



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Mar 2, 2017 – 12:42 pm GMT

PDB ID : 5K12  
EMDB ID: : EMD-8194  
Title : Cryo-EM structure of glutamate dehydrogenase at 1.8 Å resolution  
Authors : Merk, A.; Bartesaghi, A.; Banerjee, S.; Falconieri, V.; Rao, P.; Earl, L.; Milne, J.; Subramaniam, S.  
Deposited on : 2016-05-17  
Resolution : 1.80 Å (reported)  
Based on PDB ID : 1NR7

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc29047

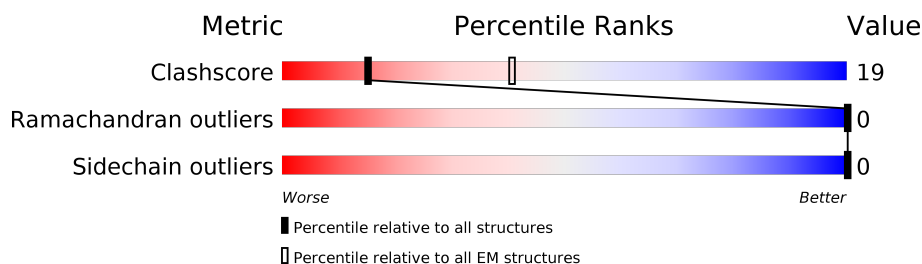
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 1.80 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)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	558	36% 16% 47%
1	B	558	36% 16% 47%
1	C	558	36% 16% 47%
1	D	558	36% 16% 47%
1	E	558	37% 16% 47%
1	F	558	36% 16% 47%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14856 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Glutamate dehydrogenase 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	294	Total	C	N	O	S	0	0
			2295	1445	409	429	12		
1	B	294	Total	C	N	O	S	0	0
			2295	1445	409	429	12		
1	C	294	Total	C	N	O	S	0	0
			2295	1445	409	429	12		
1	D	294	Total	C	N	O	S	0	0
			2295	1445	409	429	12		
1	E	294	Total	C	N	O	S	0	0
			2295	1445	409	429	12		
1	F	294	Total	C	N	O	S	0	0
			2295	1445	409	429	12		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	387	LYS	ASN	conflict	UNP P00366
B	387	LYS	ASN	conflict	UNP P00366
C	387	LYS	ASN	conflict	UNP P00366
D	387	LYS	ASN	conflict	UNP P00366
E	387	LYS	ASN	conflict	UNP P00366
F	387	LYS	ASN	conflict	UNP P00366

- Molecule 2 is water.

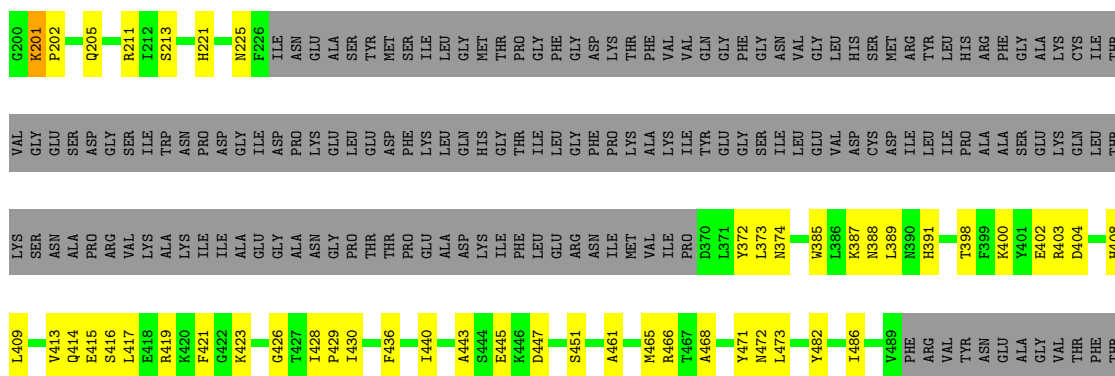
Mol	Chain	Residues	Atoms		AltConf
2	A	181	Total	O	0
			181	181	
2	B	182	Total	O	0
			182	182	
2	C	180	Total	O	0
			180	180	
2	D	181	Total	O	0
			181	181	

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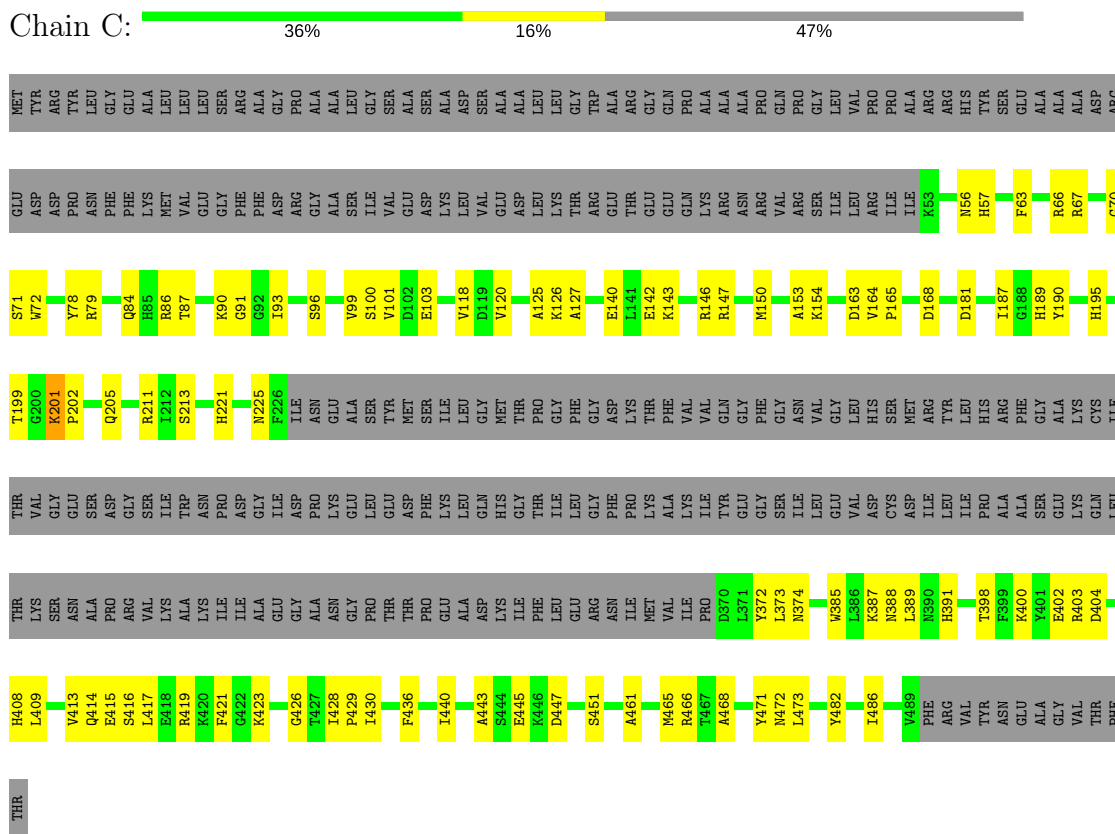
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Mol	Chain	Residues	Atoms		AltConf
2	E	181	Total 181	O 181	0
2	F	181	Total 181	O 181	0

