GLY:HA3	1:F:233:ALA:HB3	2.02	0.42
1:I:335:ILE:O	1:I:339:LYS:HG3	2.20	0.42
1:A:236:ARG:HH11	1:A:236:ARG:HD2	1.67	0.42
1:B:95:LEU:HB3	1:B:114:LYS:HG3	2.02	0.42
1:B:155:VAL:O	1:B:156:ASN:HB2	2.19	0.42
1:D:244:ARG:NH1	1:D:244:ARG:HB2	2.29	0.42
1:L:267:LEU:HA	1:L:270:VAL:CG1	2.49	0.42
1:L:277:ARG:HA	1:L:278:GLY:HA2	1.83	0.42
1:L:281:LYS:HD3	1:L:281:LYS:O	2.20	0.42
1:L:80:GLY:HA2	1:L:152:ALA:O	2.20	0.42
1:B:169:TYR:O	1:B:173:VAL:HB	2.19	0.41
1:E:82:ARG:O	1:E:116:GLY:HA2	2.20	0.41
1:J:319:ILE:HA	1:J:342:LEU:O	2.20	0.41
1:J:370:TRP:HE3	1:J:375:ILE:HD13	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:THR:O	1:D:137:THR:CG2	2.67	0.41
1:D:212:LYS:HD2	1:D:391:TRP:NE1	2.35	0.41
1:E:137:THR:HG21	1:E:165:MET:HA	2.01	0.41
1:F:51:VAL:HA	1:F:52:PRO:HD2	1.96	0.41
1:I:215:LEU:HD11	1:I:296:GLU:HB3	2.01	0.41
1:I:72:THR:O	1:I:72:THR:CG2	2.67	0.41
1:L:4:GLU:N	1:L:5:PRO:CD	2.84	0.41
1:A:10:GLY:C	1:A:12:ASP:H	2.22	0.41
1:D:354:VAL:HG21	5:D:1175:HOH:O	2.20	0.41
1:E:26:VAL:HG13	1:E:407:VAL:HG22	2.01	0.41
1:F:225:GLN:HE22	1:F:306:GLN:NE2	2.06	0.41
1:H:82:ARG:O	1:H:116:GLY:HA2	2.20	0.41
1:L:78:LYS:HD2	1:L:150:ILE:HB	2.03	0.41
1:E:308:THR:HG22	1:E:309:GLU:N	2.34	0.41
1:H:74:ARG:NH2	1:H:104:ALA:HA	2.35	0.41
1:C:13:GLY:HA3	1:C:14:GLY:HA2	1.67	0.41
1:C:252:THR:HG21	1:C:277:ARG:HB2	2.01	0.41
1:D:225:GLN:HE22	1:D:306:GLN:HE21	1.66	0.41
1:G:74:ARG:NH2	5:G:910:HOH:O	2.51	0.41
1:I:342:LEU:HD21	1:I:401:LEU:HD21	2.02	0.41
1:J:336:LEU:HD23	1:J:339:LYS:HE3	2.03	0.41
1:L:16:TRP:HZ2	1:L:41:LYS:O	2.03	0.41
1:B:134:ARG:HG2	1:B:168:THR:OG1	2.20	0.41
1:B:90:SER:HA	1:B:93:MET:HE3	1.96	0.41
1:D:313:TRP:CD1	1:D:313:TRP:C	2.94	0.41
1:H:32:ARG:HG2	1:H:33:LEU:HD13	2.01	0.41
1:K:49:VAL:HG11	1:K:139:GLU:HB3	2.01	0.41
1:K:69:HIS:CE1	1:K:143:LEU:HG	2.55	0.41
1:J:420:ARG:NH1	1:L:171:MET:CE	2.84	0.41
1:A:108:LEU:HD23	1:A:108:LEU:N	2.35	0.41
1:A:62:TYR:HB3	1:B:42:ARG:HD2	2.02	0.41
1:B:262:ASP:HA	1:B:263:PRO:HD3	1.91	0.41
1:C:307:ILE:HB	1:C:328:THR:HG22	2.02	0.41
1:F:95:LEU:CB	1:F:114:LYS:HG3	2.50	0.41
1:C:122:ARG:HA	1:C:122:ARG:HH11	1.86	0.41
1:C:30:LEU:HA	1:C:30:LEU:HD12	1.81	0.41
1:B:378:ARG:HG2	3:D:426:PO4:O2	2.20	0.41
1:G:137:THR:HG21	1:G:165:MET:HA	2.03	0.41
1:I:370:TRP:CE3	1:I:375:ILE:HD13	2.50	0.41
1:J:200:ARG:O	1:J:204:ILE:HG13	2.20	0.41
