



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 01:53 PM UTC

PDB ID : 3AOG / pdb_00003aog
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 types of validation reports are described at

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

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

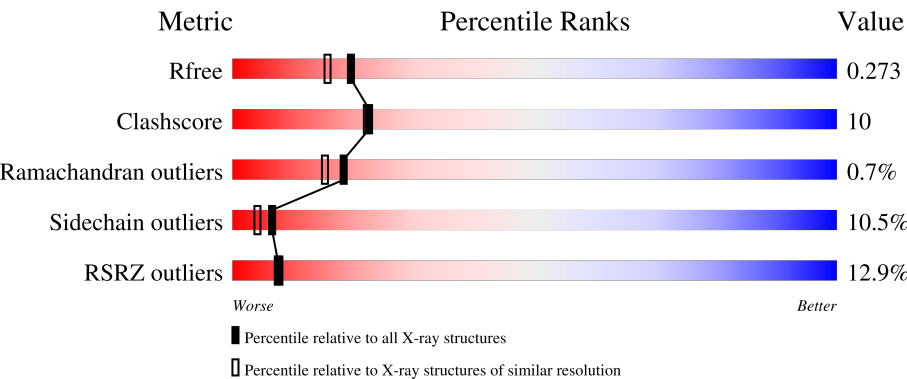
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 $\leq 5\%$. 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	5% 68%24%.
1	B	440	14% 73%20%.
1	C	440	9% 74%19%.
1	D	440	21% 70%23%.
1	E	440	10% 69%22%.

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Mol	Chain	Length	Quality of chain
1	F	440	17% 75% 19%
1	G	440	5% 71% 21%
1	H	440	11% 70% 21% 5%
1	I	440	8% 71% 21%
1	J	440	9% 71% 21%
1	K	440	24% 70% 21% 5%
1	L	440	16% 70% 21%

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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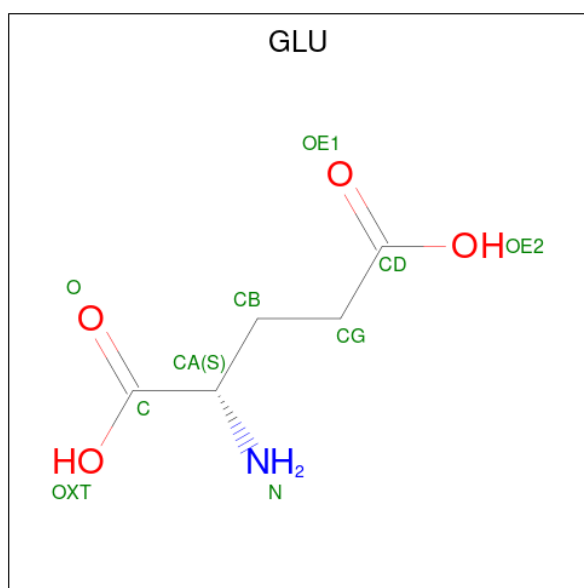
Chain	Residue	Modelled	Actual	Comment	Reference
I	-12	SER	-	expression tag	UNP Q72IC1
I	-11	HIS	-	expression tag	UNP Q72IC1
I	-10	HIS	-	expression tag	UNP Q72IC1
I	-9	HIS	-	expression tag	UNP Q72IC1
I	-8	HIS	-	expression tag	UNP Q72IC1
I	-7	HIS	-	expression tag	UNP Q72IC1
I	-6	HIS	-	expression tag	UNP 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 (CCD ID: 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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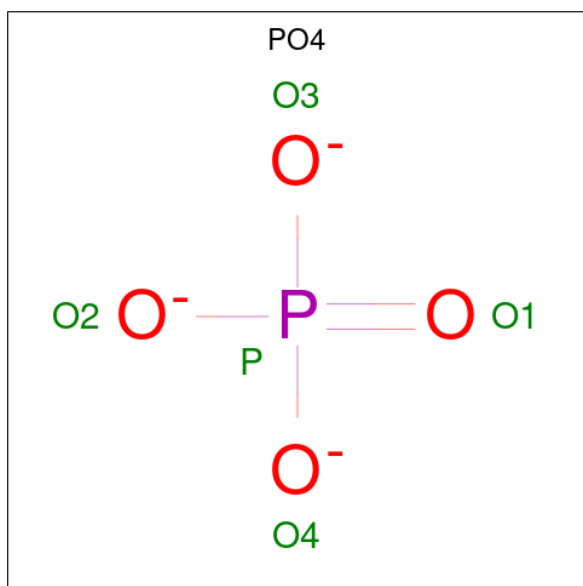
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			10	5	1	4		
2	B	1	Total	C	N	O	0	0
			10	5	1	4		
2	C	1	Total	C	N	O	0	0
			10	5	1	4		
2	C	1	Total	C	N	O	0	0
			10	5	1	4		
2	D	1	Total	C	N	O	0	0
			10	5	1	4		
2	D	1	Total	C	N	O	0	0
			10	5	1	4		
2	E	1	Total	C	N	O	0	0
			10	5	1	4		
2	E	1	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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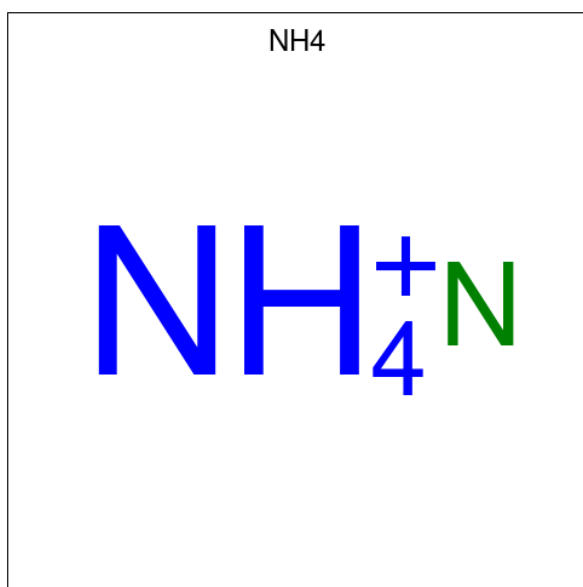
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	L	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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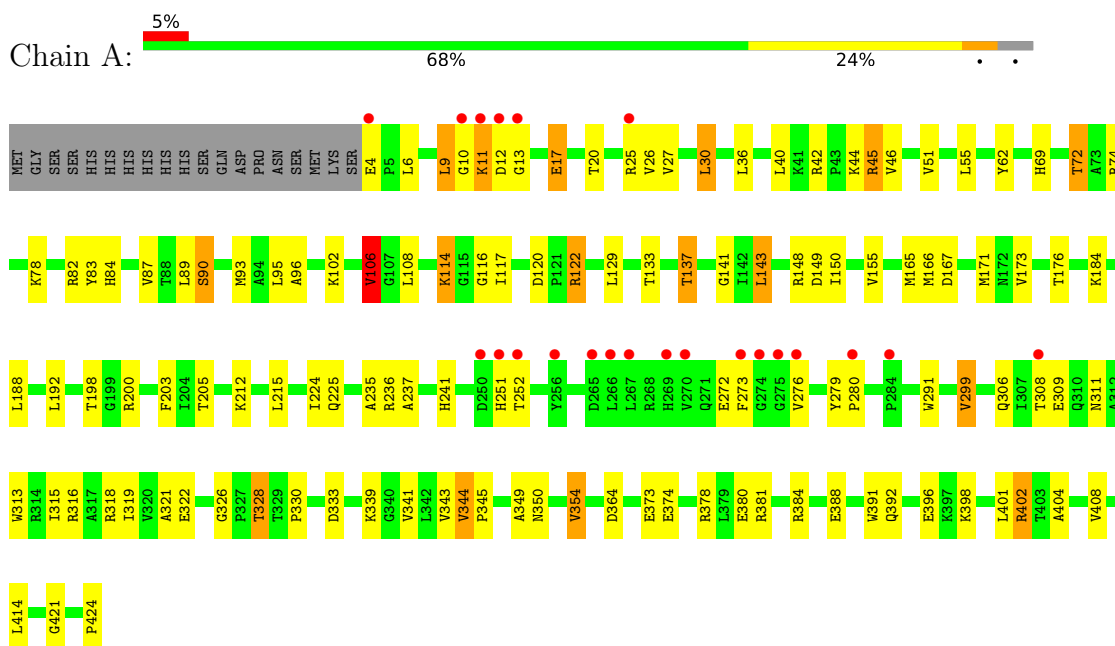
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	187	Total 187	O 187	0	0
5	H	125	Total 125	O 125	0	0
5	I	178	Total 178	O 178	0	0
5	J	157	Total 157	O 157	0	0
5	K	121	Total 121	O 121	0	0
5	L	106	Total 106	O 106	0	0

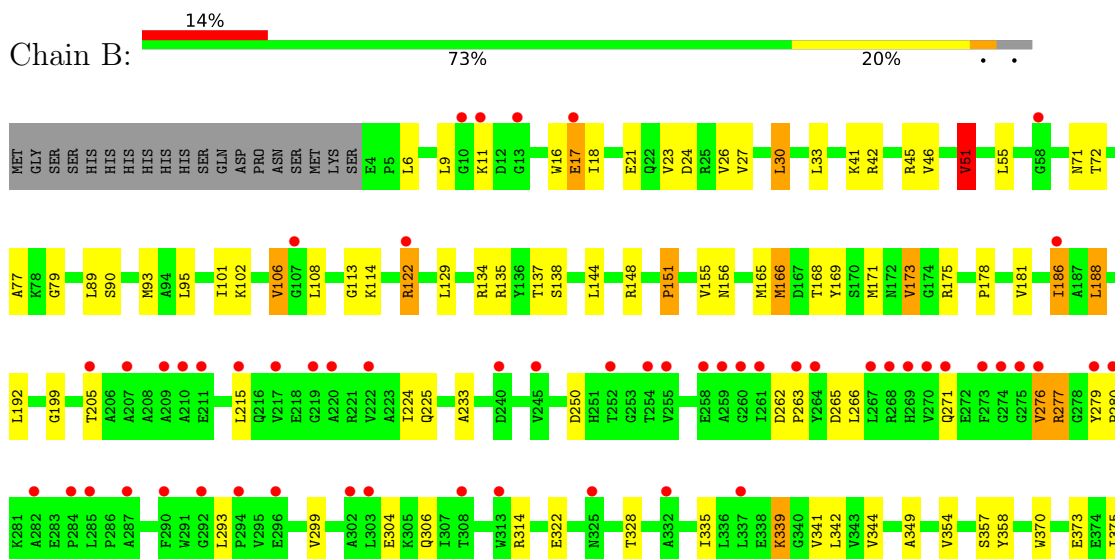
3 Residue-property plots [i](#)

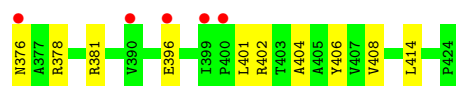
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Glutamate dehydrogenase

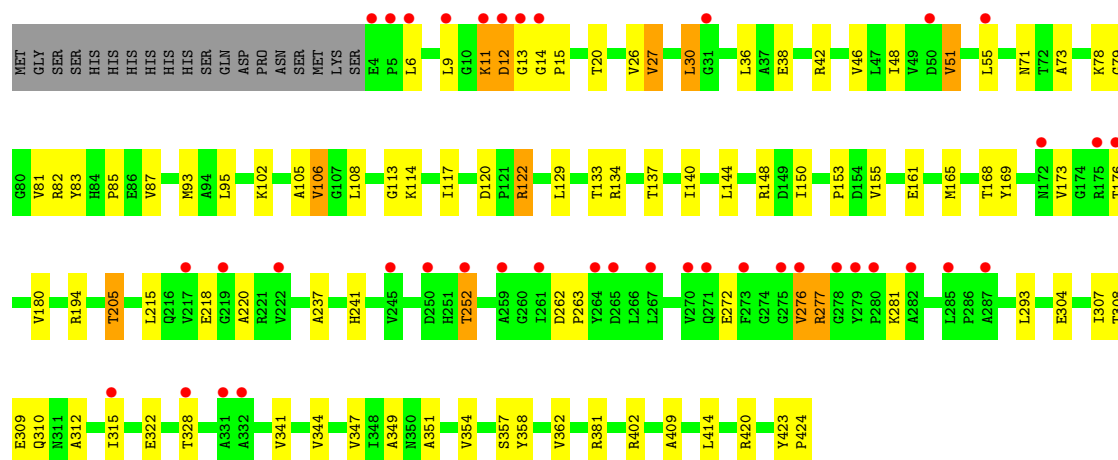
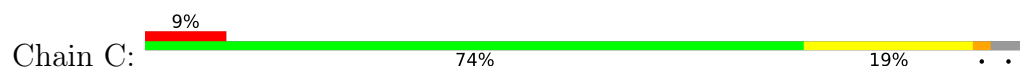