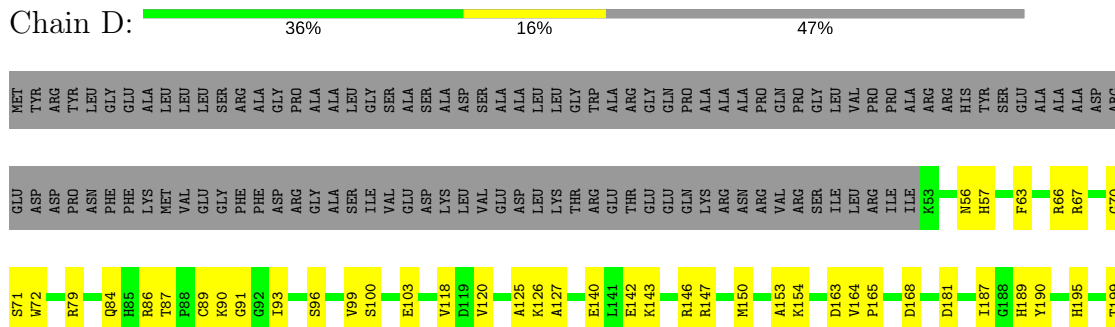


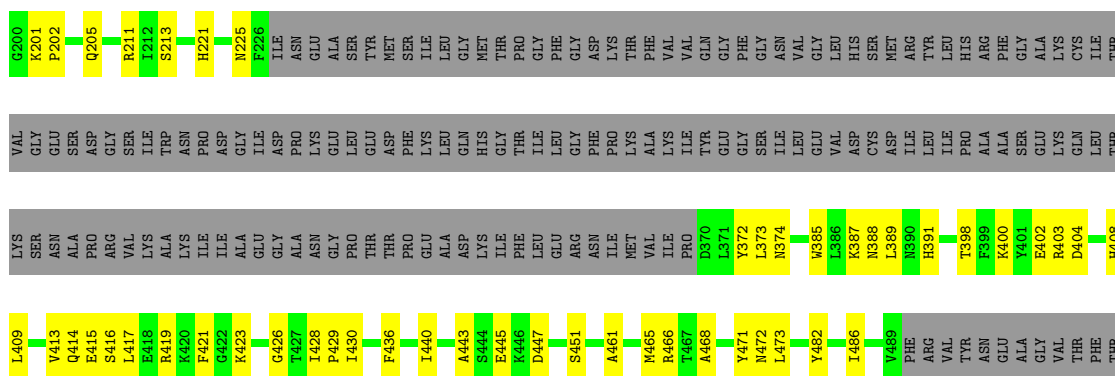


- Molecule 1: Glutamate dehydrogenase 1, mitochondrial

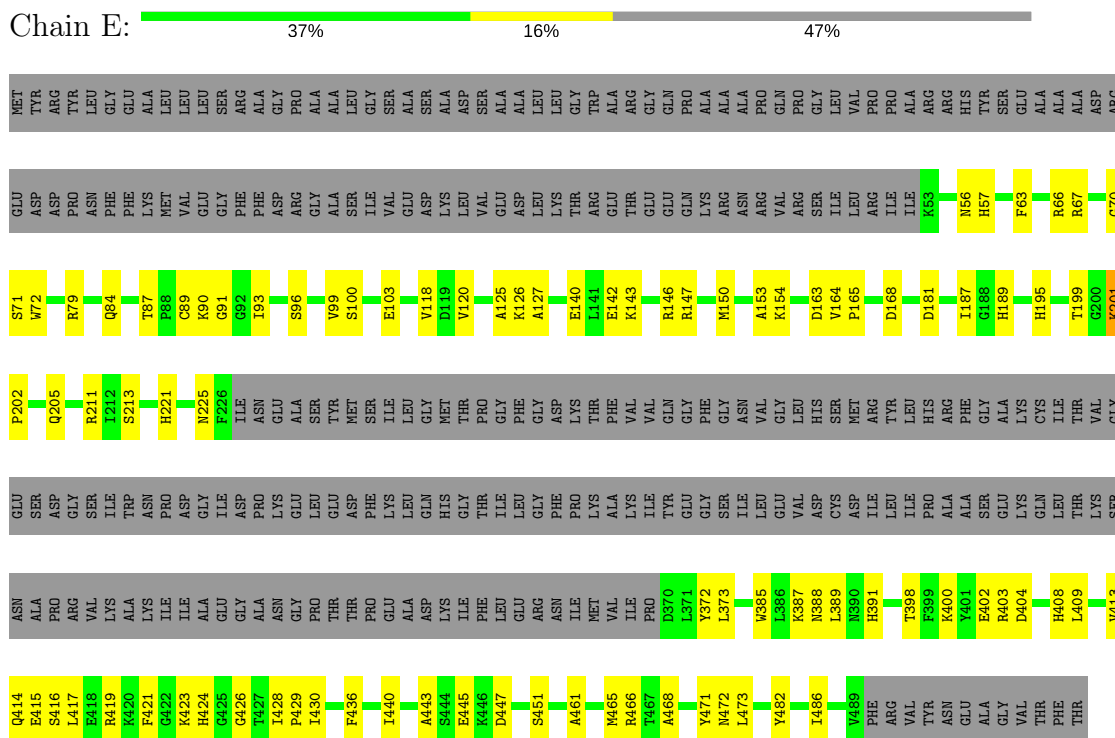


- Molecule 1: Glutamate dehydrogenase 1, mitochondrial

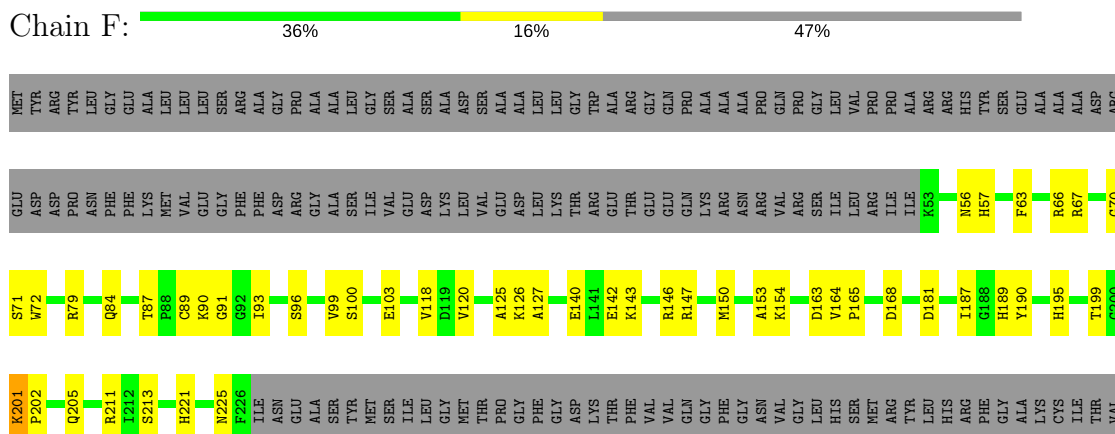




- Molecule 1: Glutamate dehydrogenase 1, mitochondrial



- Molecule 1: Glutamate dehydrogenase 1, mitochondrial



V413	SER	GLY
Q414	ASN	GLU
E415	ALA	SER
S416	PRO	ASP
L417	ARG	GLY
E418	VAL	SER
R419	LYS	ILE
K420	ALA	TRP
F421	LYS	ASN
G422	ILE	PRO
K423	ILE	ASP
H424	ALA	GLY
G425	GLU	ILE
G426	GLY	ASP
I427	ALA	PRO
I428	ASN	LYS
P429	GLY	GLU
I430	PRO	LEU
	THR	GLU
F436	THR	ASP
	PRO	PHE
I440	GLU	LYS
	ALA	LEU
A443	ASP	GLN
S444	LYS	HIS
E445	ILE	GLY
K446	PHE	THR
D447	LEU	ILE
	GLU	LEU
S451	ARG	GLY
	ASN	PHE
A461	ILE	PRO
	MET	LYS
M465	VAL	ALA
R466	ILE	LYS
T467	PRO	ILE
A468	D370	TYR
	L371	GLU
Y471	Y372	GLY
N472	L373	SER
L473		ILE
	W385	LEU
Y482	L386	GLU
	K387	VAL
I486	N388	ASP
	L389	CYS
V489	N390	ASP
PHE	H391	ILE
ARG		LEU
VAL	T398	ILE
TYR	F399	PRO
ASN	K400	ALA
GLU	Y401	ALA
ALA	E402	SER
GLY	R403	GLU
VAL	D404	LYS
THR		GLN
THR	H408	LEU