1:A:343:VAL:O	1:A:345:PRO:HD3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:ILE:CD1	1:B:186:ILE:N	2.81	0.41
1:B:79:GLY:HA3	1:B:113:GLY:O	2.21	0.41
1:D:295:VAL:O	1:D:317:ALA:HA	2.20	0.41
1:D:423:TYR:HA	1:D:424:PRO:C	2.41	0.41
1:I:346:ASP:O	1:I:347:VAL:C	2.58	0.41
1:G:378:ARG:HD3	1:I:368:TYR:OH	2.20	0.41
1:K:26:VAL:HG13	1:K:407:VAL:HG22	2.02	0.41
1:L:108:LEU:HD11	1:L:354:VAL:HG12	2.03	0.41
1:A:215:LEU:HD13	1:A:319:ILE:HD12	2.01	0.41
1:B:90:SER:CA	1:B:93:MET:HE2	2.44	0.41
1:D:34:ALA:N	1:D:35:PRO:CD	2.84	0.41
1:E:32:ARG:H	1:E:32:ARG:HG2	1.77	0.41
1:J:275:GLY:O	1:J:277:ARG:N	2.48	0.41
1:L:117:ILE:HD11	1:L:136:TYR:CG	2.55	0.41
1:B:151:PRO:HB2	1:B:181:VAL:HG12	2.03	0.41
1:B:188:LEU:HA	1:B:188:LEU:HD12	1.91	0.41
1:C:82:ARG:HG3	1:C:155:VAL:HB	2.02	0.41
1:D:423:TYR:CD1	1:D:424:PRO:HA	2.56	0.41
1:F:79:GLY:HA3	1:F:113:GLY:O	2.21	0.41
1:G:95:LEU:HB3	1:G:114:LYS:HE2	2.03	0.41
1:G:378:ARG:NE	5:G:1343:HOH:O	2.54	0.41
1:A:313:TRP:CH2	1:I:242:GLY:HA3	2.56	0.41
1:H:133:THR:O	1:H:137:THR:CG2	2.63	0.40
1:I:162:MET:HG3	1:I:182:THR:O	2.21	0.40
1:I:307:ILE:HD12	1:I:328:THR:HG22	2.01	0.40
1:A:279:TYR:HA	1:A:280:PRO:HD3	1.94	0.40
1:B:101:ILE:HG21	1:B:406:TYR:HD1	1.86	0.40
1:C:137:THR:CG2	1:C:165:MET:HG2	2.52	0.40
1:D:308:THR:C	1:D:310:GLN:H	2.25	0.40
1:D:51:VAL:HA	1:D:52:PRO:HD2	1.86	0.40
1:G:393:VAL:HG21	1:G:408:VAL:HG22	2.02	0.40
1:J:291:TRP:O	1:J:315:ILE:HA	2.21	0.40
1:K:27:VAL:HA	1:K:30:LEU:HD22	2.03	0.40
1:L:299:VAL:HG22	1:L:321:ALA:HB3	2.04	0.40
1:C:308:THR:HG22	1:C:309:GLU:N	2.37	0.40
1:I:117:ILE:HD11	1:I:136:TYR:CG	2.55	0.40
1:K:74:ARG:NH2	1:K:104:ALA:HA	2.37	0.40
1:L:234:ALA:O	1:L:238:PHE:HD2	2.04	0.40
1:A:212:LYS:HE2	1:A:391:TRP:CD1	2.56	0.40
1:E:57:ASP:OD2	1:E:59:SER:HB3	2.22	0.40
1:G:298:LEU:O	1:G:320:VAL:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:414:LEU:HD12	1:H:414:LEU:HA	1.92	0.40
1:K:47:LEU:HD23	1:K:140:ILE:HG22	2.03	0.40
1:C:262:ASP:HA	1:C:263:PRO:HD3	1.90	0.40
1:C:105:ALA:HB2	1:C:409:ALA:HB2	2.03	0.40
1:E:266:LEU:O	1:E:270:VAL:HG23	2.22	0.40
1:G:103:ASN:O	1:G:104:ALA:C	2.59	0.40
1:G:423:TYR:HA	1:G:424:PRO:C	2.42	0.40
1:I:252:THR:HB	1:I:277:ARG:HB2	2.03	0.40
1:K:301:ALA:CA	1:K:302:ALA:CB	2.99	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	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

All (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