- Molecule 1: Glutamate dehydrogenase

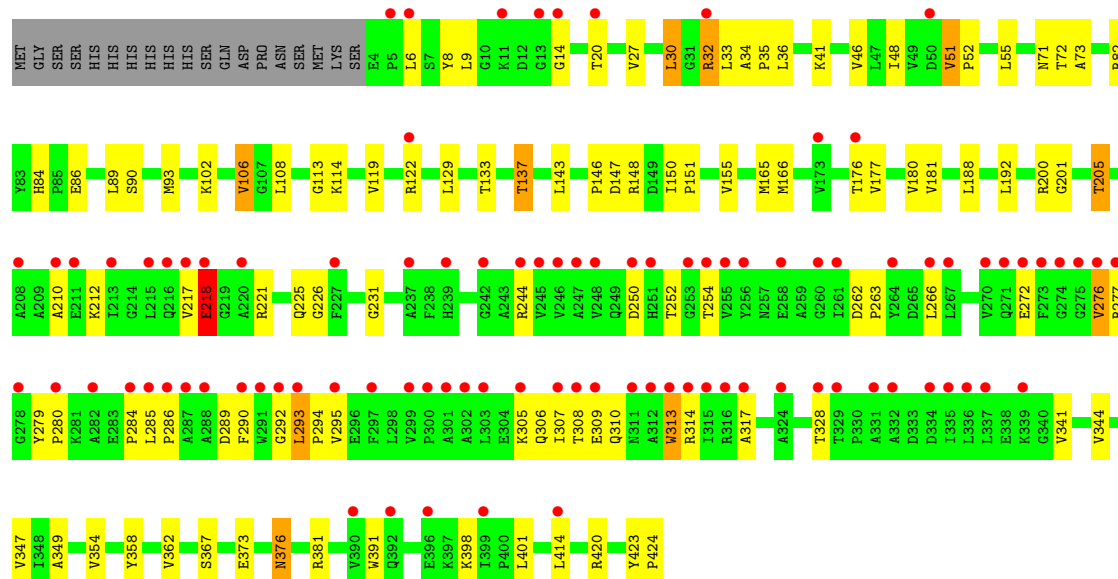




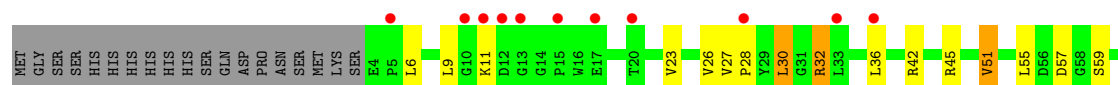
• Molecule 1: Glutamate dehydrogenase

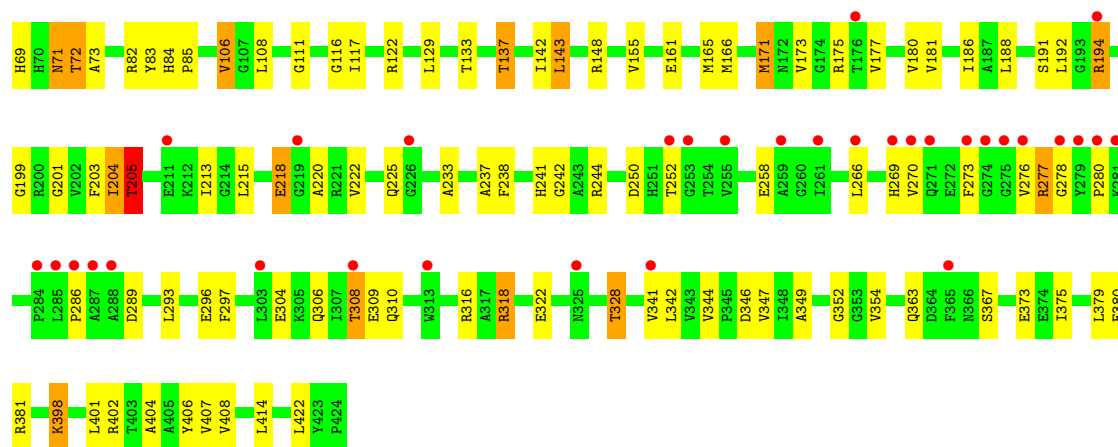


• Molecule 1: Glutamate dehydrogenase

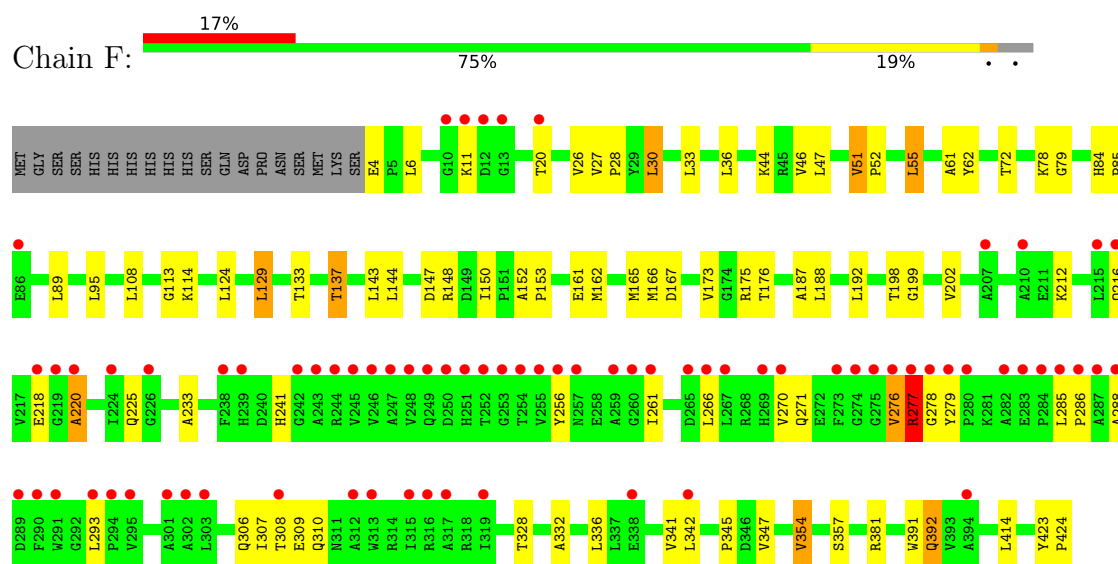


• Molecule 1: Glutamate dehydrogenase

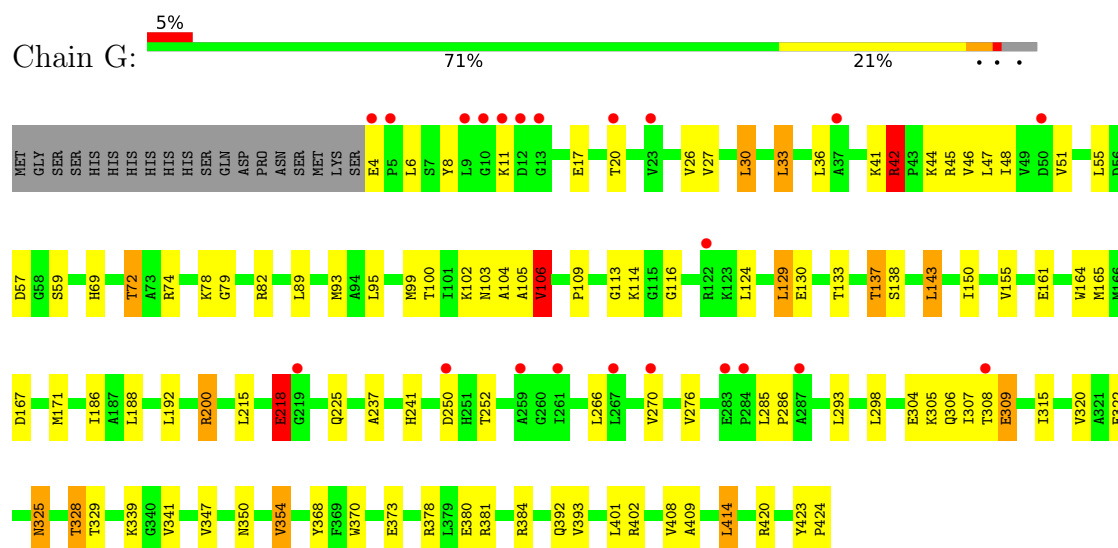




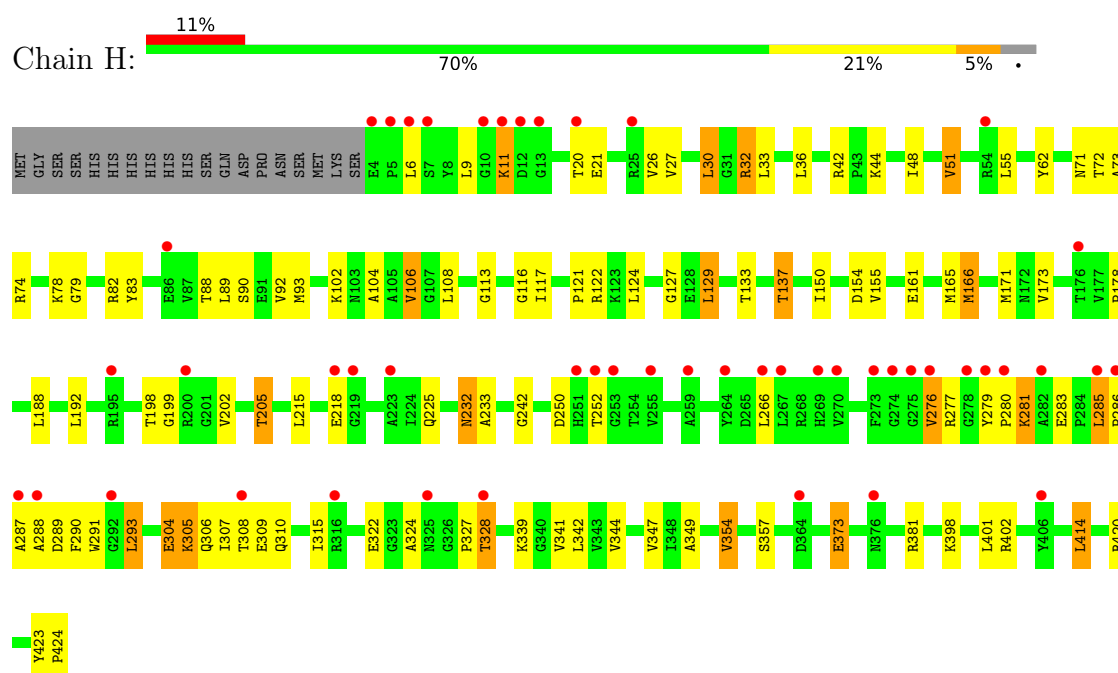
• Molecule 1: Glutamate dehydrogenase



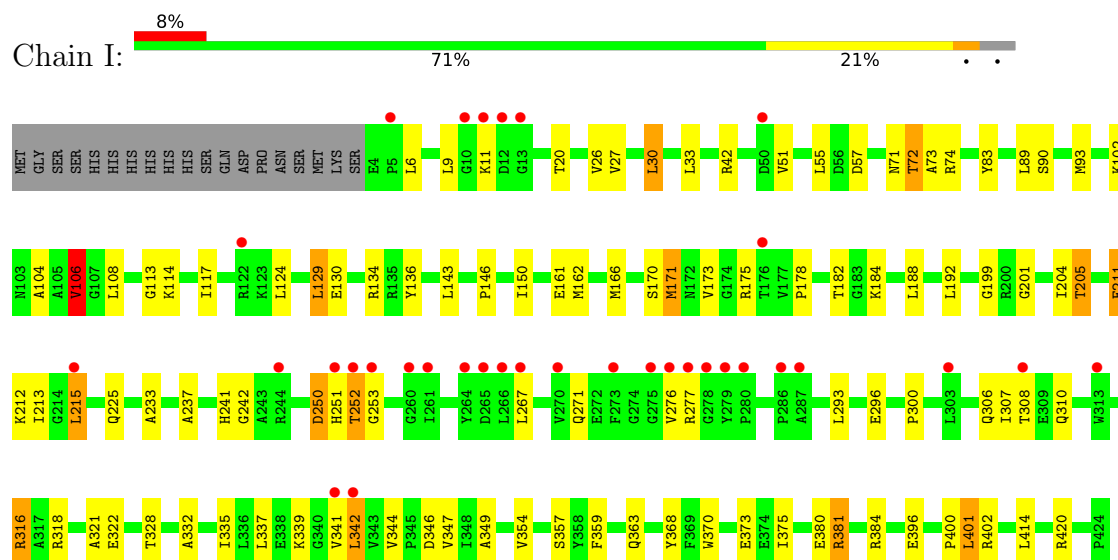
• Molecule 1: Glutamate dehydrogenase



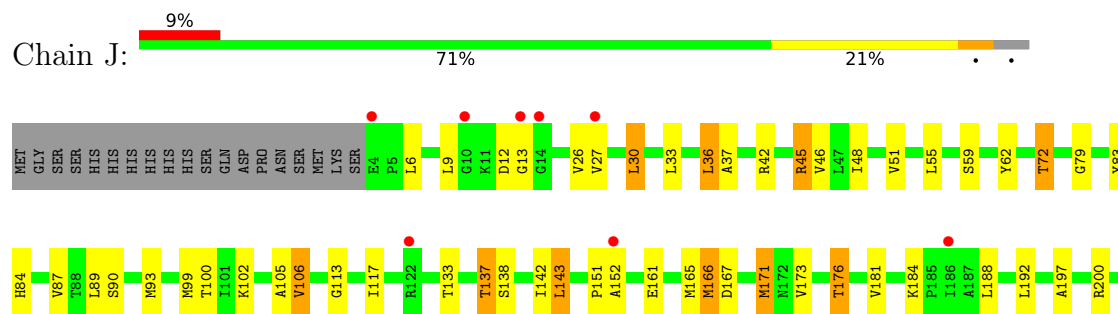
• Molecule 1: Glutamate dehydrogenase

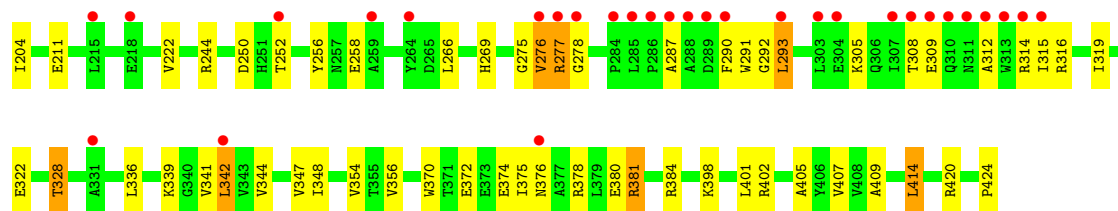


• Molecule 1: Glutamate dehydrogenase

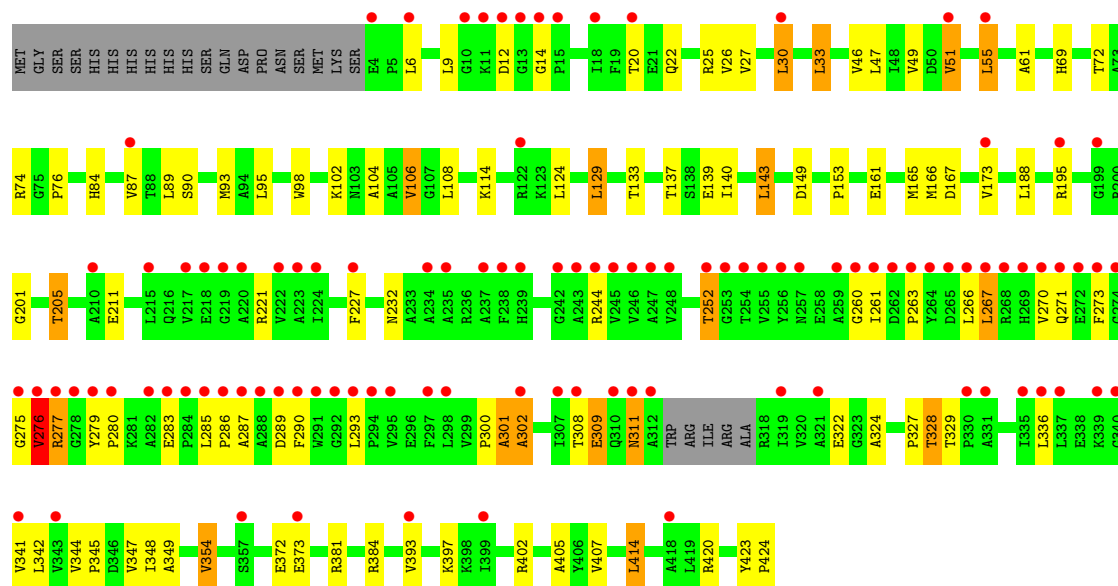


• Molecule 1: Glutamate dehydrogenase

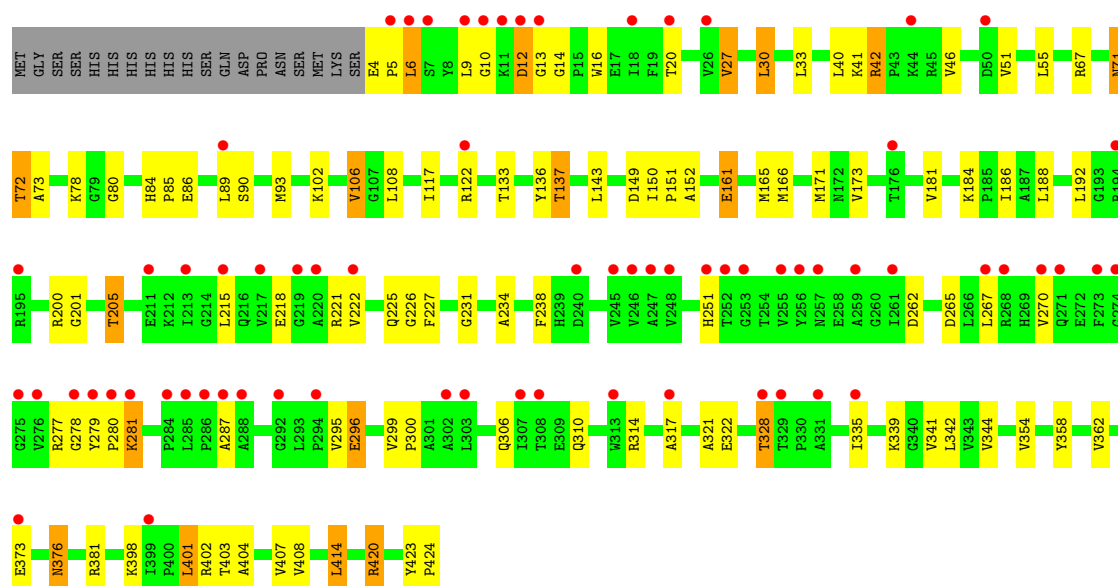




• Molecule 1: Glutamate dehydrogenase



• 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 , 48.3	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 [i](#)

5.1 Standard geometry [i](#)

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	0.92	1/3312 (0.0%)	1.09	6/4508 (0.1%)
1	B	0.80	0/3312	1.01	4/4508 (0.1%)
1	C	0.70	1/3330 (0.0%)	0.98	2/4532 (0.0%)
1	D	0.66	0/3312	0.95	2/4508 (0.0%)
1	E	0.80	1/3312 (0.0%)	1.04	9/4508 (0.2%)
1	F	0.67	0/3323	0.94	2/4522 (0.0%)
1	G	0.83	1/3323 (0.0%)	1.05	5/4522 (0.1%)
1	H	0.67	0/3334	0.95	1/4536 (0.0%)
1	I	0.74	1/3323 (0.0%)	0.95	1/4522 (0.0%)
1	J	0.74	0/3323	1.00	4/4522 (0.1%)
1	K	0.67	1/3260 (0.0%)	0.96	6/4436 (0.1%)
1	L	0.63	1/3312 (0.0%)	0.93	1/4508 (0.0%)
All	All	0.74	7/39776 (0.0%)	0.99	43/54132 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	27	VAL	CA-CB	6.71	1.57	1.54
1	C	27	VAL	CA-CB	5.99	1.57	1.53
1	G	106	VAL	CA-CB	5.75	1.62	1.54
1	A	106	VAL	CA-CB	5.53	1.60	1.54
1	I	106	VAL	CA-CB	5.20	1.60	1.54
1	E	375	ILE	CA-CB	5.19	1.60	1.54
1	K	51	VAL	CA-CB	5.03	1.60	1.54

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	301	ALA	N-CA-C	9.39	122.35	110.61
1	K	273	PHE	N-CA-C	-8.46	103.40	114.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	51	VAL	CB-CA-C	7.74	118.43	111.08
1	E	177	VAL	CA-C-N	-7.65	110.28	119.84
1	E	177	VAL	C-N-CA	-7.65	110.28	119.84
1	C	51	VAL	CB-CA-C	7.62	118.32	111.08
1	C	220	ALA	N-CA-C	7.38	120.94	110.23
1	G	42	ARG	CA-C-N	-7.24	112.52	119.76
1	G	42	ARG	C-N-CA	-7.24	112.52	119.76
1	D	14	GLY	CA-C-N	6.68	126.19	119.24
1	D	14	GLY	C-N-CA	6.68	126.19	119.24
1	K	301	ALA	CA-C-N	6.53	133.45	121.70