	L409	THR
		LYS



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	21818	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	78000	Depositor
Image detector	Not provided	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	A	0.43	0/2345	0.55	1/3166 (0.0%)
1	B	0.43	0/2345	0.55	1/3166 (0.0%)
1	C	0.43	0/2345	0.55	1/3166 (0.0%)
1	D	0.43	0/2345	0.55	0/3166
1	E	0.43	0/2345	0.55	1/3166 (0.0%)
1	F	0.43	0/2345	0.55	1/3166 (0.0%)
All	All	0.43	0/14070	0.55	5/18996 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	201	LYS	C-N-CD	5.02	138.94	128.40
1	A	201	LYS	C-N-CD	5.01	138.93	128.40
1	F	201	LYS	C-N-CD	5.01	138.92	128.40
1	E	201	LYS	C-N-CD	5.00	138.91	128.40
1	C	201	LYS	C-N-CD	5.00	138.90	128.40

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2295	0	2261	94	0
1	B	2295	0	2261	93	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2295	0	2261	93	0
1	D	2295	0	2261	92	0
1	E	2295	0	2261	89	0
1	F	2295	0	2261	92	0
2	A	181	0	0	18	0
2	B	182	0	0	20	0
2	C	180	0	0	18	0
2	D	181	0	0	20	0
2	E	181	0	0	16	0
2	F	181	0	0	16	0
All	All	14856	0	13566	512	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 19.