1	J	277	ARG
1	J	305	LYS
1	K	12	ASP
1	K	276	VAL
1	K	302	ALA
1	L	251	HIS
1	A	11	LYS
1	C	12	ASP
1	C	252	THR
1	F	288	ALA
1	J	276	VAL
1	J	287	ALA
1	K	311	ASN
1	D	272	GLU
1	E	277	ARG
1	K	309	GLU
1	L	6	LEU
1	H	279	TYR
1	J	13	GLY
1	L	279	TYR
1	L	287	ALA
1	E	273	PHE
1	I	252	THR
1	L	14	GLY
1	E	280	PRO
1	L	10	GLY
1	L	13	GLY
1	I	253	GLY
1	A	141	GLY

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

All (354) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	6	LEU
1	A	9	LEU
1	A	11	LYS
1	A	17	GLU
1	A	26	VAL
1	A	30	LEU
1	A	40	LEU
1	A	42	ARG
1	A	45	ARG
1	A	51	VAL
1	A	55	LEU
1	A	72	THR
1	A	90	SER
1	A	106	VAL
1	A	114	LYS
1	A	122	ARG
1	A	129	LEU
1	A	137	THR
1	A	143	LEU

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Mol	Chain	Res	Type
1	A	173	VAL
1	A	188	LEU
1	A	192	LEU
1	A	200	ARG
1	A	252	THR
1	A	273	PHE
1	A	276	VAL
1	A	328	THR
1	A	341	VAL
1	A	354	VAL
1	A	398	LYS
1	A	414	LEU
1	B	6	LEU
1	B	11	LYS
1	B	17	GLU
1	B	26	VAL
1	B	30	LEU
1	B	51	VAL
1	B	55	LEU
1	B	72	THR
1	B	106	VAL
1	B	122	ARG
1	B	129	LEU
1	B	151	PRO
1	B	166	MET
1	B	173	VAL
1	B	188	LEU
1	B	192	LEU
1	B	215	LEU
1	B	265	ASP
1	B	271	GLN
1	B	276	VAL
1	B	277	ARG
1	B	293	LEU
1	B	304	GLU
1	B	328	THR
1	B	339	LYS
1	B	341	VAL
1	B	342	LEU
1	B	357	SER
1	B	373	GLU
1	B	376	ASN

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Mol	Chain	Res	Type
1	B	396	GLU
1	B	401	LEU
1	B	414	LEU
1	C	6	LEU
1	C	11	LYS
1	C	20	THR
1	C	30	LEU
1	C	42	ARG
1	C	51	VAL
1	C	55	LEU
1	C	106	VAL
1	C	122	ARG
1	C	129	LEU
1	C	173	VAL
1	C	176	THR
1	C	205	THR
1	C	215	LEU
1	C	272	GLU
1	C	281	LYS
1	C	293	LEU
1	C	304	GLU
1	C	341	VAL
1	C	347	VAL
1	C	357	SER
1	C	398	LYS
1	C	414	LEU
1	D	6	LEU
1	D	30	LEU
1	D	32	ARG
1	D	33	LEU
1	D	36	LEU
1	D	51	VAL
1	D	72	THR
1	D	106	VAL
1	D	137	THR
1	D	143	LEU
1	D	166	MET
1	D	188	LEU
1	D	192	LEU
1	D	205	THR
1	D	276	VAL
1	D	289	ASP

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Mol	Chain	Res	Type
1	D	305	LYS
1	D	309	GLU
1	D	313	TRP
1	D	341	VAL
1	D	347	VAL
1	D	367	SER
1	D	373	GLU
1	D	376	ASN
1	D	381	ARG
1	D	398	LYS
1	D	401	LEU
1	D	414	LEU
1	E	6	LEU
1	E	11	LYS
1	E	30	LEU
1	E	32	ARG
1	E	36	LEU
1	E	51	VAL
1	E	55	LEU
1	E	71	ASN
1	E	72	THR
1	E	106	VAL
1	E	122	ARG
1	E	129	LEU
1	E	137	THR
1	E	143	LEU
1	E	188	LEU
1	E	192	LEU
1	E	194	ARG
1	E	205	THR
1	E	215	LEU