1	K	301	ALA	C-N-CA	6.53	133.45	121.70
1	G	354	VAL	CB-CA-C	6.34	120.97	112.22
1	J	152	ALA	CA-C-N	-6.28	114.30	120.52
1	J	152	ALA	C-N-CA	-6.28	114.30	120.52
1	E	51	VAL	CB-CA-C	6.04	116.82	111.08
1	L	218	GLU	N-CA-C	5.99	118.30	111.11
1	A	344	VAL	CA-C-N	5.99	125.95	119.78
1	A	344	VAL	C-N-CA	5.99	125.95	119.78
1	F	277	ARG	N-CA-C	5.89	121.03	111.37
1	B	358	TYR	N-CA-C	-5.80	104.87	111.14
1	G	347	VAL	CB-CA-C	-5.64	104.66	112.04
1	B	77	ALA	N-CA-C	-5.61	102.59	110.50
1	E	111	GLY	N-CA-C	-5.57	104.05	112.41
1	E	363	GLN	CA-C-N	5.29	128.11	120.38
1	E	363	GLN	C-N-CA	5.29	128.11	120.38
1	E	204	ILE	CA-C-N	5.27	127.77	120.29
1	E	204	ILE	C-N-CA	5.27	127.77	120.29
1	I	250	ASP	N-CA-C	5.25	116.26	108.86
1	A	45	ARG	N-CA-C	5.16	117.10	108.99
1	K	14	GLY	CA-C-N	5.12	124.73	119.05
1	K	14	GLY	C-N-CA	5.12	124.73	119.05
1	F	220	ALA	N-CA-C	5.10	121.67	110.80
1	B	51	VAL	CA-C-N	5.10	125.50	119.99
1	B	51	VAL	C-N-CA	5.10	125.50	119.99
1	A	326	GLY	N-CA-C	5.07	122.69	112.34
1	G	218	GLU	N-CA-C	5.07	117.46	111.33
1	A	299	VAL	N-CA-C	5.06	113.16	108.15
1	E	205	THR	N-CA-CB	-5.05	102.68	110.16
1	J	344	VAL	CA-C-N	5.03	124.78	119.76
1	J	344	VAL	C-N-CA	5.03	124.78	119.76
1	A	402	ARG	NE-CZ-NH1	-5.01	116.49	121.50

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	87	0
1	B	3236	0	3229	63	0
1	C	3248	0	3243	55	0
1	D	3236	0	3229	72	0
1	E	3236	0	3229	67	0
1	F	3244	0	3242	68	0
1	G	3244	0	3242	85	0
1	H	3252	0	3255	67	0
1	I	3244	0	3242	71	0
1	J	3244	0	3242	78	0
1	K	3187	0	3176	74	0
1	L	3236	0	3229	68	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	1	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	5	0
5	F	133	0	0	4	0
5	G	187	0	0	13	0
5	H	125	0	0	2	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	816	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 (816) 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:H:89:LEU:HG	1:H:93:MET:HE2	1.26	1.13
1:K:89:LEU:HG	1:K:93:MET:HE2	1.26	1.13
1:A:9:LEU:HD11	1:A:93:MET:HE1	1.24	1.09
1:A:90:SER:HA	1:A:93:MET:HE3	1.31	1.08
1:I:9:LEU:HD21	1:I:93:MET:HE1	1.26	1.07
1:K:9:LEU:HD21	1:K:93:MET:HE1	1.36	1.07
1:J:89:LEU:HG	1:J:93:MET:HE2	1.26	1.07
1:B:9:LEU:HD21	1:B:93:MET:HE1	1.36	1.06
1:L:205:THR:HG23	1:L:344:VAL:HG11	1.37	1.06
1:J:171:MET:HE2	1:J:171:MET:HA	1.38	1.05
1:G:89:LEU:HG	1:G:93:MET:HE3	1.34	1.05
1:D:89:LEU:HG	1:D:93:MET:HE2	1.37	1.03
1:H:205:THR:HG23	1:H:344:VAL:HG11	1.40	1.03
1:F:162:MET:CE	1:F:165:MET:HE2	1.89	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