All (512) 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:B:142:GLU:O	1:B:146:ARG:HG3	1.62	0.99
1:D:142:GLU:O	1:D:146:ARG:HG3	1.62	0.99
1:A:142:GLU:O	1:A:146:ARG:HG3	1.62	0.99
1:C:142:GLU:O	1:C:146:ARG:HG3	1.62	0.99
1:E:142:GLU:O	1:E:146:ARG:HG3	1.62	0.98
1:F:142:GLU:O	1:F:146:ARG:HG3	1.62	0.98
1:E:90:LYS:HE3	2:E:721:HOH:O	1.76	0.85
1:F:90:LYS:HE3	2:F:721:HOH:O	1.76	0.85
1:B:90:LYS:HE3	2:B:722:HOH:O	1.76	0.85
1:D:90:LYS:HE3	2:D:721:HOH:O	1.76	0.85
1:E:201:LYS:HZ1	1:E:388:ASN:HD21	1.23	0.85
1:C:90:LYS:HE3	2:C:720:HOH:O	1.76	0.84
1:F:201:LYS:HZ1	1:F:388:ASN:HD21	1.23	0.84
1:A:90:LYS:HE3	2:A:722:HOH:O	1.76	0.84
1:C:201:LYS:HZ3	1:C:388:ASN:HD21	1.24	0.83
1:A:201:LYS:HZ3	1:A:388:ASN:HD21	1.24	0.83
1:F:211:ARG:NH2	2:F:603:HOH:O	2.13	0.82
1:E:211:ARG:NH2	2:E:603:HOH:O	2.13	0.82
1:B:211:ARG:NH2	2:B:603:HOH:O	2.13	0.81
1:D:211:ARG:NH2	2:D:603:HOH:O	2.13	0.81
1:A:211:ARG:NH2	2:A:603:HOH:O	2.13	0.80
1:C:211:ARG:NH2	2:C:603:HOH:O	2.13	0.80
1:E:201:LYS:NZ	1:E:388:ASN:HD21	1.81	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:201:LYS:NZ	1:F:388:ASN:HD21	1.81	0.78
1:A:201:LYS:NZ	1:A:388:ASN:HD21	1.81	0.78
1:C:201:LYS:NZ	1:C:388:ASN:HD21	1.81	0.78
1:B:201:LYS:HZ3	1:B:388:ASN:HD21	1.29	0.77
1:D:201:LYS:HZ3	1:D:388:ASN:HD21	1.29	0.77
1:A:201:LYS:NZ	1:A:388:ASN:ND2	2.33	0.76
1:C:201:LYS:NZ	1:C:388:ASN:ND2	2.33	0.76
1:B:201:LYS:NZ	1:B:388:ASN:HD21	1.81	0.76
1:D:201:LYS:NZ	1:D:388:ASN:HD21	1.81	0.76
1:B:201:LYS:NZ	1:B:388:ASN:ND2	2.33	0.76
1:D:201:LYS:NZ	1:D:388:ASN:ND2	2.33	0.76
1:E:201:LYS:NZ	1:E:388:ASN:ND2	2.33	0.75
1:F:150:MET:HE3	2:F:775:HOH:O	1.86	0.75
1:F:201:LYS:NZ	1:F:388:ASN:ND2	2.33	0.75
1:E:150:MET:HE3	2:E:775:HOH:O	1.86	0.75
1:A:414:GLN:HG2	1:A:429:PRO:HD2	1.69	0.75
1:C:414:GLN:HG2	1:C:429:PRO:HD2	1.69	0.75
1:F:79:ARG:NE	1:F:163:ASP:OD2	2.20	0.75
1:E:79:ARG:NE	1:E:163:ASP:OD2	2.20	0.74
1:A:211:ARG:O	2:A:601:HOH:O	2.05	0.74
1:B:211:ARG:O	2:B:601:HOH:O	2.05	0.74
1:A:150:MET:CE	2:A:775:HOH:O	2.35	0.74
1:D:211:ARG:O	2:D:601:HOH:O	2.05	0.74
1:B:142:GLU:OE1	2:B:602:HOH:O	2.06	0.74
1:C:211:ARG:O	2:C:601:HOH:O	2.05	0.74
1:D:142:GLU:OE1	2:D:602:HOH:O	2.06	0.74
1:C:150:MET:CE	2:C:774:HOH:O	2.35	0.74
1:C:79:ARG:NE	1:C:163:ASP:OD2	2.20	0.74
1:F:150:MET:CE	2:F:775:HOH:O	2.35	0.73
1:E:150:MET:CE	2:E:775:HOH:O	2.35	0.73
1:F:211:ARG:O	2:F:601:HOH:O	2.05	0.73
1:A:142:GLU:OE1	2:A:602:HOH:O	2.06	0.73
1:C:142:GLU:OE1	2:C:602:HOH:O	2.06	0.73
1:E:211:ARG:O	2:E:601:HOH:O	2.05	0.73
1:B:150:MET:CE	2:B:776:HOH:O	2.35	0.73
1:D:150:MET:CE	2:D:775:HOH:O	2.35	0.73
1:E:414:GLN:HG2	1:E:429:PRO:HD2	1.69	0.73
1:B:414:GLN:HG2	1:B:429:PRO:HD2	1.69	0.72
1:F:142:GLU:OE1	2:F:602:HOH:O	2.06	0.72
1:F:126:LYS:NZ	1:F:168:ASP:OD2	2.22	0.72
1:E:126:LYS:NZ	1:E:168:ASP:OD2	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:142:GLU:OE1	2:E:602:HOH:O	2.06	0.72
1:F:423:LYS:HD3	1:F:426:GLY:HA3	1.71	0.72
1:F:414:GLN:HG2	1:F:429:PRO:HD2	1.69	0.72
1:A:423:LYS:HD3	1:A:426:GLY:HA3	1.71	0.72
1:B:423:LYS:HD3	1:B:426:GLY:HA3	1.71	0.72
1:D:414:GLN:HG2	1:D:429:PRO:HD2	1.69	0.72
1:E:423:LYS:HD3	1:E:426:GLY:HA3	1.72	0.72
1:D:423:LYS:HD3	1:D:426:GLY:HA3	1.72	0.72
1:C:423:LYS:HD3	1:C:426:GLY:HA3	1.72	0.72
1:A:126:LYS:NZ	1:A:168:ASP:OD2	2.22	0.71