1	E	218	GLU
1	E	252	THR
1	E	277	ARG
1	E	293	LEU
1	E	316	ARG
1	E	318	ARG
1	E	328	THR
1	E	341	VAL
1	E	342	LEU
1	E	354	VAL
1	E	367	SER

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Mol	Chain	Res	Type
1	E	373	GLU
1	E	398	LYS
1	E	401	LEU
1	E	414	LEU
1	F	6	LEU
1	F	11	LYS
1	F	20	THR
1	F	26	VAL
1	F	30	LEU
1	F	33	LEU
1	F	36	LEU
1	F	55	LEU
1	F	72	THR
1	F	129	LEU
1	F	137	THR
1	F	143	LEU
1	F	166	MET
1	F	173	VAL
1	F	176	THR
1	F	188	LEU
1	F	271	GLN
1	F	277	ARG
1	F	296	GLU
1	F	310	GLN
1	F	328	THR
1	F	341	VAL
1	F	342	LEU
1	F	354	VAL
1	F	357	SER
1	F	381	ARG
1	F	392	GLN
1	F	414	LEU
1	G	6	LEU
1	G	11	LYS
1	G	17	GLU
1	G	30	LEU
1	G	33	LEU
1	G	36	LEU
1	G	42	ARG
1	G	51	VAL
1	G	55	LEU
1	G	71	ASN

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Mol	Chain	Res	Type
1	G	72	THR
1	G	106	VAL
1	G	109	PRO
1	G	129	LEU
1	G	137	THR
1	G	143	LEU
1	G	192	LEU
1	G	200	ARG
1	G	215	LEU
1	G	293	LEU
1	G	309	GLU
1	G	325	ASN
1	G	328	THR
1	G	354	VAL
1	G	414	LEU
1	H	6	LEU
1	H	11	LYS
1	H	20	THR
1	H	30	LEU
1	H	32	ARG
1	H	36	LEU
1	H	42	ARG
1	H	51	VAL
1	H	55	LEU
1	H	71	ASN
1	H	106	VAL
1	H	122	ARG
1	H	129	LEU
1	H	137	THR
1	H	166	MET
1	H	173	VAL
1	H	188	LEU
1	H	192	LEU
1	H	205	THR
1	H	215	LEU
1	H	232	ASN
1	H	276	VAL
1	H	280	PRO
1	H	283	GLU
1	H	285	LEU
1	H	293	LEU
1	H	304	GLU

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Mol	Chain	Res	Type
1	H	305	LYS
1	H	309	GLU
1	H	328	THR
1	H	341	VAL
1	H	342	LEU
1	H	347	VAL
1	H	354	VAL
1	H	357	SER
1	H	381	ARG
1	H	398	LYS
1	H	414	LEU
1	I	6	LEU
1	I	11	LYS
1	I	12	ASP
1	I	51	VAL
1	I	55	LEU
1	I	72	THR
1	I	106	VAL
1	I	129	LEU
1	I	143	LEU
1	I	171	MET
1	I	188	LEU
1	I	192	LEU
1	I	205	THR
1	I	211	GLU
1	I	215	LEU
1	I	227	PHE
1	I	251	HIS
1	I	271	GLN
1	I	293	LEU
1	I	316	ARG
1	I	341	VAL
1	I	342	LEU
1	I	354	VAL
1	I	381	ARG
1	I	401	LEU
1	I	414	LEU
1	J	6	LEU
1	J	12	ASP
1	J	30	LEU
1	J	33	LEU
1	J	36	LEU

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Mol	Chain	Res	Type
1	J	42	ARG
1	J	45	ARG
1	J	51	VAL
1	J	55	LEU
1	J	59	SER
1	J	72	THR
1	J	106	VAL
1	J	122	ARG
1	J	137	THR
1	J	143	LEU
1	J	166	MET
1	J	171	MET
1	J	173	VAL
1	J	176	THR
1	J	188	LEU
1	J	192	LEU
1	J	211	GLU
1	J	218	GLU
1	J	250	ASP
1	J	277	ARG
1	J	293	LEU
1	J	328	THR
1	J	341	VAL
1	J	342	LEU
1	J	372	GLU
1	J	376	ASN
1	J	401	LEU
1	J	414	LEU
1	K	6	LEU
1	K	20	THR
1	K	30	LEU