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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:A:381:ARG:HD3	5:A:453:HOH:O	1.63	0.97
1:L:420:ARG:HG2	1:L:420:ARG:HH11	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:L:9:LEU:HD21	1:L:93:MET:HE1	1.46	0.97
1:K:201:GLY:O	1:K:205:THR:HG22	1.63	0.96
1:A:89:LEU:HG	1:A:93:MET:HE2	1.48	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:9:LEU:HD21	1:H:93:MET:HE1	1.48	0.93
1:H:308:THR:HG22	1:H:310:GLN:H	1.33	0.92
1:J:420:ARG:HH12	1:L:171:MET:HE3	1.36	0.91
1:J:9:LEU:HD21	1:J:93:MET:HE1	1.51	0.91
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:K:308:THR:HG22	1:K:309:GLU:H	1.36	0.90
1:I:89:LEU:HG	1:I:93:MET:HE2	1.54	0.90
1:B:166:MET:HE2	1:B:178:PRO:HA	1.54	0.89
1:A:205:THR:CG2	1:A:344:VAL:HG11	2.03	0.88
1:A:9:LEU:CD1	1:A:93:MET:HE1	2.03	0.87
1:A:225:GLN:HE22	1:A:306:GLN:HE21	1.22	0.87
1:J:90:SER:HA	1:J:93:MET:HE3	1.57	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: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:F:162:MET:HE1	1:F:165:MET:CE	2.06	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:F:162:MET:HE2	1:F:165:MET:HE2	1.58	0.83
1:I:90:SER:HA	1:I:93:MET:HE3	1.59	0.83
1:L:133:THR:O	1:L:137:THR:HG23	1.77	0.83
1:I:171:MET:HA	1:I:171:MET:HE2	1.58	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:SER:HA	1:B:93:MET:HE3	1.59	0.82
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:D:9:LEU:HD21	1:D:93:MET:HE1	1.61	0.82
1:K:275:GLY:O	1:K:276:VAL:HB	1.77	0.82
1:A:90:SER:HA	1:A:93:MET:CE	2.10	0.81
1:A:380:GLU:OE2	1:G:218:GLU:HG3	1.80	0.81
1:B:90:SER:HA	1:B:93:MET:CE	2.10	0.81
1:F:162:MET:SD	1:F:165:MET:CE	2.69	0.81
1:J:420:ARG:NH1	1:L:171:MET:HE3	1.95	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:D:205:THR:HG23	1:D:344:VAL:HG11	1.63	0.79
1:I:171:MET:HA	1:I:171:MET:CE	2.11	0.79
1:G:89:LEU:HG	1:G:93:MET:CE	2.10	0.79
5:A:1218:HOH:O	1:B:45:ARG:HD3	1.82	0.79
1:E:322:GLU:CD	1:E:402:ARG:HH12	1.89	0.79
1:A:9:LEU:HD11	1:A:93:MET:CE	2.11	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:89:LEU:HG	1:B:93:MET:HE2	1.64	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:K:90:SER:HA	1:K:93:MET:HE3	1.66	0.78
1:A:380:GLU:OE1	1:A:384:ARG:NH1	2.17	0.78
1:H:11:LYS:HD3	1:H:11:LYS:C	2.09	0.77
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:G:171:MET:HE2	1:G:171:MET:HA	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:F:162:MET:HE1	1:F:165:MET:HE1	1.69	0.75
1:H:133:THR:O	1:H:137:THR:HG23	1.86	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:L:72:THR:HG21	5:L:440:HOH:O	1.87	0.74
1:K:9:LEU:HD21	1:K:93:MET:CE	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:308:THR:HG22	1:F:309:GLU:H	1.54	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:H:225:GLN:HE22	1:H:306:GLN:HE21	1.38	0.72
1:G:89:LEU:CG	1:G:93:MET:HE3	2.15	0.71
1:H:9:LEU:HD21	1:H:93:MET:CE	2.19	0.71
1:K:244:ARG:HD2	1:K:260:GLY:HA3	1.72	0.71
1:G:44:LYS:HZ3	1:G:45:ARG:NH1	1.89	0.71
1:G:325:ASN:ND2	1:G:350:ASN:HD21	1.89	0.71
1:C:9:LEU:HD11	1:C:93:MET:HE1	1.73	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:K:221:ARG:NH2	5:K:1185:HOH:O	2.23	0.70
1:A:322:GLU:CD	1:A:402:ARG:HH12	1.99	0.70
1:D:205:THR:HG21	1:D:349:ALA:HA	1.74	0.70
1:L:420:ARG:HG2	1:L:420:ARG:NH1	2.04	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:HB2	1:D:244:ARG:HH11	1.58	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: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
1:G:42:ARG:HD2	1:J:62:TYR:HB3	1.77	0.67
1:A:133:THR:O	1:A:137:THR:HG23	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:PRO:HG2	1:C:194:ARG:HH12	1.59	0.67
1:D:89:LEU:HG	1:D:93:MET:CE	2.21	0.67
1:B:277:ARG:HG3	1:B:277:ARG:NH1	2.04	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:G:42:ARG:HD2	1:J:62:TYR:CB	2.25	0.66
1:H:285:LEU:HD22	1:H:286:PRO:HD2	1.77	0.66
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:9:LEU:HD21	1:I:93:MET:CE	2.17	0.65
1:G:322:GLU:CD	1:G:402:ARG:HH12	2.04	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:C:276:VAL:O	1:C:277:ARG:HB2	1.96	0.64
1:G:325:ASN:HD22	1:G:350:ASN:HD21	1.45	0.64
1:F:162:MET:CE	1:F:165:MET:HE1	2.26	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: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:H:89:LEU:CG	1:H:93:MET:HE2	2.17	0.62
1:B:186:ILE:HD12	1:B:186:ILE:N	2.14	0.62
1:E:71:ASN:ND2	1:E:73:ALA:H	1.97	0.62
1:K:300:PRO:C	1:K:302:ALA:HB2	2.24	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
1:C:237:ALA:O	1:C:241:HIS:HD2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:ILE:H	1:B:186:ILE:CD1	2.12	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:F:162:MET:HE1	1:F:165:MET:HE2	1.70	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: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:K:285:LEU:HG	1:K:286:PRO:HD2	1.84	0.60
1:K:133:THR:O	1:K:137:THR:HG23	2.02	0.60
1:J:171:MET:HE2	1:J:171:MET:CA	2.21	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:I:322:GLU:CD	1:I:402:ARG:HH12	2.11	0.59
1:C:322:GLU:OE2	1:C:402:ARG:NH1	2.34	0.59
1:E:171:MET:HE2	1:E:171:MET:HA	1.85	0.59
1:L:89:LEU:HG	1:L:93:MET:HE2	1.84	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:J:89:LEU:CG	1:J:93:MET:HE2	2.17	0.59
1:K:277:ARG:HG3	1:K:277:ARG:NH1	1.99	0.59
1:G:47:LEU:HD11	1:J:45:ARG:HG2	1.84	0.59
1:I:90:SER:HA	1:I:93:MET:CE	2.32	0.59
1:D:276:VAL:CG2	5:D:1163:HOH:O	2.47	0.58
1:A:166:MET:HE3	1:A:184:LYS:HD2	1.84	0.58
1:B:9:LEU:CD2	1:B:93:MET:HE1	2.23	0.58
1:B:102:LYS:O	1:B:106:VAL:HG13	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:78:LYS:HD2	1:F:150:ILE:HB	1.85	0.58
1:F:124:LEU:HD12	1:F:129:LEU:HD13	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:G:315:ILE:O	1:G:339:LYS:NZ	2.28	0.57
1:H:171:MET:HE2	1:H:171:MET:HA	1.86	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: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: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: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: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: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:42:ARG:HD2	1:F:62:TYR:CD1	2.41	0.56
1:E:205:THR:HG23	1:E:344:VAL:HG11	1.87	0.56
1:F:162:MET:SD	1:F:165:MET:HE1	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:J:133:THR:O	1:J:137:THR:HG22	2.05	0.55
1:J:322:GLU:CD	1:J:402:ARG:HH12	2.13	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: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:G:8:TYR:HE2	1:G:93:MET:HE1	1.72	0.55
1:F:152:ALA:HB1	1:F:153:PRO:HD2	1.87	0.55
1:J:171:MET:HA	1:J:171:MET:CE	2.23	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:HE3	2.47	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:J:102:LYS:O	1:J:106:VAL:CG1	2.54	0.55
1:A:316:ARG:NH2	1:I:384:ARG:HH12	2.05	0.54
1:C:312:ALA:HA	1:C:315:ILE:HD12	1.88	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: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: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
1:J:167:ASP:OD1	1:K:420:ARG:NH1	2.40	0.54
1:A:315:ILE:O	1:A:339:LYS:NZ	2.38	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ARG:HG3	1:A:155:VAL:HB	1.90	0.54
1:A:137:THR:HG21	1:A:165:MET:HA	1.89	0.54
1:K:22:GLN:HG2	1:K:98:TRP:HH2	1.73	0.54
1:A:316:ARG:HH22	1:I:384:ARG:HH12	1.56	0.53
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:H:373:GLU:CD	1:H:373:GLU:H	2.16	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: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: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: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:322:GLU:CD	1:B:402:ARG:HH12	2.16	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
1:F:277:ARG:HG2	1:F:277:ARG:NH1	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:G:89:LEU:HD11	1:G:93:MET:HE2	1.91	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:H:171:MET:HE3	1:I:420:ARG:HH22	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:LEU:HG	1:A:93:MET:CE	2.32	0.51
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: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:G:89:LEU:CG	1:G:93:MET:CE	2.82	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:176:THR:HG21	1:K:76:PRO:CD	2.39	0.51
1:J:256:TYR:CZ	1:J:258:GLU:HG2	2.45	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
1:I:368:TYR:OH	3:I:426:PO4:O4	2.26	0.50
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:I:166:MET:HE3	1:I:184:LYS:HD2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:46:VAL:HB	1:D:48:ILE:HB	1.95	0.49
1:C:71:ASN:ND2	1:C:73:ALA:H	2.10	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:A:10:GLY:C	1:A:12:ASP:N	2.71	0.49
1:G:200:ARG:HD2	5:G:1072:HOH:O	2.12	0.49
1:H:11:LYS:HD3	1:H:11:LYS:O	2.13	0.49
1:J:420:ARG:HH12	1:L:171:MET:CE	2.16	0.49
1:C:9:LEU:HD11	1:C:93:MET:CE	2.40	0.49
1:J:380:GLU:O	1:J:384:ARG:HB2	2.11	0.49
1:L:90:SER:HA	1:L:93:MET:HE3	1.95	0.49
1:I:106:VAL:HG22	1:I:108:LEU:HG	1.94	0.49
1:J:37:ALA:HA	1:J:414:LEU:HD21	1.93	0.49
1:J:102:LYS:O	1:J:106:VAL:HG12	2.11	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
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:I:57:ASP:OD2	1:I:57:ASP:C	2.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:266:LEU:HD11	1:B:276:VAL:CG2	2.44	0.48
1:D:82:ARG:HG3	1:D:155:VAL:HB	1.96	0.48
1:D:113:GLY:O	1:D:114:LYS:HG2	2.12	0.48
1:F:278:GLY:O	1:F:279:TYR:C	2.57	0.48
1:H:48:ILE:HB	1:L:46:VAL:HB	1.95	0.48
1:B:108:LEU:CD1	1:B:354:VAL:HG12	2.44	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:D:90:SER:HA	1:D:93:MET:HE3	1.96	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:C:322:GLU:CD	1:C:402:ARG:HH12	2.22	0.47
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:H:166:MET:HE2	1:H:178:PRO:HA	1.95	0.47
1:A:72:THR:CB	5:A:1313:HOH:O	2.52	0.47
1:F:277:ARG:CG	1:F:277:ARG:NH1	2.69	0.47
1:G:69:HIS:CE1	1:G:143:LEU:HG	2.49	0.47
1:G:89:LEU:CD1	1:G:93:MET:CE	2.92	0.47
1:C:81:VAL:HG21	1:C:165:MET:HE1	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:291:TRP:CD1	1:A:311:ASN:HD22	2.33	0.47
1:C:27:VAL:HA	1:C:30:LEU:HD22	1.96	0.47
1:C:102:LYS:O	1:C:106:VAL:HG13	2.14	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:H:90:SER:HA	1:H:93:MET:HE3	1.97	0.47
1:J:171:MET:HG3	1:K:423:TYR:O	2.15	0.47
1:A:13:GLY:HA3	1:A:17:GLU:HB2	1.97	0.47
1:A:224:ILE:HD12	1:A:235:ALA:HB2	1.96	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: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:J:9:LEU:HD21	1:J:93:MET:CE	2.35	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:E:203:PHE:CD1	1:E:203:PHE:C	2.93	0.47
1:F:44:LYS:HE2	5:F:445:HOH:O	2.14	0.47
1:G:42:ARG:CD	1:J:62:TYR:HB3	2.44	0.47
1:G:124:LEU:HD12	1:G:129:LEU:HD13	1.97	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:F:152:ALA:HB1	1:F:153:PRO:CD	2.45	0.46
1:G:89:LEU:CD1	1:G:93:MET:HE3	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
1:I:316:ARG:HH11	1:I:316:ARG:HB3	1.79	0.46
1:A:308:THR:HG22	1:A:309:GLU:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:10:GLY:C	1:A:12:ASP:H	2.22	0.46
1:D:71:ASN:ND2	1:D:73:ALA:H	2.14	0.46
1:D:226:GLY:O	1:D:231:GLY:HA3	2.16	0.46
1:D:313:TRP:CD1	1:D:313:TRP:C	2.94	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:HH21	1:L:402:ARG:HB2	1.81	0.46
1:A:184:LYS:NZ	1:A:364:ASP:OD2	2.45	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:D:423:TYR:HA	1:D:424:PRO:C	2.41	0.45
1:I:346:ASP:O	1:I:347:VAL:C	2.58	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:B:166:MET:HE2	1:B:178:PRO:CA	2.37	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:8:TYR:CE2	1:G:93:MET:HE1	2.52	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:J:171:MET:CA	1:J:171:MET:CE	2.91	0.45
1:C:169:TYR:CG	1:C:180:VAL:HG21	2.52	0.45
1:E:171:MET:HE3	5:E:1708:HOH:O	2.16	0.45
1:K:252:THR:CG2	1:K:277:ARG:HB2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:308:THR:C	1:D:310:GLN:H	2.25	0.45
1:G:103:ASN:O	1:G:104:ALA:C	2.59	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:A:69:HIS:CE1	1:A:143:LEU:HG	2.51	0.45
1:A:133:THR:O	1:A:137:THR:CG2	2.64	0.45
1:E:72:THR:HG23	1:E:72:THR:O	2.16	0.45
1:G:392:GLN:HG2	5:G:687:HOH:O	2.17	0.45
1:G:423:TYR:HA	1:G:424:PRO:C	2.42	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:O	1:J:72:THR:CG2	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: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:13:GLY:HA3	1:A:17:GLU:HG3	1.99	0.44
1:E:346:ASP:O	1:E:347:VAL:C	2.59	0.44
1:K:322:GLU:CD	1:K:402:ARG:HH12	2.25	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:36:LEU:HB3	1:J:414:LEU:HG	2.00	0.44
1:J:105:ALA:HB2	1:J:409:ALA:HB2	2.00	0.44
1:J:347:VAL:HG21	1:J:405:ALA:HB1	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:84:HIS:HB3	1:K:87:VAL:HG23	2.00	0.44
1:L:84:HIS:CG	1:L:85:PRO:HD2	2.53	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: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
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:H:154:ASP:CG	1:H:155:VAL:H	2.25	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:287:ALA:C	1:K:289:ASP:H	2.26	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:H:322:GLU:CD	1:H:402:ARG:HH12	2.26	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:69:HIS:CE1	1:E:143:LEU:HG	2.53	0.43
1:E:404:ALA:O	1:E:408:VAL:HG23	2.18	0.43
1:F:307:ILE:HG22	1:F:332:ALA:HB1	1.99	0.43
1:G:33:LEU:HG	1:G:414:LEU:HB3	2.01	0.43
1:G:237:ALA:O	1:G:241:HIS:HD2	2.01	0.43
1:H:315:ILE:O	1:H:339:LYS:NZ	2.33	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:307:ILE:HB	1:D:328:THR:HG22	2.00	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:99:MET:O	1:G:100:THR:C	2.61	0.43
1:G:420:ARG:NH2	5:G:1332:HOH:O	2.51	0.43
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: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:G:325:ASN:CG	5:G:1107:HOH:O	2.62	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:9:LEU:HD23	1:E:9:LEU:HA	1.89	0.42
1:E:71:ASN:HD21	1:E:73:ALA:HB3	1.83	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:204:ILE:HD13	1:I:380:GLU:HA	2.01	0.42
1:I:359:PHE:O	1:I:363:GLN:HG3	2.19	0.42
1:C:194:ARG:NE	5:C:1253:HOH:O	2.52	0.42
1:D:284:PRO:C	1:D:286:PRO:HD3	2.43	0.42
1:E:250:ASP:OD2	1:E:250:ASP:C	2.62	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:79:GLY:HA3	1:J:113:GLY:O	2.19	0.42
1:J:290:PHE:HA	1:J:293:LEU:HD22	2.01	0.42
1:L:133:THR:O	1:L:137:THR:CG2	2.58	0.42
1:L:166:MET:HE3	1:L:184:LYS:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:89:LEU:CG	1:D:93:MET:HE2	2.27	0.42
1:E:180:VAL:HG13	1:E:181:VAL:HG13	2.01	0.42
1:I:182:THR:HG1	1:I:357:SER:HG	1.65	0.42
1:L:122:ARG:CZ	1:L:122:ARG:HA	2.49	0.42
1:D:32:ARG:HH11	1:D:32:ARG:HB3	1.84	0.42
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:71:ASN:HD21	1:I:73:ALA:CB	2.32	0.42
1:J:99:MET:O	1:J:100:THR:C	2.63	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: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:B:279:TYR:HA	1:B:280:PRO:HD3	1.81	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:G:79:GLY:HA3	1:G:113:GLY:O	2.20	0.42
1:G:378:ARG:CZ	5:G:1343:HOH:O	2.67	0.42
1:H:171:MET:HE3	1:I:420:ARG:NH2	2.34	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:L:12:ASP:CG	1:L:12:ASP:O	2.62	0.42
1:A:167:ASP:O	1:A:171:MET:HG2	2.19	0.42
1:E:27:VAL:N	1:E:28:PRO:CD	2.82	0.42
1:E:244:ARG:NH2	1:E:258:GLU:O	2.51	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:308:THR:CG2	1:C:309:GLU:N	2.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:VAL:O	1:B:156:ASN:HB2	2.19	0.42
1:D:244:ARG:HB2	1:D:244:ARG:NH1	2.29	0.42
5:J:1545:HOH:O	1:L:171:MET:HE1	2.20	0.42
1:L:80:GLY:HA2	1:L:152:ALA:O	2.20	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:O	1:L:281:LYS:HD3	2.20	0.42
1:L:423:TYR:HA	1:L:424:PRO:C	2.45	0.42
1:B:89:LEU:HG	1:B:93:MET:CE	2.42	0.41
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
1:D:133:THR:O	1:D:137:THR:CG2	2.67	0.41
1:D:210:ALA:C	1:D:212:LYS:H	2.28	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:72:THR:O	1:I:72:THR:CG2	2.67	0.41
1:I:215:LEU:HD11	1:I:296:GLU:HB3	2.01	0.41
1:L:4:GLU:N	1:L:5:PRO:CD	2.84	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:K:69:HIS:HE2	1:K:149:ASP:CG	2.28	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:E:276:VAL:C	1:E:278:GLY:H	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:TYR:HB3	1:B:42:ARG:HD2	2.02	0.41
1:A:108:LEU:N	1:A:108:LEU:HD23	2.35	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:B:378:ARG:HG2	3:D:426:PO4:O2	2.20	0.41
1:C:30:LEU:HD12	1:C:30:LEU:HA	1.81	0.41
1:C:122:ARG:HA	1:C:122:ARG:HH11	1.86	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:69:HIS:HE2	1:A:149:ASP:CG	2.26	0.41
1:A:215:LEU:HD13	1:A:319:ILE:HD12	2.01	0.41
1:A:343:VAL:O	1:A:345:PRO:HD3	2.21	0.41
1:B:79:GLY:HA3	1:B:113:GLY:O	2.21	0.41
1:B:186:ILE:N	1:B:186:ILE:CD1	2.81	0.41
1:D:34:ALA:N	1:D:35:PRO:CD	2.84	0.41
1:D:295:VAL:O	1:D:317:ALA:HA	2.20	0.41
1:E:32:ARG:H	1:E:32:ARG:HG2	1.77	0.41
1:G:378:ARG:HD3	1:I:368:TYR:OH	2.20	0.41
1:J:275:GLY:O	1:J:277:ARG:N	2.48	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:L:117:ILE:HD11	1:L:136:TYR:CG	2.55	0.41
1:A:313:TRP:CH2	1:I:242:GLY:HA3	2.56	0.41
1:B:151:PRO:HB2	1:B:181:VAL:HG12	2.03	0.41
1:B:188:LEU:HD12	1:B:188:LEU:HA	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:G:44:LYS:NZ	1:G:45:ARG:NH1	2.66	0.40
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:423:TYR:HA	1:F:424:PRO:C	2.46	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
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:105:ALA:HB2	1:C:409:ALA:HB2	2.03	0.40
1:C:262:ASP:HA	1:C:263:PRO:HD3	1.90	0.40
1:E:266:LEU:O	1:E:270:VAL:HG23	2.22	0.40
1:H:232:ASN:OD1	1:H:232:ASN:C	2.65	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
1:L:215:LEU:C	1:L:215:LEU:HD23	2.47	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%)	24	22
1	B	419/440 (95%)	405 (97%)	14 (3%)	0	100	100
1	C	421/440 (96%)	407 (97%)	11 (3%)	3 (1%)	18	15
1	D	419/440 (95%)	397 (95%)	20 (5%)	2 (0%)	24	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	419/440 (95%)	397 (95%)	19 (4%)	3 (1%)	18	15
1	F	420/440 (96%)	398 (95%)	20 (5%)	2 (0%)	24	22
1	G	420/440 (96%)	409 (97%)	11 (3%)	0	100	100
1	H	421/440 (96%)	403 (96%)	15 (4%)	3 (1%)	18	15
1	I	420/440 (96%)	401 (96%)	17 (4%)	2 (0%)	24	22
1	J	420/440 (96%)	398 (95%)	17 (4%)	5 (1%)	10	7
1	K	412/440 (94%)	386 (94%)	21 (5%)	5 (1%)	10	7
1	L	419/440 (95%)	396 (94%)	16 (4%)	7 (2%)	7	3
All	All	5029/5280 (95%)	4797 (95%)	198 (4%)	34 (1%)	18	15