1:A:79:ARG:NE	1:A:163:ASP:OD2	2.20	0.71
1:C:126:LYS:NZ	1:C:168:ASP:OD2	2.22	0.71
1:C:90:LYS:NZ	1:C:199:THR:OG1	2.22	0.71
1:A:90:LYS:NZ	1:A:199:THR:OG1	2.22	0.71
1:B:201:LYS:HZ1	1:B:388:ASN:ND2	1.88	0.71
1:D:201:LYS:HZ1	1:D:388:ASN:ND2	1.88	0.70
1:D:126:LYS:NZ	1:D:168:ASP:OD2	2.22	0.70
1:D:79:ARG:NE	1:D:163:ASP:OD2	2.20	0.70
1:B:126:LYS:NZ	1:B:168:ASP:OD2	2.22	0.70
1:B:79:ARG:NE	1:B:163:ASP:OD2	2.20	0.70
1:E:90:LYS:NZ	1:E:199:THR:OG1	2.22	0.70
1:A:150:MET:HE3	2:A:775:HOH:O	1.90	0.69
1:F:90:LYS:NZ	1:F:199:THR:OG1	2.22	0.69
1:B:90:LYS:NZ	1:B:199:THR:OG1	2.22	0.69
1:D:90:LYS:NZ	1:D:199:THR:OG1	2.22	0.69
1:F:415:GLU:O	1:F:419:ARG:HG2	1.93	0.68
1:E:415:GLU:O	1:E:419:ARG:HG2	1.93	0.68
1:C:150:MET:HE3	2:C:774:HOH:O	1.92	0.68
1:D:415:GLU:O	1:D:419:ARG:HG2	1.93	0.68
1:B:415:GLU:O	1:B:419:ARG:HG2	1.93	0.68
1:A:415:GLU:O	1:A:419:ARG:HG2	1.93	0.67
1:C:415:GLU:O	1:C:419:ARG:HG2	1.93	0.67
1:E:221:HIS:O	1:E:225:ASN:ND2	2.29	0.66
1:F:221:HIS:O	1:F:225:ASN:ND2	2.29	0.66
1:C:63:PHE:HB2	1:C:147:ARG:HE	1.61	0.66
1:A:63:PHE:HB2	1:A:147:ARG:HE	1.61	0.66
1:B:63:PHE:HB2	1:B:147:ARG:HE	1.61	0.66
1:D:63:PHE:HB2	1:D:147:ARG:HE	1.61	0.65
1:A:221:HIS:O	1:A:225:ASN:ND2	2.29	0.65
1:E:63:PHE:HB2	1:E:147:ARG:HE	1.61	0.65
1:F:63:PHE:HB2	1:F:147:ARG:HE	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:HIS:O	1:C:225:ASN:ND2	2.29	0.65
1:D:221:HIS:O	1:D:225:ASN:ND2	2.29	0.65
1:B:221:HIS:O	1:B:225:ASN:ND2	2.29	0.65
1:C:201:LYS:HZ1	1:C:388:ASN:ND2	1.94	0.64
1:A:201:LYS:HZ1	1:A:388:ASN:ND2	1.94	0.64
1:D:100:SER:OG	1:D:103:GLU:HG2	1.98	0.64
1:A:100:SER:OG	1:A:103:GLU:HG2	1.98	0.64
1:B:100:SER:OG	1:B:103:GLU:HG2	1.98	0.64
1:C:100:SER:OG	1:C:103:GLU:HG2	1.97	0.64
1:F:146:ARG:NH1	1:F:181:ASP:OD2	2.32	0.63
1:E:146:ARG:NH1	1:E:181:ASP:OD2	2.32	0.63
1:D:150:MET:HE3	2:D:775:HOH:O	1.98	0.63
1:B:150:MET:HE3	2:B:776:HOH:O	1.98	0.63
1:B:146:ARG:NH1	1:B:181:ASP:OD2	2.32	0.63
1:D:146:ARG:NH1	1:D:181:ASP:OD2	2.32	0.63
1:E:100:SER:OG	1:E:103:GLU:HG2	1.98	0.62
1:B:414:GLN:HE21	1:B:428:ILE:HA	1.64	0.62
1:F:100:SER:OG	1:F:103:GLU:HG2	1.98	0.62
1:A:146:ARG:NH1	1:A:181:ASP:OD2	2.32	0.62
1:C:146:ARG:NH1	1:C:181:ASP:OD2	2.32	0.62
1:D:414:GLN:HE21	1:D:428:ILE:HA	1.64	0.62
1:A:414:GLN:HE21	1:A:428:ILE:HA	1.64	0.62
1:B:189:HIS:HB3	2:B:761:HOH:O	2.00	0.62
1:C:414:GLN:HE21	1:C:428:ILE:HA	1.64	0.62
1:D:189:HIS:HB3	2:D:760:HOH:O	1.99	0.62
1:A:189:HIS:HB3	2:A:760:HOH:O	1.99	0.62
1:C:189:HIS:HB3	2:C:759:HOH:O	1.99	0.62
1:E:201:LYS:HZ2	1:E:388:ASN:ND2	1.96	0.62
1:F:201:LYS:HZ2	1:F:388:ASN:ND2	1.96	0.61
1:E:90:LYS:HD2	1:E:164:VAL:O	2.00	0.61
1:F:90:LYS:HD2	1:F:164:VAL:O	2.01	0.61
1:A:90:LYS:HD2	1:A:164:VAL:O	2.00	0.61
1:E:414:GLN:HE21	1:E:428:ILE:HA	1.64	0.61
1:F:189:HIS:HB3	2:F:760:HOH:O	1.99	0.61
1:C:90:LYS:HD2	1:C:164:VAL:O	2.00	0.61
1:E:189:HIS:HB3	2:E:760:HOH:O	1.99	0.61
1:F:414:GLN:HE21	1:F:428:ILE:HA	1.64	0.61
1:D:90:LYS:HD2	1:D:164:VAL:O	2.00	0.60
1:B:90:LYS:HD2	1:B:164:VAL:O	2.01	0.60
1:E:202:PRO:HD2	1:E:205:GLN:HB2	1.83	0.60
1:F:202:PRO:HD2	1:F:205:GLN:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:PRO:HD2	1:A:205:GLN:HB2	1.83	0.60
1:C:202:PRO:HD2	1:C:205:GLN:HB2	1.83	0.60
1:A:195:HIS:HE1	1:A:391:HIS:CD2	2.21	0.59
1:C:195:HIS:HE1	1:C:391:HIS:CD2	2.21	0.59