1	K	33	LEU
1	K	51	VAL
1	K	55	LEU
1	K	71	ASN
1	K	72	THR
1	K	129	LEU
1	K	143	LEU
1	K	161	GLU
1	K	166	MET
1	K	173	VAL
1	K	188	LEU

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Mol	Chain	Res	Type
1	K	195	ARG
1	K	205	THR
1	K	211	GLU
1	K	232	ASN
1	K	238	PHE
1	K	252	THR
1	K	267	LEU
1	K	276	VAL
1	K	277	ARG
1	K	283	GLU
1	K	311	ASN
1	K	328	THR
1	K	342	LEU
1	K	354	VAL
1	K	381	ARG
1	K	384	ARG
1	K	414	LEU
1	L	6	LEU
1	L	12	ASP
1	L	30	LEU
1	L	33	LEU
1	L	42	ARG
1	L	51	VAL
1	L	55	LEU
1	L	71	ASN
1	L	86	GLU
1	L	137	THR
1	L	143	LEU
1	L	173	VAL
1	L	186	ILE
1	L	188	LEU
1	L	192	LEU
1	L	205	THR
1	L	281	LYS
1	L	328	THR
1	L	339	LYS
1	L	341	VAL
1	L	376	ASN
1	L	414	LEU
1	L	420	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	71	ASN
1	A	241	HIS
1	A	306	GLN
1	A	376	ASN
1	B	71	ASN
1	B	251	HIS
1	B	269	HIS
1	B	306	GLN
1	C	71	ASN
1	C	216	GLN
1	C	229	ASN
1	C	241	HIS
1	C	376	ASN
1	D	71	ASN
1	D	306	GLN
1	E	71	ASN
1	E	241	HIS
1	E	306	GLN
1	F	22	GLN
1	F	71	ASN
1	F	216	GLN
1	F	241	HIS
1	F	306	GLN
1	F	392	GLN
1	G	22	GLN
1	G	71	ASN
1	G	241	HIS
1	G	269	HIS
1	G	306	GLN
1	G	325	ASN
1	G	376	ASN
1	H	71	ASN
1	H	216	GLN
1	H	241	HIS
1	H	306	GLN
1	H	310	GLN
1	I	71	ASN
1	I	241	HIS
1	I	271	GLN
1	I	306	GLN
1	I	310	GLN
1	J	22	GLN

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Mol	Chain	Res	Type
1	J	71	ASN
1	J	241	HIS
1	J	269	HIS
1	K	71	ASN
1	K	306	GLN
1	L	22	GLN
1	L	71	ASN
1	L	216	GLN
1	L	241	HIS
1	L	306	GLN
1	L	310	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [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	$\# Z > 2$
3	PO4	I	426	-	4,4,4	0.97	0	6,6,6	0.51	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	$\# Z > 2$
3	PO4	F	426	-	0,3,4	0.00	-	0,3,6	0.00	-
3	PO4	I	427	-	4,4,4	0.90	0	6,6,6	0.74	0
3	PO4	C	426	-	4,4,4	0.83	0	6,6,6	0.48	0
3	PO4	A	426	-	4,4,4	0.91	0	6,6,6	0.87	0
3	PO4	D	426	-	4,4,4	0.91	0	6,6,6	0.64	0
3	PO4	G	426	-	4,4,4	0.75	0	6,6,6	0.85	0
3	PO4	K	426	-	4,4,4	0.82	0	6,6,6	0.66	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	426	PO4	1	0
3	G	426	PO4	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, 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	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%)

All (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
1	K	264	TYR	6.0
1	L	273	PHE	5.9
1	E	11	LYS	5.9