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

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Mol	Chain	Res	Type
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 [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%)	287 (88%)	38 (12%)	5	3
1	B	325/343 (95%)	291 (90%)	34 (10%)	6	4
1	C	327/343 (95%)	297 (91%)	30 (9%)	8	6
1	D	325/343 (95%)	293 (90%)	32 (10%)	7	5
1	E	325/343 (95%)	283 (87%)	42 (13%)	4	2
1	F	326/343 (95%)	294 (90%)	32 (10%)	7	5
1	G	326/343 (95%)	293 (90%)	33 (10%)	7	5
1	H	327/343 (95%)	286 (88%)	41 (12%)	4	2
1	I	326/343 (95%)	296 (91%)	30 (9%)	8	6
1	J	326/343 (95%)	292 (90%)	34 (10%)	7	4
1	K	321/343 (94%)	289 (90%)	32 (10%)	7	5
1	L	325/343 (95%)	293 (90%)	32 (10%)	7	5
All	All	3904/4116 (95%)	3494 (90%)	410 (10%)	6	4

All (410) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	6	LEU

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Mol	Chain	Res	Type
1	A	9	LEU
1	A	11	LYS
1	A	17	GLU
1	A	20	THR
1	A	26	VAL
1	A	30	LEU
1	A	36	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
1	A	173	VAL
1	A	188	LEU
1	A	192	LEU
1	A	200	ARG
1	A	251	HIS
1	A	252	THR
1	A	272	GLU
1	A	273	PHE
1	A	276	VAL
1	A	328	THR
1	A	341	VAL
1	A	354	VAL
1	A	373	GLU
1	A	398	LYS
1	A	401	LEU
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	33	LEU

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Mol	Chain	Res	Type
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	186	ILE
1	B	188	LEU
1	B	192	LEU
1	B	215	LEU
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
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	26	VAL
1	C	30	LEU
1	C	36	LEU
1	C	38	GLU
1	C	42	ARG
1	C	51	VAL
1	C	55	LEU
1	C	87	VAL
1	C	106	VAL
1	C	122	ARG
1	C	129	LEU

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Mol	Chain	Res	Type
1	C	161	GLU
1	C	173	VAL
1	C	176	THR
1	C	205	THR
1	C	215	LEU
1	C	218	GLU
1	C	272	GLU
1	C	276	VAL
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	381	ARG
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	55	LEU
1	D	72	THR
1	D	106	VAL
1	D	129	LEU
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	218	GLU
1	D	276	VAL
1	D	289	ASP
1	D	293	LEU
1	D	305	LYS
1	D	309	GLU
1	D	313	TRP
1	D	341	VAL
1	D	347	VAL
1	D	367	SER

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Mol	Chain	Res	Type
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	161	GLU
1	E	166	MET
1	E	171	MET
1	E	173	VAL
1	E	186	ILE
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	304	GLU
1	E	308	THR
1	E	316	ARG
1	E	318	ARG
1	E	328	THR
1	E	341	VAL
1	E	342	LEU
1	E	354	VAL

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Mol	Chain	Res	Type
1	E	367	SER
1	E	373	GLU
1	E	381	ARG
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	51	VAL
1	F	55	LEU
1	F	72	THR
1	F	129	LEU
1	F	137	THR
1	F	143	LEU
1	F	161	GLU
1	F	166	MET
1	F	173	VAL
1	F	176	THR
1	F	188	LEU
1	F	192	LEU
1	F	271	GLN
1	F	276	VAL
1	F	277	ARG
1	F	293	LEU
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	26	VAL

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Mol	Chain	Res	Type
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	72	THR
1	G	106	VAL
1	G	109	PRO
1	G	129	LEU
1	G	137	THR
1	G	143	LEU
1	G	161	GLU
1	G	186	ILE
1	G	188	LEU
1	G	192	LEU
1	G	200	ARG
1	G	215	LEU
1	G	218	GLU
1	G	293	LEU
1	G	309	GLU
1	G	325	ASN
1	G	328	THR
1	G	341	VAL
1	G	354	VAL
1	G	373	GLU
1	G	381	ARG
1	G	401	LEU
1	G	414	LEU
1	H	6	LEU
1	H	11	LYS
1	H	20	THR
1	H	21	GLU
1	H	26	VAL
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	106	VAL
1	H	122	ARG

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Mol	Chain	Res	Type
1	H	129	LEU
1	H	137	THR
1	H	161	GLU
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	283	GLU
1	H	285	LEU
1	H	293	LEU
1	H	304	GLU
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	373	GLU
1	H	381	ARG
1	H	398	LYS
1	H	401	LEU
1	H	414	LEU
1	I	6	LEU
1	I	11	LYS
1	I	20	THR
1	I	30	LEU
1	I	33	LEU
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	161	GLU
1	I	171	MET
1	I	173	VAL