1:B:91:GLY:O	1:B:165:PRO:HA	2.03	0.58
1:B:195:HIS:HE1	1:B:391:HIS:CD2	2.21	0.58
1:D:91:GLY:O	1:D:165:PRO:HA	2.03	0.58
1:D:195:HIS:HE1	1:D:391:HIS:CD2	2.21	0.58
1:F:91:GLY:O	1:F:165:PRO:HA	2.03	0.58
1:E:91:GLY:O	1:E:165:PRO:HA	2.03	0.58
1:E:195:HIS:HE1	1:E:391:HIS:CD2	2.21	0.58
1:F:195:HIS:HE1	1:F:391:HIS:CD2	2.21	0.58
1:B:202:PRO:HD2	1:B:205:GLN:HB2	1.83	0.58
1:D:202:PRO:HD2	1:D:205:GLN:HB2	1.83	0.58
1:C:91:GLY:O	1:C:165:PRO:HA	2.03	0.58
1:E:56:ASN:OD1	1:E:57:HIS:N	2.37	0.58
1:B:56:ASN:OD1	1:B:57:HIS:N	2.37	0.58
1:D:56:ASN:OD1	1:D:57:HIS:N	2.37	0.58
1:F:56:ASN:OD1	1:F:57:HIS:N	2.37	0.58
1:A:372:TYR:HD2	1:A:373:LEU:HD12	1.69	0.58
1:A:91:GLY:O	1:A:165:PRO:HA	2.03	0.58
1:C:372:TYR:HD2	1:C:373:LEU:HD12	1.69	0.58
1:B:372:TYR:HD2	1:B:373:LEU:HD12	1.69	0.57
1:C:56:ASN:OD1	1:C:57:HIS:N	2.37	0.57
1:E:372:TYR:HD2	1:E:373:LEU:HD12	1.69	0.57
1:F:372:TYR:HD2	1:F:373:LEU:HD12	1.69	0.57
1:A:56:ASN:OD1	1:A:57:HIS:N	2.37	0.57
1:D:372:TYR:HD2	1:D:373:LEU:HD12	1.69	0.57
1:D:387:LYS:HD2	1:D:445:GLU:OE2	2.04	0.57
1:B:387:LYS:HD2	1:B:445:GLU:OE2	2.04	0.57
1:A:471:TYR:HB3	1:A:473:LEU:HD12	1.87	0.57
1:C:471:TYR:HB3	1:C:473:LEU:HD12	1.87	0.57
1:D:471:TYR:HB3	1:D:473:LEU:HD12	1.87	0.57
1:B:471:TYR:HB3	1:B:473:LEU:HD12	1.87	0.57
1:C:387:LYS:HD2	1:C:445:GLU:OE2	2.04	0.57
1:E:471:TYR:HB3	1:E:473:LEU:HD12	1.87	0.57
1:F:471:TYR:HB3	1:F:473:LEU:HD12	1.87	0.57
1:E:387:LYS:HD2	1:E:445:GLU:OE2	2.04	0.56
1:F:387:LYS:HD2	1:F:445:GLU:OE2	2.04	0.56
1:A:387:LYS:HD2	1:A:445:GLU:OE2	2.04	0.56
1:A:79:ARG:HH11	1:A:127:ALA:HB2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:ARG:HH11	1:C:127:ALA:HB2	1.70	0.56
1:D:79:ARG:HH11	1:D:127:ALA:HB2	1.70	0.55
1:F:79:ARG:HH11	1:F:127:ALA:HB2	1.70	0.55
1:B:79:ARG:HH11	1:B:127:ALA:HB2	1.70	0.55
1:E:79:ARG:HH11	1:E:127:ALA:HB2	1.70	0.55
1:A:451:SER:HB2	1:B:400:LYS:HB3	1.89	0.54
1:B:190:TYR:OH	1:E:154:LYS:O	2.15	0.54
1:B:87:THR:HG22	2:B:658:HOH:O	2.07	0.54
1:C:87:THR:HG22	2:C:658:HOH:O	2.07	0.54
1:D:87:THR:HG22	2:D:658:HOH:O	2.07	0.54
1:A:87:THR:HG22	2:A:657:HOH:O	2.07	0.54
1:E:403:ARG:NE	2:E:616:HOH:O	2.41	0.54
1:F:403:ARG:NE	2:F:616:HOH:O	2.41	0.54
1:F:87:THR:HG22	2:F:657:HOH:O	2.07	0.54
1:C:403:ARG:NE	2:C:616:HOH:O	2.41	0.53
1:D:403:ARG:NE	2:D:616:HOH:O	2.41	0.53
1:E:87:THR:HG22	2:E:658:HOH:O	2.07	0.53
1:A:403:ARG:NE	2:A:616:HOH:O	2.41	0.53
1:B:403:ARG:NE	2:B:616:HOH:O	2.41	0.53
1:C:153:ALA:HB1	1:C:187:ILE:HG13	1.90	0.53
1:A:153:ALA:HB1	1:A:187:ILE:HG13	1.90	0.53
1:B:451:SER:HB2	1:F:400:LYS:HB3	1.89	0.53
1:E:153:ALA:HB1	1:E:187:ILE:HG13	1.90	0.53
1:F:153:ALA:HB1	1:F:187:ILE:HG13	1.90	0.52
1:D:140:GLU:OE1	1:D:143:LYS:HD2	2.10	0.52
1:B:140:GLU:OE1	1:B:143:LYS:HD2	2.10	0.52
1:A:140:GLU:OE1	1:A:143:LYS:HD2	2.10	0.52
1:B:153:ALA:HB1	1:B:187:ILE:HG13	1.90	0.52
1:C:140:GLU:OE1	1:C:143:LYS:HD2	2.10	0.52
1:E:140:GLU:OE1	1:E:143:LYS:HD2	2.10	0.52
1:D:153:ALA:HB1	1:D:187:ILE:HG13	1.90	0.51
1:C:451:SER:HB2	1:D:400:LYS:HB3	1.92	0.51
1:F:140:GLU:OE1	1:F:143:LYS:HD2	2.10	0.51
1:E:398:THR:HG22	1:E:402:GLU:HG2	1.92	0.51
1:F:90:LYS:HZ3	1:F:164:VAL:HG12	1.74	0.51
1:B:398:THR:HG22	1:B:402:GLU:HG2	1.92	0.51
1:C:400:LYS:HB3	1:E:451:SER:HB2	1.92	0.51
1:F:398:THR:HG22	1:F:402:GLU:HG2	1.92	0.51