1	E	280	PRO	5.8
1	K	271	GLN	5.8
1	L	270	VAL	5.6

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Mol	Chain	Res	Type	RSRZ
1	D	285	LEU	5.5
1	A	273	PHE	5.4
1	E	273	PHE	5.3
1	C	273	PHE	5.1
1	A	12	ASP	5.1
1	K	245	VAL	5.1
1	B	273	PHE	5.1
1	B	270	VAL	5.0
1	L	271	GLN	4.9
1	K	268	ARG	4.9
1	F	11	LYS	4.8
1	C	11	LYS	4.7
1	K	239	HIS	4.7
1	L	268	ARG	4.7
1	K	267	LEU	4.6
1	L	274	GLY	4.5
1	G	11	LYS	4.5
1	L	10	GLY	4.4
1	L	313	TRP	4.3
1	I	270	VAL	4.3
1	K	222	VAL	4.2
1	K	11	LYS	4.2
1	L	11	LYS	4.2
1	D	173	VAL	4.2
1	G	13	GLY	4.2
1	K	273	PHE	4.2
1	L	257	ASN	4.2
1	G	4	GLU	4.2
1	E	251	HIS	4.1
1	F	218	GLU	4.1
1	C	274	GLY	4.1
1	D	256	TYR	4.0
1	L	278	GLY	4.0
1	F	247	ALA	4.0
1	D	11	LYS	3.9
1	F	259	ALA	3.9
1	C	280	PRO	3.9
1	F	317	ALA	3.8
1	J	12	ASP	3.8
1	F	316	ARG	3.8
1	C	13	GLY	3.8
1	H	267	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	I	274	GLY	3.8
1	K	10	GLY	3.8
1	F	264	TYR	3.7
1	L	256	TYR	3.7
1	B	10	GLY	3.7
1	A	251	HIS	3.7
1	B	272	GLU	3.7
1	E	277	ARG	3.7
1	K	272	GLU	3.7
1	G	12	ASP	3.7
1	I	272	GLU	3.7
1	J	218	GLU	3.7
1	H	278	GLY	3.6
1	D	271	GLN	3.6
1	F	265	ASP	3.6
1	K	218	GLU	3.6
1	D	217	VAL	3.6
1	F	216	GLN	3.6
1	A	13	GLY	3.6
1	K	4	GLU	3.6
1	I	275	GLY	3.6
1	E	283	GLU	3.5
1	D	272	GLU	3.5
1	H	271	GLN	3.5
1	E	252	THR	3.5
1	K	274	GLY	3.5
1	I	252	THR	3.4
1	J	11	LYS	3.4
1	D	268	ARG	3.4
1	J	10	GLY	3.4
1	D	4	GLU	3.4
1	K	217	VAL	3.4
1	F	261	ILE	3.4
1	H	272	GLU	3.3
1	D	263	PRO	3.3
1	K	244	ARG	3.3
1	F	211	GLU	3.3
1	A	252	THR	3.3
1	F	239	HIS	3.3
1	L	173	VAL	3.3
1	A	271	GLN	3.3
1	K	297	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	276	VAL	3.3
1	K	275	GLY	3.2
1	I	251	HIS	3.2
1	G	10	GLY	3.2
1	C	12	ASP	3.2
1	I	280	PRO	3.2
1	L	122	ARG	3.2
1	K	216	GLN	3.2
1	H	277	ARG	3.2
1	D	276	VAL	3.2
1	F	244	ARG	3.2
1	C	259	ALA	3.1
1	F	220	ALA	3.1
1	C	276	VAL	3.1
1	C	278	GLY	3.1
1	F	260	GLY	3.1
1	J	169	TYR	3.1
1	H	251	HIS	3.1
1	C	4	GLU	3.1
1	B	271	GLN	3.1
1	K	295	VAL	3.1
1	B	13	GLY	3.1
1	F	242	GLY	3.1
1	C	271	GLN	3.1
1	D	215	LEU	3.1
1	D	32	ARG	3.1
1	F	217	VAL	3.1
1	K	13	GLY	3.0
1	D	396	GLU	3.0
1	B	277	ARG	3.0
1	I	12	ASP	3.0
1	I	11	LYS	3.0
1	A	10	GLY	3.0
1	D	174	GLY	3.0
1	H	122	ARG	3.0
1	K	335	ILE	3.0
1	E	272	GLU	3.0
1	K	293	LEU	3.0
1	F	13	GLY	3.0
1	I	277	ARG	3.0
1	F	267	LEU	3.0
1	D	274	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	271	GLN	2.9