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Mol	Chain	Res	Type
1	I	188	LEU
1	I	192	LEU
1	I	205	THR
1	I	211	GLU
1	I	215	LEU
1	I	251	HIS
1	I	293	LEU
1	I	316	ARG
1	I	341	VAL
1	I	342	LEU
1	I	354	VAL
1	I	373	GLU
1	I	381	ARG
1	I	396	GLU
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
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	137	THR
1	J	143	LEU
1	J	161	GLU
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	222	VAL
1	J	293	LEU
1	J	316	ARG
1	J	328	THR

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Mol	Chain	Res	Type
1	J	341	VAL
1	J	342	LEU
1	J	354	VAL
1	J	372	GLU
1	J	376	ASN
1	J	381	ARG
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	72	THR
1	K	106	VAL
1	K	129	LEU
1	K	143	LEU
1	K	161	GLU
1	K	166	MET
1	K	173	VAL
1	K	188	LEU
1	K	195	ARG
1	K	205	THR
1	K	211	GLU
1	K	232	ASN
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	372	GLU
1	K	373	GLU
1	K	381	ARG
1	K	384	ARG
1	K	414	LEU
1	L	6	LEU
1	L	12	ASP

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Mol	Chain	Res	Type
1	L	20	THR
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	72	THR
1	L	86	GLU
1	L	106	VAL
1	L	137	THR
1	L	143	LEU
1	L	161	GLU
1	L	173	VAL
1	L	186	ILE
1	L	188	LEU
1	L	192	LEU
1	L	205	THR
1	L	222	VAL
1	L	281	LYS
1	L	296	GLU
1	L	328	THR
1	L	341	VAL
1	L	373	GLU
1	L	376	ASN
1	L	381	ARG
1	L	398	LYS
1	L	401	LEU
1	L	414	LEU
1	L	420	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	239	HIS
1	A	241	HIS
1	A	306	GLN
1	B	22	GLN
1	B	251	HIS
1	B	269	HIS
1	B	271	GLN
1	B	306	GLN

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Mol	Chain	Res	Type
1	B	392	GLN
1	C	22	GLN
1	C	71	ASN
1	C	216	GLN
1	C	229	ASN
1	C	239	HIS
1	C	241	HIS
1	C	251	HIS
1	C	376	ASN
1	D	22	GLN
1	D	71	ASN
1	D	251	HIS
1	D	306	GLN
1	E	22	GLN
1	E	71	ASN
1	E	241	HIS
1	E	251	HIS
1	E	269	HIS
1	E	306	GLN
1	E	376	ASN
1	F	22	GLN
1	F	216	GLN
1	F	241	HIS
1	F	251	HIS
1	F	269	HIS
1	F	271	GLN
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	239	HIS
1	H	306	GLN
1	H	310	GLN
1	H	325	ASN
1	I	22	GLN

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Mol	Chain	Res	Type
1	I	71	ASN
1	I	241	HIS
1	I	269	HIS
1	I	271	GLN
1	I	306	GLN
1	I	310	GLN
1	J	22	GLN
1	J	241	HIS
1	J	251	HIS
1	J	269	HIS
1	J	392	GLN
1	K	71	ASN
1	K	229	ASN
1	K	306	GLN
1	K	395	GLN
1	L	22	GLN
1	L	71	ASN
1	L	216	GLN
1	L	239	HIS
1	L	249	GLN
1	L	257	ASN
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 oligosaccharides 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	F	425	-	8,9,9	1.06	0	8,11,11	0.79	0
2	GLU	H	425	-	8,9,9	1.29	1 (12%)	8,11,11	1.23	1 (12%)
2	GLU	D	425	-	8,9,9	1.17	1 (12%)	8,11,11	1.60	1 (12%)
2	GLU	C	425	-	8,9,9	1.07	1 (12%)	8,11,11	1.45	1 (12%)
3	PO4	K	426	-	4,4,4	0.86	0	6,6,6	0.70	0
2	GLU	G	425	-	8,9,9	1.11	0	8,11,11	0.99	0
2	GLU	A	425	-	8,9,9	0.95	0	8,11,11	1.02	1 (12%)
2	GLU	H	500	-	8,9,9	1.12	1 (12%)	8,11,11	1.04	1 (12%)
2	GLU	I	500	-	8,9,9	1.18	1 (12%)	8,11,11	1.45	1 (12%)
2	GLU	K	500	-	8,9,9	0.95	1 (12%)	8,11,11	1.22	1 (12%)
3	PO4	G	426	-	4,4,4	0.79	0	6,6,6	0.89	0
2	GLU	G	500	-	8,9,9	1.04	1 (12%)	8,11,11	1.10	0
2	GLU	J	500	-	8,9,9	1.22	1 (12%)	8,11,11	1.21	1 (12%)
2	GLU	L	425	-	8,9,9	1.06	1 (12%)	8,11,11	1.66	1 (12%)
2	GLU	E	425	-	8,9,9	1.13	1 (12%)	8,11,11	1.32	2 (25%)
2	GLU	K	425	-	8,9,9	1.05	1 (12%)	8,11,11	1.15	1 (12%)
2	GLU	I	425	-	8,9,9	1.29	1 (12%)	8,11,11	0.90	0
2	GLU	B	500	-	8,9,9	1.08	1 (12%)	8,11,11	1.58	1 (12%)
2	GLU	F	500	-	8,9,9	1.04	1 (12%)	8,11,11	0.91	0
2	GLU	D	500	-	8,9,9	1.25	1 (12%)	8,11,11	1.38	1 (12%)
2	GLU	C	500	-	8,9,9	1.12	1 (12%)	8,11,11	0.85	0
3	PO4	J	426	-	4,4,4	0.89	0	6,6,6	0.72	0
2	GLU	A	500	-	8,9,9	1.23	1 (12%)	8,11,11	1.47	1 (12%)
3	PO4	F	426	-	0,3,4	-	-	0,3,6	-	-
3	PO4	A	426	-	4,4,4	0.96	0	6,6,6	0.91	0
3	PO4	D	426	-	4,4,4	0.95	0	6,6,6	0.68	0
3	PO4	C	426	-	4,4,4	0.88	0	6,6,6	0.50	0
3	PO4	I	426	-	4,4,4	1.01	0	6,6,6	0.53	0
3	PO4	I	427	-	4,4,4	0.95	0	6,6,6	0.77	0
2	GLU	L	500	-	8,9,9	1.11	1 (12%)	8,11,11	1.22	1 (12%)
2	GLU	B	425	-	8,9,9	1.05	0	8,11,11	1.19	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLU	J	425	-	8,9,9	1.10	0	8,11,11	1.20	1 (12%)
2	GLU	E	500	-	8,9,9	1.13	1 (12%)	8,11,11	1.29	1 (12%)

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	F	425	-	-	0/9/9/9	-
2	GLU	H	425	-	-	0/9/9/9	-
2	GLU	D	425	-	-	0/9/9/9	-
2	GLU	C	425	-	-	1/9/9/9	-
2	GLU	G	425	-	-	0/9/9/9	-
2	GLU	A	425	-	-	1/9/9/9	-
2	GLU	H	500	-	-	2/9/9/9	-
2	GLU	I	500	-	-	4/9/9/9	-
2	GLU	K	500	-	-	3/9/9/9	-
2	GLU	G	500	-	-	4/9/9/9	-
2	GLU	J	500	-	-	0/9/9/9	-
2	GLU	L	425	-	-	1/9/9/9	-
2	GLU	E	425	-	-	2/9/9/9	-
2	GLU	K	425	-	-	0/9/9/9	-
2	GLU	I	425	-	-	4/9/9/9	-
2	GLU	B	500	-	-	2/9/9/9	-
2	GLU	F	500	-	-	7/9/9/9	-
2	GLU	D	500	-	-	2/9/9/9	-
2	GLU	C	500	-	-	1/9/9/9	-
2	GLU	A	500	-	-	2/9/9/9	-
2	GLU	L	500	-	-	1/9/9/9	-
2	GLU	B	425	-	-	4/9/9/9	-
2	GLU	J	425	-	-	0/9/9/9	-
2	GLU	E	500	-	-	4/9/9/9	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	GLU	OXT-C	-2.63	1.22	1.30
2	H	425	GLU	OXT-C	-2.57	1.22	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	500	GLU	OXT-C	-2.55	1.22	1.30
2	L	500	GLU	OXT-C	-2.45	1.22	1.30
2	I	425	GLU	OXT-C	-2.43	1.22	1.30
2	B	500	GLU	OXT-C	-2.40	1.23	1.30
2	I	500	GLU	OXT-C	-2.33	1.23	1.30
2	C	425	GLU	OXT-C	-2.33	1.23	1.30
2	E	500	GLU	OXT-C	-2.30	1.23	1.30
2	G	500	GLU	OXT-C	-2.28	1.23	1.30
2	E	425	GLU	OXT-C	-2.24	1.23	1.30
2	H	500	GLU	OXT-C	-2.20	1.23	1.30
2	D	425	GLU	OXT-C	-2.13	1.23	1.30
2	A	500	GLU	OXT-C	-2.10	1.24	1.30
2	C	500	GLU	OXT-C	-2.10	1.24	1.30
2	L	425	GLU	OXT-C	-2.06	1.24	1.30
2	K	500	GLU	OXT-C	-2.03	1.24	1.30
2	F	500	GLU	OXT-C	-2.02	1.24	1.30
2	K	425	GLU	OXT-C	-2.01	1.24	1.30

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	425	GLU	OXT-C-O	-3.98	115.06	124.08
2	B	500	GLU	OXT-C-O	-3.75	115.58	124.08
2	L	425	GLU	OXT-C-O	-3.55	116.02	124.08
2	I	500	GLU	OXT-C-O	-3.39	116.38	124.08
2	D	500	GLU	OXT-C-O	-3.28	116.64	124.08
2	H	425	GLU	OXT-C-O	-3.07	117.11	124.08
2	E	500	GLU	OXT-C-O	-2.99	117.31	124.08
2	C	425	GLU	OXT-C-O	-2.86	117.59	124.08
2	A	500	GLU	OXT-C-O	-2.63	118.10	124.08
2	E	425	GLU	OXT-C-O	-2.51	118.39	124.08
2	J	425	GLU	OXT-C-O	-2.48	118.45	124.08
2	J	500	GLU	OXT-C-O	-2.46	118.50	124.08
2	K	500	GLU	OXT-C-O	-2.32	118.81	124.08
2	L	500	GLU	OXT-C-O	-2.31	118.83	124.08
2	K	425	GLU	OXT-C-O	-2.27	118.93	124.08
2	H	500	GLU	OXT-C-O	-2.12	119.27	124.08
2	A	425	GLU	OXT-C-O	-2.12	119.27	124.08
2	B	425	GLU	OXT-C-O	-2.01	119.51	124.08
2	E	425	GLU	OE2-CD-CG	2.01	120.35	114.00

There are no chirality outliers.

All (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	G	500	GLU	C-CA-CB-CG
2	I	425	GLU	C-CA-CB-CG
2	F	500	GLU	OXT-C-CA-N
2	K	500	GLU	OXT-C-CA-N
2	F	500	GLU	C-CA-CB-CG
2	E	500	GLU	N-CA-CB-CG
2	K	500	GLU	CA-CB-CG-CD
2	F	500	GLU	O-C-CA-CB
2	I	500	GLU	O-C-CA-CB
2	I	500	GLU	OXT-C-CA-CB
2	C	500	GLU	CA-CB-CG-CD
2	F	500	GLU	OXT-C-CA-CB
2	D	500	GLU	OE2-CD-CG-CB
2	D	500	GLU	OE1-CD-CG-CB
2	E	500	GLU	OE1-CD-CG-CB
2	I	500	GLU	OE1-CD-CG-CB
2	E	500	GLU	OE2-CD-CG-CB
2	A	500	GLU	OE1-CD-CG-CB
2	B	500	GLU	OE2-CD-CG-CB
2	F	500	GLU	OE2-CD-CG-CB
2	I	500	GLU	OE2-CD-CG-CB
2	H	500	GLU	OE2-CD-CG-CB
2	B	500	GLU	OE1-CD-CG-CB
2	F	500	GLU	OE1-CD-CG-CB
2	I	425	GLU	OE2-CD-CG-CB
2	H	500	GLU	OE1-CD-CG-CB
2	E	425	GLU	OE2-CD-CG-CB
2	I	425	GLU	OE1-CD-CG-CB
2	E	500	GLU	C-CA-CB-CG
2	A	500	GLU	OE2-CD-CG-CB
2	G	500	GLU	OE1-CD-CG-CB
2	G	500	GLU	OE2-CD-CG-CB
2	B	425	GLU	OE1-CD-CG-CB
2	E	425	GLU	OE1-CD-CG-CB
2	G	500	GLU	N-CA-CB-CG
2	I	425	GLU	N-CA-CB-CG
2	L	425	GLU	OE2-CD-CG-CB
2	L	500	GLU	CA-CB-CG-CD
2	C	425	GLU	OE2-CD-CG-CB
2	A	425	GLU	OXT-C-CA-N

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Mol	Chain	Res	Type	Atoms
2	F	500	GLU	O-C-CA-N
2	K	500	GLU	O-C-CA-N
2	B	425	GLU	OE2-CD-CG-CB

There are no ring outliers.