1:A:429:PRO:HA	1:B:416:SER:HB3	1.92	0.51
1:D:190:TYR:OH	1:F:154:LYS:O	2.18	0.51
1:D:398:THR:HG22	1:D:402:GLU:HG2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:LYS:HB3	1:F:451:SER:HB2	1.92	0.51
1:D:187:ILE:HG23	2:D:766:HOH:O	2.11	0.51
1:B:187:ILE:HG23	2:B:767:HOH:O	2.11	0.51
1:F:187:ILE:HG23	2:F:766:HOH:O	2.11	0.50
1:E:187:ILE:HG23	2:E:767:HOH:O	2.11	0.50
1:E:90:LYS:HZ3	1:E:164:VAL:HG12	1.75	0.50
1:A:398:THR:HG22	1:A:402:GLU:HG2	1.92	0.50
1:C:398:THR:HG22	1:C:402:GLU:HG2	1.92	0.50
1:C:187:ILE:HG23	2:C:765:HOH:O	2.11	0.50
1:D:154:LYS:O	1:F:190:TYR:OH	2.18	0.50
1:F:436:PHE:CZ	1:F:440:ILE:HD11	2.47	0.50
1:A:187:ILE:HG23	2:A:766:HOH:O	2.11	0.50
1:B:142:GLU:O	1:B:146:ARG:CG	2.50	0.50
1:E:436:PHE:CZ	1:E:440:ILE:HD11	2.47	0.50
1:A:436:PHE:CG	1:B:408:HIS:HB3	2.47	0.50
1:C:142:GLU:O	1:C:146:ARG:CG	2.50	0.50
1:D:436:PHE:CZ	1:D:440:ILE:HD11	2.47	0.50
1:A:429:PRO:HA	1:B:416:SER:CB	2.42	0.50
1:B:436:PHE:CZ	1:B:440:ILE:HD11	2.47	0.50
1:D:451:SER:HB2	1:E:400:LYS:HB3	1.93	0.50
1:D:142:GLU:O	1:D:146:ARG:CG	2.50	0.49
1:E:430:ILE:HD12	2:E:710:HOH:O	2.13	0.49
1:B:482:TYR:O	1:B:486:ILE:HD12	2.12	0.49
1:F:430:ILE:HD12	2:F:710:HOH:O	2.13	0.49
1:A:90:LYS:HZ3	1:A:164:VAL:HG12	1.76	0.49
1:C:372:TYR:CD2	1:C:373:LEU:HD12	2.48	0.49
1:C:482:TYR:O	1:C:486:ILE:HD12	2.12	0.49
1:D:482:TYR:O	1:D:486:ILE:HD12	2.12	0.49
1:B:150:MET:HE2	2:B:776:HOH:O	2.08	0.49
1:C:436:PHE:CZ	1:C:440:ILE:HD11	2.47	0.49
1:E:482:TYR:O	1:E:486:ILE:HD12	2.12	0.49
1:A:372:TYR:CD2	1:A:373:LEU:HD12	2.48	0.48
1:A:436:PHE:CZ	1:A:440:ILE:HD11	2.47	0.48
1:A:482:TYR:O	1:A:486:ILE:HD12	2.12	0.48
1:A:436:PHE:HB2	1:B:408:HIS:CD2	2.48	0.48
1:C:90:LYS:HZ3	1:C:164:VAL:HG12	1.76	0.48
1:E:372:TYR:CD2	1:E:373:LEU:HD12	2.48	0.48
1:F:372:TYR:CD2	1:F:373:LEU:HD12	2.48	0.48
1:A:416:SER:HB3	1:F:429:PRO:HA	1.95	0.48
1:F:482:TYR:O	1:F:486:ILE:HD12	2.12	0.48
1:A:66:ARG:HD3	1:A:72:TRP:CZ2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:ILE:HD12	2:B:711:HOH:O	2.13	0.48
1:C:66:ARG:HD3	1:C:72:TRP:CZ2	2.48	0.48
1:D:150:MET:HE2	2:D:775:HOH:O	2.08	0.48
1:D:430:ILE:HD12	2:D:710:HOH:O	2.13	0.48
1:A:430:ILE:HD12	2:A:710:HOH:O	2.13	0.48
1:D:404:ASP:O	1:D:408:HIS:ND1	2.32	0.48
1:C:430:ILE:HD12	2:C:709:HOH:O	2.13	0.48
1:B:436:PHE:CG	1:F:408:HIS:HB3	2.49	0.48
1:C:404:ASP:O	1:C:408:HIS:ND1	2.32	0.48
1:E:66:ARG:HD3	1:E:72:TRP:CZ2	2.48	0.48
1:B:404:ASP:O	1:B:408:HIS:ND1	2.32	0.48
1:F:66:ARG:HD3	1:F:72:TRP:CZ2	2.48	0.48
1:A:404:ASP:O	1:A:408:HIS:ND1	2.32	0.48
1:A:190:TYR:OH	1:C:154:LYS:O	2.18	0.47
1:D:66:ARG:HD3	1:D:72:TRP:CZ2	2.48	0.47
1:B:56:ASN:HD22	1:B:84:GLN:H	1.63	0.47
1:B:66:ARG:HD3	1:B:72:TRP:CZ2	2.48	0.47
1:C:416:SER:HB3	1:E:429:PRO:HA	1.97	0.47
1:D:372:TYR:CD2	1:D:373:LEU:HD12	2.48	0.47
1:D:56:ASN:HD22	1:D:84:GLN:N	2.12	0.47
1:A:56:ASN:HD22	1:A:84:GLN:N	2.12	0.47
1:C:56:ASN:HD22	1:C:84:GLN:N	2.12	0.47
1:D:56:ASN:HD22	1:D:84:GLN:H	1.63	0.47
1:A:56:ASN:HD22	1:A:84:GLN:H	1.63	0.47
1:B:372:TYR:CD2	1:B:373:LEU:HD12	2.48	0.47
1:B:56:ASN:HD22	1:B:84:GLN:N	2.12	0.47
1:F:56:ASN:HD22	1:F:84:GLN:H	1.63	0.47
1:B:56:ASN:CG	1:B:57:HIS:HD1	2.18	0.47
1:C:56:ASN:HD22	1:C:84:GLN:H	1.63	0.47
1:D:56:ASN:CG	1:D:57:HIS:HD1	2.18	0.47
1:E:56:ASN:HD22	1:E:84:GLN:H	1.63	0.47