1	D	255	VAL	2.9
1	B	264	TYR	2.9
1	L	251	HIS	2.9
1	K	237	ALA	2.9
1	I	276	VAL	2.9
1	K	246	VAL	2.9
1	K	213	ILE	2.9
1	G	175[A]	ARG	2.9
1	E	274	GLY	2.8
1	I	13	GLY	2.8
1	A	4	GLU	2.8
1	E	271	GLN	2.8
1	K	391	TRP	2.8
1	A	173	VAL	2.8
1	E	173	VAL	2.8
1	F	337	LEU	2.8
1	D	277	ARG	2.8
1	K	399	ILE	2.8
1	C	265	ASP	2.8
1	E	279	TYR	2.8
1	I	173	VAL	2.8
1	L	286	PRO	2.8
1	H	10	GLY	2.8
1	F	246	VAL	2.7
1	B	278	GLY	2.7
1	H	218	GLU	2.7
1	F	276	VAL	2.7
1	F	295	VAL	2.7
1	G	122	ARG	2.7
1	H	4	GLU	2.7
1	I	271	GLN	2.7
1	F	214	GLY	2.7
1	J	308	THR	2.7
1	H	269	HIS	2.7
1	J	13	GLY	2.7
1	F	222	VAL	2.7
1	K	243	ALA	2.7
1	A	277	ARG	2.7
1	J	142	ILE	2.7
1	D	280	PRO	2.7
1	K	318	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	215	LEU	2.7
1	E	270	VAL	2.6
1	F	248	VAL	2.6
1	E	12	ASP	2.6
1	F	219	GLY	2.6
1	H	280	PRO	2.6
1	L	284	PRO	2.6
1	F	297	PHE	2.6
1	D	262	ASP	2.6
1	B	285	LEU	2.6
1	K	173	VAL	2.6
1	K	279	TYR	2.6
1	C	277	ARG	2.6
1	F	243	ALA	2.5
1	H	270	VAL	2.5
1	K	210	ALA	2.5
1	F	338	GLU	2.5
1	L	12	ASP	2.5
1	K	276	VAL	2.5
1	J	4	GLU	2.5
1	J	259	ALA	2.5
1	K	215	LEU	2.5
1	F	279	TYR	2.5
1	C	272	GLU	2.5
1	F	296	GLU	2.5
1	F	396	GLU	2.5
1	C	143	LEU	2.4
1	H	265	ASP	2.4
1	K	265	ASP	2.4
1	K	256	TYR	2.4
1	K	5	PRO	2.4
1	K	294	PRO	2.4
1	D	293	LEU	2.4
1	K	341	VAL	2.4
1	E	13	GLY	2.4
1	H	316	ARG	2.4
1	B	398	LYS	2.4
1	B	269	HIS	2.4
1	G	273	PHE	2.4
1	G	268	ARG	2.4
1	C	270	VAL	2.4
1	B	12	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	L	259	ALA	2.4
1	D	313	TRP	2.4
1	J	315	ILE	2.4
1	E	275	GLY	2.4
1	B	211	GLU	2.4
1	D	278	GLY	2.4
1	E	313	TRP	2.4
1	A	272	GLU	2.3
1	C	267	LEU	2.3
1	D	269	HIS	2.3
1	J	331	ALA	2.3
1	L	253	GLY	2.3
1	D	334	ASP	2.3
1	H	253	GLY	2.3
1	D	10	GLY	2.3
1	L	57	ASP	2.3
1	J	173	VAL	2.3
1	F	4	GLU	2.3
1	A	270	VAL	2.3
1	H	276	VAL	2.3
1	H	274	GLY	2.3
1	H	54	ARG	2.3
1	D	331	ALA	2.3
1	K	270	VAL	2.3
1	L	338	GLU	2.3
1	D	270	VAL	2.2
1	K	122	ARG	2.2
1	K	224	ILE	2.2
1	K	319	ILE	2.2
1	E	4	GLU	2.2
1	I	10	GLY	2.2
1	C	283	GLU	2.2
1	C	251	HIS	2.2
1	C	252	THR	2.2
1	D	216	GLN	2.2
1	K	277	ARG	2.2
1	F	285	LEU	2.2
1	F	268	ARG	2.2
1	K	259	ALA	2.2
1	B	169	TYR	2.2
1	D	317	ALA	2.2
1	K	260	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	122	ARG	2.2
1	F	251	HIS	2.2
1	J	309	GLU	2.2
1	B	274	GLY	2.2
1	B	281	LYS	2.2
1	D	175	ARG	2.2
1	D	244	ARG	2.2
1	C	219	GLY	2.1
1	I	278	GLY	2.1
1	K	278	GLY	2.1