12 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	425	GLU	1	0
2	H	425	GLU	1	0
2	C	425	GLU	1	0
2	G	425	GLU	1	0
2	A	425	GLU	1	0
2	K	500	GLU	1	0
3	G	426	PO4	1	0
2	F	500	GLU	2	0
2	A	500	GLU	1	0
3	D	426	PO4	1	0
3	I	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, 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%)	0.61	22 (5%) 33 35	18, 35, 62, 75	1 (0%)
1	B	421/440 (95%)	0.94	60 (14%) 6 6	20, 42, 75, 93	0
1	C	421/440 (95%)	0.94	40 (9%) 14 14	22, 44, 70, 85	3 (0%)
1	D	421/440 (95%)	1.20	94 (22%) 2 2	25, 51, 87, 94	1 (0%)
1	E	421/440 (95%)	0.80	44 (10%) 11 12	16, 41, 75, 91	2 (0%)
1	F	421/440 (95%)	1.05	75 (17%) 4 4	17, 46, 79, 84	2 (0%)
1	G	421/440 (95%)	0.65	22 (5%) 33 35	20, 37, 59, 71	2 (0%)
1	H	421/440 (95%)	0.96	48 (11%) 10 10	23, 47, 75, 89	4 (0%)
1	I	421/440 (95%)	0.69	34 (8%) 18 19	19, 41, 70, 86	2 (0%)
1	J	421/440 (95%)	0.81	38 (9%) 15 16	23, 41, 63, 76	3 (0%)
1	K	416/440 (94%)	1.35	106 (25%) 1 2	26, 52, 81, 89	1 (0%)
1	L	421/440 (95%)	1.18	69 (16%) 4 4	28, 54, 87, 96	1 (0%)
All	All	5047/5280 (95%)	0.93	652 (12%) 7 8	16, 43, 78, 96	22 (0%)

All (652) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	273	PHE	6.9
1	D	285	LEU	6.5
1	K	270	VAL	5.9
1	L	313	TRP	5.9
1	K	276	VAL	5.8
1	K	267	LEU	5.7
1	H	273	PHE	5.6
1	K	312	ALA	5.6
1	K	273	PHE	5.4
1	K	284	PRO	5.4
1	C	276	VAL	5.2

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Mol	Chain	Res	Type	RSRZ
1	D	313	TRP	5.1
1	D	286	PRO	5.1
1	E	313	TRP	5.0
1	D	217	VAL	5.0
1	E	11	LYS	4.9
1	B	273	PHE	4.9
1	E	252	THR	4.8
1	C	11	LYS	4.8
1	J	308	THR	4.8
1	K	256	TYR	4.7
1	L	287	ALA	4.6
1	L	286	PRO	4.6
1	L	122	ARG	4.6
1	D	273	PHE	4.6
1	D	315	ILE	4.6
1	H	200	ARG	4.6
1	E	273	PHE	4.6
1	G	13	GLY	4.5
1	K	279	TYR	4.5
1	L	270	VAL	4.5
1	E	280	PRO	4.5
1	K	260	GLY	4.5
1	I	13	GLY	4.4
1	A	12	ASP	4.4
1	A	13	GLY	4.3
1	E	278	GLY	4.3
1	A	270	VAL	4.3
1	F	278	GLY	4.3
1	A	251	HIS	4.3
1	K	335	ILE	4.3
1	C	219	GLY	4.2
1	D	244	ARG	4.2
1	F	248	VAL	4.2
1	D	11	LYS	4.1
1	K	246	VAL	4.1
1	K	255	VAL	4.1
1	D	288	ALA	4.1
1	F	220	ALA	4.1
1	K	294	PRO	4.1
1	K	266	LEU	4.1
1	K	223	ALA	4.0
1	A	275	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	275	GLY	4.0
1	K	13	GLY	4.0
1	B	285	LEU	4.0
1	L	273	PHE	4.0
1	L	280	PRO	4.0
1	I	252	THR	4.0
1	F	279	TYR	4.0
1	K	264	TYR	4.0
1	C	252	THR	3.9
1	L	284	PRO	3.9
1	D	287	ALA	3.9
1	J	122	ARG	3.9
1	F	261	ILE	3.9
1	I	270	VAL	3.9
1	D	250	ASP	3.9
1	G	10	GLY	3.9
1	K	282	ALA	3.9
1	L	267	LEU	3.9
1	D	396	GLU	3.9
1	K	271	GLN	3.9
1	D	276	VAL	3.8
1	G	4	GLU	3.8
1	K	287	ALA	3.8
1	H	251	HIS	3.8
1	F	11	LYS	3.8
1	F	259	ALA	3.8
1	A	274	GLY	3.8
1	F	247	ALA	3.7
1	I	251	HIS	3.7
1	C	6	LEU	3.7
1	H	4	GLU	3.7
1	L	10	GLY	3.7
1	K	261	ILE	3.7
1	D	303	LEU	3.7
1	C	270	VAL	3.7
1	L	257	ASN	3.7
1	F	287	ALA	3.7
1	I	275	GLY	3.7
1	K	217	VAL	3.7
1	A	252	THR	3.7
1	F	267	LEU	3.6
1	K	286	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	280	PRO	3.6
1	F	10	GLY	3.6
1	K	4	GLU	3.6
1	F	290	PHE	3.6
1	K	308	THR	3.6
1	D	122	ARG	3.6
1	G	270	VAL	3.6
1	K	224	ILE	3.6
1	C	331	ALA	3.6
1	H	266	LEU	3.6
1	D	256	TYR	3.6
1	I	10	GLY	3.6
1	E	308	THR	3.5
1	J	311	ASN	3.5
1	K	340	GLY	3.5
1	L	274	GLY	3.5
1	D	312	ALA	3.5
1	F	13	GLY	3.5
1	F	260	GLY	3.5
1	K	275	GLY	3.5
1	F	280	PRO	3.5
1	C	13	GLY	3.5
1	J	13	GLY	3.5
1	G	12	ASP	3.5
1	H	270	VAL	3.5
1	D	308	THR	3.5
1	B	13	GLY	3.4
1	K	254	THR	3.4
1	E	284	PRO	3.4
1	B	219	GLY	3.4
1	F	282	ALA	3.4
1	L	292	GLY	3.4
1	F	284	PRO	3.4
1	J	286	PRO	3.4
1	D	220	ALA	3.4
1	E	211	GLU	3.4
1	J	288	ALA	3.4
1	H	267	LEU	3.4
1	B	270	VAL	3.4
1	B	276	VAL	3.4
1	L	253	GLY	3.4
1	B	259	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	261	ILE	3.4
1	A	4	GLU	3.3
1	I	308	THR	3.3
1	F	317	ALA	3.3
1	K	302	ALA	3.3
1	C	267	LEU	3.3
1	L	271	GLN	3.3
1	F	245	VAL	3.3
1	J	259	ALA	3.3
1	L	307	ILE	3.3
1	K	277	ARG	3.3
1	B	11	LYS	3.3
1	H	253	GLY	3.3
1	I	278	GLY	3.3
1	D	307	ILE	3.3
1	D	216	GLN	3.3
1	G	308	THR	3.2
1	B	287	ALA	3.2
1	H	11	LYS	3.2
1	H	12	ASP	3.2
1	J	278	GLY	3.2
1	K	269	HIS	3.2
1	E	287	ALA	3.2
1	K	331	ALA	3.2
1	J	307	ILE	3.2
1	F	273	PHE	3.2
1	K	268	ARG	3.2
1	L	373	GLU	3.2
1	L	11	LYS	3.2
1	F	276	VAL	3.2
1	K	235	ALA	3.2
1	I	273	PHE	3.2
1	H	10	GLY	3.2
1	F	257	ASN	3.2
1	F	313	TRP	3.1
1	D	282	ALA	3.1
1	L	276	VAL	3.1
1	D	335	ILE	3.1
1	K	337	LEU	3.1
1	J	264	TYR	3.1
1	F	251	HIS	3.1
1	H	278	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	H	280	PRO	3.1
1	K	311	ASN	3.1
1	K	245	VAL	3.1
1	K	259	ALA	3.1
1	K	293	LEU	3.1
1	K	278	GLY	3.1
1	J	276	VAL	3.1
1	K	295	VAL	3.1
1	B	279	TYR	3.1
1	E	279	TYR	3.1
1	D	275	GLY	3.1
1	H	292	GLY	3.1
1	C	273	PHE	3.1
1	D	280	PRO	3.1
1	K	263	PRO	3.1
1	I	277	ARG	3.1
1	C	4	GLU	3.1
1	L	240	ASP	3.1
1	D	237	ALA	3.1
1	F	224	ILE	3.1
1	D	328	THR	3.0
1	A	25	ARG	3.0
1	I	5	PRO	3.0
1	K	283	GLU	3.0
1	B	240	ASP	3.0
1	L	12	ASP	3.0
1	K	339	LYS	3.0
1	K	321	ALA	3.0
1	D	337	LEU	3.0
1	F	303	LEU	3.0
1	L	6	LEU	3.0
1	F	219	GLY	3.0
1	K	244	ARG	3.0
1	J	290	PHE	3.0
1	K	239	HIS	3.0
1	F	210	ALA	3.0
1	E	255	VAL	3.0
1	K	285	LEU	3.0
1	E	219	GLY	3.0
1	B	396	GLU	3.0
1	C	280	PRO	3.0
1	F	277	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	K	234	ALA	3.0
1	E	13	GLY	3.0
1	K	10	GLY	3.0
1	L	278	GLY	3.0
1	I	313	TRP	3.0
1	I	267	LEU	2.9
1	L	303	LEU	2.9
1	D	292	GLY	2.9
1	K	18	ILE	2.9
1	E	17	GLU	2.9
1	B	220	ALA	2.9
1	L	302	ALA	2.9
1	E	285	LEU	2.9
1	I	253	GLY	2.9
1	K	11	LYS	2.9
1	L	275	GLY	2.9
1	B	255	VAL	2.9
1	B	269	HIS	2.9
1	K	257	ASN	2.9
1	F	207	ALA	2.9
1	J	312	ALA	2.9
1	K	243	ALA	2.9
1	D	267	LEU	2.9
1	F	275	GLY	2.9
1	L	13	GLY	2.9
1	L	215	LEU	2.9
1	D	248	VAL	2.9
1	B	308	THR	2.9
1	C	5	PRO	2.9
1	J	284	PRO	2.9
1	K	280	PRO	2.9
1	G	11	LYS	2.9
1	L	256	TYR	2.9
1	L	247	ALA	2.9
1	F	253	GLY	2.9
1	H	255	VAL	2.8
1	L	20	THR	2.8
1	L	329	THR	2.8
1	G	284	PRO	2.8
1	K	330	PRO	2.8
1	K	310	GLN	2.8
1	F	250	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	302	ALA	2.8
1	F	255	VAL	2.8
1	K	252	THR	2.8
1	J	315	ILE	2.8
1	A	250	ASP	2.8
1	B	260	GLY	2.8
1	E	275	GLY	2.8
1	D	258	GLU	2.8
1	J	309	GLU	2.8
1	K	6	LEU	2.8
1	D	255	VAL	2.8
1	L	255	VAL	2.8
1	B	399	ILE	2.8
1	C	172	ASN	2.8
1	K	12	ASP	2.8
1	B	274	GLY	2.8
1	B	284	PRO	2.8
1	K	222	VAL	2.8
1	G	50	ASP	2.7
1	H	219	GLY	2.7
1	C	332	ALA	2.7
1	F	312	ALA	2.7
1	H	288	ALA	2.7
1	D	215	LEU	2.7
1	K	298	LEU	2.7
1	B	400	PRO	2.7
1	H	276	VAL	2.7
1	I	261	ILE	2.7
1	L	399	ILE	2.7
1	J	313	TRP	2.7
1	L	211	GLU	2.7
1	B	282	ALA	2.7
1	K	290	PHE	2.7
1	C	328	THR	2.7
1	E	276	VAL	2.7
1	K	307	ILE	2.7
1	K	215	LEU	2.7
1	D	284	PRO	2.7
1	D	295	VAL	2.7
1	E	274	GLY	2.7
1	A	267	LEU	2.6
1	D	266	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	266	LEU	2.6
1	F	269	HIS	2.6
1	D	242	GLY	2.6
1	K	14	GLY	2.6
1	K	253	GLY	2.6
1	K	274	GLY	2.6
1	D	309	GLU	2.6
1	B	325	ASN	2.6
1	D	329	THR	2.6
1	E	20	THR	2.6
1	E	325	ASN	2.6
1	J	331	ALA	2.6
1	F	252	THR	2.6
1	F	308	THR	2.6
1	D	6	LEU	2.6
1	F	215	LEU	2.6
1	H	6	LEU	2.6
1	D	272	GLU	2.6
1	J	304	GLU	2.6
1	L	251	HIS	2.6
1	H	376	ASN	2.6
1	A	308	THR	2.6
1	F	286	PRO	2.6
1	L	5	PRO	2.6
1	D	314	ARG	2.6
1	I	279	TYR	2.6
1	L	213	ILE	2.6
1	B	10	GLY	2.6
1	H	13	GLY	2.6
1	K	219	GLY	2.6
1	I	11	LYS	2.6
1	D	301	ALA	2.6
1	H	282	ALA	2.6
1	H	308	THR	2.6
1	C	12	ASP	2.6
1	K	55	LEU	2.6
1	K	218	GLU	2.5
1	C	217	VAL	2.5
1	F	315	ILE	2.5
1	D	251	HIS	2.5
1	C	176	THR	2.5
1	F	254	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	20	THR	2.5
1	G	250	ASP	2.5
1	L	328	THR	2.5
1	F	294	PRO	2.5
1	K	357	SER	2.5
1	F	285	LEU	2.5
1	F	293	LEU	2.5
1	J	285	LEU	2.5
1	B	275	GLY	2.5
1	D	274	GLY	2.5
1	H	406	TYR	2.5
1	L	279	TYR	2.5
1	J	252	THR	2.5
1	B	294	PRO	2.5
1	C	259	ALA	2.5
1	E	288	ALA	2.5
1	H	286	PRO	2.5
1	B	303	LEU	2.5
1	B	337	LEU	2.5
1	J	342	LEU	2.5
1	K	291	TRP	2.5
1	C	222	VAL	2.5
1	J	277	ARG	2.5
1	K	319	ILE	2.5
1	I	12	ASP	2.5
1	C	271	GLN	2.5
1	F	249	GLN	2.5
1	B	254	THR	2.5
1	K	20	THR	2.5
1	L	220	ALA	2.5
1	K	292	GLY	2.5
1	A	276	VAL	2.4
1	D	173	VAL	2.4
1	D	299	VAL	2.4
1	E	270	VAL	2.4
1	E	341	VAL	2.4
1	F	319	ILE	2.5
1	D	50	ASP	2.4
1	D	211	GLU	2.4
1	K	289	ASP	2.4
1	B	264	TYR	2.4
1	F	256	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	I	176	THR	2.4
1	G	5	PRO	2.4
1	B	332	ALA	2.4
1	D	317	ALA	2.4
1	D	332	ALA	2.4
1	D	305	LYS	2.4
1	I	342	LEU	2.4
1	J	215	LEU	2.4
1	K	30	LEU	2.4
1	B	268	ARG	2.4
1	I	122	ARG	2.4
1	D	13	GLY	2.4
1	F	242	GLY	2.4
1	J	376	ASN	2.4
1	B	313	TRP	2.4
1	C	250	ASP	2.4
1	D	390	VAL	2.4
1	J	27	VAL	2.4
1	K	341	VAL	2.4
1	L	18	ILE	2.4
1	D	20	THR	2.4
1	L	294	PRO	2.4
1	K	288	ALA	2.4
1	L	281	LYS	2.4
1	L	288	ALA	2.4
1	B	107	GLY	2.4
1	C	14	GLY	2.4
1	D	278	GLY	2.4
1	E	10	GLY	2.4
1	H	275	GLY	2.4
1	B	290	PHE	2.4
1	D	290	PHE	2.4
1	C	261	ILE	2.4
1	L	248	VAL	2.4
1	C	279	TYR	2.4
1	E	286	PRO	2.4
1	G	259	ALA	2.4
1	F	338	GLU	2.4
1	H	218	GLU	2.4
1	E	226	GLY	2.4
1	G	219	GLY	2.4
1	H	274	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	L	219	GLY	2.4
1	H	364	ASP	2.4
1	E	365	PHE	2.4
1	F	238	PHE	2.4
1	K	297	PHE	2.4
1	C	245	VAL	2.4
1	L	217	VAL	2.4
1	D	5	PRO	2.4
1	E	5	PRO	2.4
1	H	264	TYR	2.3
1	B	207	ALA	2.3
1	D	324	ALA	2.3
1	D	331	ALA	2.3
1	F	301	ALA	2.3
1	J	218	GLU	2.3
1	K	210	ALA	2.3
1	A	266	LEU	2.3
1	C	55	LEU	2.3
1	F	342	LEU	2.3
1	L	9	LEU	2.3
1	D	14	GLY	2.3
1	J	14	GLY	2.3
1	D	227	PHE	2.3
1	E	194	ARG	2.3
1	K	195	ARG	2.3
1	B	186	ILE	2.3
1	B	390	VAL	2.3
1	K	87	VAL	2.3
1	K	173	VAL	2.3
1	E	269	HIS	2.3
1	F	283	GLU	2.3
1	I	264	TYR	2.3
1	K	237	ALA	2.3
1	B	58	GLY	2.3
1	D	293	LEU	2.3
1	D	32	ARG	2.3
1	A	11	LYS	2.3
1	K	227	PHE	2.3
1	L	335	ILE	2.3
1	K	343	VAL	2.3
1	L	26	VAL	2.3
1	D	254	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	28	PRO	2.3
1	F	216	GLN	2.3
1	H	20	THR	2.3
1	B	376	ASN	2.3
1	B	210	ALA	2.3
1	I	287	ALA	2.3
1	C	285	LEU	2.3
1	E	253	GLY	2.3
1	I	50	ASP	2.3
1	I	260	GLY	2.3
1	J	314	ARG	2.3
1	K	242	GLY	2.3
1	L	194	ARG	2.3
1	L	268	ARG	2.3
1	B	296	GLU	2.3
1	H	269	HIS	2.3
1	K	373	GLU	2.3
1	D	392	GLN	2.3
1	D	399	ILE	2.3
1	D	246	VAL	2.3
1	D	270	VAL	2.3
1	K	51	VAL	2.3
1	I	280	PRO	2.3
1	G	122	ARG	2.3
1	C	265	ASP	2.3
1	F	243	ALA	2.3
1	G	37	ALA	2.3
1	K	247	ALA	2.3
1	L	50	ASP	2.3
1	D	414	LEU	2.3
1	E	33	LEU	2.3
1	D	271	GLN	2.2
1	K	399	ILE	2.2
1	B	205	THR	2.2
1	D	300	PRO	2.2
1	F	295	VAL	2.2
1	L	176	THR	2.2
1	L	246	VAL	2.2
1	B	122	ARG	2.2
1	F	244	ARG	2.2
1	A	265	ASP	2.2
1	C	50	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	265	ASP	2.2
1	B	302	ALA	2.2
1	B	215	LEU	2.2
1	B	267	LEU	2.2
1	A	256	TYR	2.2
1	J	4	GLU	2.2
1	B	271	GLN	2.2
1	D	316	ARG	2.2
1	D	311	ASN	2.2
1	F	20	THR	2.2
1	L	261	ILE	2.2
1	B	245	VAL	2.2
1	F	246	VAL	2.2
1	A	10	GLY	2.2
1	D	260	GLY	2.2
1	F	226	GLY	2.2
1	F	274	GLY	2.2
1	D	210	ALA	2.2
1	D	247	ALA	2.2
1	H	287	ALA	2.2
1	J	152	ALA	2.2
1	J	287	ALA	2.2
1	K	220	ALA	2.2
1	L	259	ALA	2.2
1	L	331	ALA	2.2
1	L	89	LEU	2.2
1	A	269	HIS	2.2
1	D	264	TYR	2.2
1	L	7	SER	2.2
1	D	291	TRP	2.2
1	B	261	ILE	2.2
1	D	176	THR	2.2
1	H	328	THR	2.2
1	K	265	ASP	2.2
1	B	222	VAL	2.2
1	I	341	VAL	2.2
1	K	248	VAL	2.2
1	D	253	GLY	2.2
1	G	283	GLU	2.2
1	J	10	GLY	2.2
1	D	302	ALA	2.2
1	F	288	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	287	ALA	2.2
1	J	303	LEU	2.2
1	I	244	ARG	2.2
1	L	308	THR	2.2
1	J	186	ILE	2.1
1	D	245	VAL	2.1
1	C	278	GLY	2.1
1	E	259	ALA	2.1
1	L	317	ALA	2.1
1	D	277	ARG	2.1
1	E	266	LEU	2.1
1	J	293	LEU	2.1
1	H	7	SER	2.1
1	E	281	LYS	2.1
1	H	279	TYR	2.1
1	B	211	GLU	2.1
1	F	12	ASP	2.1
1	F	289	ASP	2.1
1	K	262	ASP	2.1
1	B	252	THR	2.1
1	F	291	TRP	2.1
1	E	261	ILE	2.1
1	E	271	GLN	2.1
1	K	238	PHE	2.1
1	B	292	GLY	2.1
1	F	239	HIS	2.1
1	G	23	VAL	2.1
1	I	276	VAL	2.1
1	K	199	GLY	2.1
1	D	208	ALA	2.1
1	F	394	ALA	2.1
1	C	9	LEU	2.1
1	H	285	LEU	2.1
1	I	303	LEU	2.1
1	K	272	GLU	2.1
1	F	265	ASP	2.1
1	J	289	ASP	2.1
1	I	286	PRO	2.1
1	L	252	THR	2.1
1	C	31	GLY	2.1
1	D	213	ILE	2.1
1	H	25	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	54	ARG	2.1
1	K	393	VAL	2.1
1	L	44	LYS	2.1
1	H	223	ALA	2.1
1	G	267	LEU	2.1
1	I	266	LEU	2.1
1	L	285	LEU	2.1
1	F	218	GLU	2.1
1	A	284	PRO	2.1
1	C	264	TYR	2.1
1	D	239	HIS	2.1
1	H	252	THR	2.1
1	K	15	PRO	2.1
1	D	297	PHE	2.1
1	F	270	VAL	2.1
1	L	222	VAL	2.1
1	L	245	VAL	2.1
1	F	86	GLU	2.0
1	H	86	GLU	2.0
1	H	259	ALA	2.1
1	K	418	ALA	2.1
1	D	336	LEU	2.0
1	K	336	LEU	2.0
1	D	334	ASP	2.0
1	E	12	ASP	2.0
1	J	310	GLN	2.0
1	F	316	ARG	2.0
1	H	195	ARG	2.0
1	H	316	ARG	2.0
1	L	195	ARG	2.0
1	E	15	PRO	2.0
1	H	176	THR	2.0
1	C	315	ILE	2.0
1	G	261	ILE	2.0
1	B	17	GLU	2.0
1	B	217	VAL	2.0
1	B	258	GLU	2.0
1	D	218	GLU	2.0
1	B	209	ALA	2.0
1	C	282	ALA	2.0
1	C	287	ALA	2.0
1	H	325	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	36	LEU	2.0
1	E	303	LEU	2.0
1	G	9	LEU	2.0
1	I	215	LEU	2.0
1	C	175	ARG	2.0
1	K	122	ARG	2.0
1	D	339	LYS	2.0
1	A	280	PRO	2.0
1	B	263	PRO	2.0
1	E	176	THR	2.0
1	H	5	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NH4	J	427	1/1	0.75	0.20	40,40,40,40	0
3	PO4	G	426	5/5	0.79	0.15	62,63,64,64	0
3	PO4	A	426	5/5	0.79	0.21	75,76,77,77	0
3	PO4	K	426	5/5	0.80	0.13	67,68,69,69	0
4	NH4	B	426	1/1	0.83	0.28	51,51,51,51	0
2	GLU	D	425	10/10	0.85	0.12	36,38,39,42	0
3	PO4	D	426	5/5	0.85	0.14	79,80,80,80	0
2	GLU	K	425	10/10	0.85	0.14	40,40,46,48	0
2	GLU	K	500	10/10	0.86	0.18	56,57,58,60	0
4	NH4	H	426	1/1	0.86	0.22	34,34,34,34	0
2	GLU	C	425	10/10	0.86	0.15	42,43,46,49	0
2	GLU	F	500	10/10	0.87	0.19	62,63,65,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GLU	J	500	10/10	0.88	0.12	47,48,54,55	0
2	GLU	E	425	10/10	0.88	0.13	37,38,43,45	0
2	GLU	F	425	10/10	0.89	0.13	31,34,44,45	0
2	GLU	G	500	10/10	0.89	0.14	42,42,46,50	0
2	GLU	I	500	10/10	0.89	0.13	50,51,55,55	0
3	PO4	J	426	5/5	0.89	0.12	62,62,63,64	0
2	GLU	I	425	10/10	0.89	0.12	38,39,41,44	0
2	GLU	E	500	10/10	0.89	0.12	39,42,47,49	0
2	GLU	A	500	10/10	0.89	0.13	43,45,46,46	0
2	GLU	B	425	10/10	0.89	0.12	35,36,49,51	0
2	GLU	L	500	10/10	0.90	0.13	52,53,53,54	0
2	GLU	D	500	10/10	0.90	0.10	43,46,46,49	0
4	NH4	A	427	1/1	0.90	0.28	17,17,17,17	0
2	GLU	B	500	10/10	0.91	0.10	35,37,38,39	0
2	GLU	L	425	10/10	0.91	0.12	49,49,52,53	0
2	GLU	A	425	10/10	0.91	0.12	28,29,32,34	0
2	GLU	H	500	10/10	0.91	0.12	50,53,53,54	0
3	PO4	F	426	4/5	0.91	0.13	71,71,72,72	0
2	GLU	C	500	10/10	0.91	0.12	42,43,46,48	0
4	NH4	L	426	1/1	0.91	0.15	44,44,44,44	0
2	GLU	H	425	10/10	0.92	0.10	34,36,41,42	0
2	GLU	G	425	10/10	0.92	0.09	28,30,33,33	0
3	PO4	I	427	5/5	0.92	0.10	61,62,62,62	0
3	PO4	C	426	5/5	0.92	0.12	57,58,58,58	0
2	GLU	J	425	10/10	0.92	0.10	36,37,43,43	0
4	NH4	F	427	1/1	0.93	0.24	41,41,41,41	0
3	PO4	I	426	5/5	0.95	0.08	56,56,57,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.