1	K	292	GLY	2.1
1	B	329	THR	2.1
1	H	252	THR	2.1
1	J	144	LEU	2.1
1	J	277	ARG	2.1
1	F	146	PRO	2.1
1	K	254	THR	2.1
1	F	12	ASP	2.1
1	G	57	ASP	2.1
1	L	399	ILE	2.1
1	H	32	ARG	2.1
1	K	214	GLY	2.1
1	E	259	ALA	2.1
1	C	281	LYS	2.1
1	H	286	PRO	2.1
1	F	391	TRP	2.1
1	H	175[A]	ARG	2.1
1	D	239	HIS	2.1
1	F	398	LYS	2.1
1	G	142	ILE	2.1
1	E	32	ARG	2.1
1	E	122	ARG	2.1
1	F	245	VAL	2.1
1	B	4	GLU	2.0
1	B	255	VAL	2.0
1	K	331	ALA	2.0
1	K	340	GLY	2.0
1	F	263	PRO	2.0
1	H	143	LEU	2.0
1	B	280	PRO	2.0
1	H	396	GLU	2.0
1	A	11	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	219	GLY	2.0
1	F	255	VAL	2.0
1	J	181	VAL	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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
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
2	GLU	F	500	10/10	0.89	0.20	62,63,65,66	0
3	PO4	A	426	5/5	0.89	0.20	75,76,77,77	0
2	GLU	C	425	10/10	0.89	0.17	42,43,46,49	0
4	NH4	A	427	1/1	0.90	0.46	17,17,17,17	0
4	NH4	J	427	1/1	0.90	0.14	40,40,40,40	0
2	GLU	K	425	10/10	0.90	0.16	40,40,46,48	0
2	GLU	I	425	10/10	0.91	0.13	38,39,41,44	0
2	GLU	L	425	10/10	0.91	0.14	49,49,52,53	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	I	500	10/10	0.92	0.14	50,51,55,55	0
2	GLU	A	500	10/10	0.92	0.15	43,45,46,46	0
2	GLU	E	425	10/10	0.92	0.16	37,38,43,45	0
2	GLU	C	500	10/10	0.92	0.13	42,43,46,48	0
3	PO4	G	426	5/5	0.92	0.14	62,63,64,64	0
3	PO4	K	426	5/5	0.93	0.11	67,68,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GLU	J	500	10/10	0.93	0.17	47,48,54,55	0
2	GLU	F	425	10/10	0.93	0.15	31,34,44,45	0
2	GLU	L	500	10/10	0.93	0.15	52,53,53,54	0
2	GLU	E	500	10/10	0.93	0.12	39,42,47,49	0
4	NH4	H	426	1/1	0.93	0.28	34,34,34,34	0
2	GLU	A	425	10/10	0.94	0.13	28,29,32,34	0
3	PO4	D	426	5/5	0.94	0.14	79,80,80,80	0
2	GLU	G	425	10/10	0.94	0.13	28,30,33,33	0
3	PO4	J	426	5/5	0.94	0.19	62,62,63,64	0
2	GLU	H	500	10/10	0.94	0.14	50,53,53,54	0
2	GLU	B	500	10/10	0.94	0.10	35,37,38,39	0
2	GLU	D	500	10/10	0.95	0.12	43,46,46,49	0
2	GLU	J	425	10/10	0.95	0.11	36,37,43,43	0
3	PO4	I	427	5/5	0.95	0.14	61,62,62,62	0
2	GLU	H	425	10/10	0.96	0.10	34,36,41,42	0
3	PO4	F	426	4/5	0.96	0.11	71,71,72,72	0
3	PO4	C	426	5/5	0.97	0.10	57,58,58,58	0
3	PO4	I	426	5/5	0.98	0.15	56,56,57,58	0
4	NH4	F	427	1/1	0.98	0.18	41,41,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.