1:E:56:ASN:HD22	1:E:84:GLN:N	2.12	0.47
1:A:154:LYS:O	1:C:190:TYR:OH	2.20	0.46
1:F:56:ASN:HD22	1:F:84:GLN:N	2.12	0.46
1:A:56:ASN:CG	1:A:57:HIS:HD1	2.18	0.46
1:D:429:PRO:HA	1:E:416:SER:HB3	1.96	0.46
1:C:56:ASN:CG	1:C:57:HIS:HD1	2.18	0.46
1:C:429:PRO:HA	1:D:416:SER:HB3	1.97	0.46
1:E:430:ILE:HG12	2:E:631:HOH:O	2.16	0.46
1:F:430:ILE:HG12	2:F:631:HOH:O	2.16	0.46
1:D:430:ILE:HG12	2:D:631:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:ILE:HG12	2:B:631:HOH:O	2.16	0.45
1:F:56:ASN:CG	1:F:57:HIS:HD1	2.18	0.45
1:B:436:PHE:HB2	1:F:408:HIS:CD2	2.51	0.45
1:C:430:ILE:HG12	2:C:631:HOH:O	2.16	0.45
1:E:56:ASN:CG	1:E:57:HIS:HD1	2.18	0.45
1:A:430:ILE:HG12	2:A:631:HOH:O	2.16	0.45
1:B:461:ALA:O	1:B:465:MET:HG3	2.17	0.45
1:D:461:ALA:O	1:D:465:MET:HG3	2.17	0.45
1:C:461:ALA:O	1:C:465:MET:HG3	2.17	0.45
1:E:461:ALA:O	1:E:465:MET:HG3	2.17	0.45
1:A:461:ALA:O	1:A:465:MET:HG3	2.17	0.45
1:D:409:LEU:O	1:D:413:VAL:HG23	2.17	0.45
1:D:423:LYS:HD3	1:D:426:GLY:CA	2.44	0.45
1:E:421:PHE:CD2	1:E:423:LYS:HE2	2.52	0.45
1:F:421:PHE:CD2	1:F:423:LYS:HE2	2.52	0.45
1:F:461:ALA:O	1:F:465:MET:HG3	2.17	0.45
1:A:409:LEU:O	1:A:413:VAL:HG23	2.17	0.45
1:B:409:LEU:O	1:B:413:VAL:HG23	2.17	0.45
1:B:423:LYS:HD3	1:B:426:GLY:CA	2.44	0.45
1:C:409:LEU:O	1:C:413:VAL:HG23	2.17	0.45
1:E:91:GLY:HA3	1:E:125:ALA:O	2.17	0.45
1:E:142:GLU:HG2	1:E:146:ARG:HD2	1.99	0.45
1:B:400:LYS:HA	1:B:403:ARG:HG2	1.99	0.44
1:B:414:GLN:NE2	1:B:428:ILE:HA	2.31	0.44
1:D:400:LYS:HA	1:D:403:ARG:HG2	1.99	0.44
1:F:142:GLU:HG2	1:F:146:ARG:HD2	1.99	0.44
1:A:408:HIS:CD2	1:F:436:PHE:HB2	2.53	0.44
1:B:142:GLU:HG2	1:B:146:ARG:HD2	1.99	0.44
1:D:414:GLN:NE2	1:D:428:ILE:HA	2.31	0.44
1:F:91:GLY:HA3	1:F:125:ALA:O	2.18	0.44
1:A:142:GLU:HG2	1:A:146:ARG:HD2	1.99	0.44
1:C:142:GLU:HG2	1:C:146:ARG:HD2	1.99	0.44
1:E:213:SER:HB2	2:E:642:HOH:O	2.17	0.44
1:E:423:LYS:HD3	1:E:426:GLY:CA	2.44	0.44
1:E:414:GLN:NE2	1:E:428:ILE:HA	2.31	0.44
1:F:213:SER:HB2	2:F:642:HOH:O	2.17	0.44
1:A:118:VAL:HG23	1:A:120:VAL:HG23	2.00	0.44
1:A:436:PHE:HB2	1:B:408:HIS:HD2	1.81	0.44
1:B:398:THR:O	1:B:402:GLU:HG2	2.18	0.44
1:B:421:PHE:CD2	1:B:423:LYS:HE2	2.52	0.44
1:C:118:VAL:HG23	1:C:120:VAL:HG23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:142:GLU:HG2	1:D:146:ARG:HD2	1.99	0.44
1:E:417:LEU:HD12	1:E:429:PRO:HG2	1.99	0.44
1:F:423:LYS:HD3	1:F:426:GLY:CA	2.44	0.44
1:F:417:LEU:HD12	1:F:429:PRO:HG2	1.99	0.44
1:C:400:LYS:HA	1:C:403:ARG:HG2	1.99	0.44
1:C:408:HIS:CD2	1:E:436:PHE:HB2	2.53	0.44
1:C:414:GLN:NE2	1:C:428:ILE:HA	2.31	0.44
1:D:421:PHE:CD2	1:D:423:LYS:HE2	2.52	0.44
1:A:400:LYS:HA	1:A:403:ARG:HG2	1.99	0.44
1:A:417:LEU:HD12	1:A:429:PRO:HG2	1.99	0.44
1:C:213:SER:HB2	2:C:642:HOH:O	2.17	0.44
1:D:398:THR:O	1:D:402:GLU:HG2	2.18	0.44
1:F:142:GLU:O	1:F:146:ARG:CG	2.50	0.44
1:F:414:GLN:NE2	1:F:428:ILE:HA	2.31	0.44
1:A:91:GLY:HA3	1:A:125:ALA:O	2.18	0.44
1:A:414:GLN:NE2	1:A:428:ILE:HA	2.31	0.44
1:B:91:GLY:HA3	1:B:125:ALA:O	2.18	0.44
1:C:403:ARG:NH2	2:C:616:HOH:O	2.51	0.44
1:A:213:SER:HB2	2:A:642:HOH:O	2.17	0.44
1:A:398:THR:O	1:A:402:GLU:HG2	2.18	0.44
1:A:403:ARG:NH2	2:A:616:HOH:O	2.51	0.44
1:A:408:HIS:HB3	1:F:436:PHE:CG	2.53	0.44
1:A:416:SER:CB	1:F:429:PRO:HA	2.47	0.44
1:A:421:PHE:CD2	1:A:423:LYS:HE2	2.52	0.44
1:B:213:SER:HB2	2:B:641:HOH:O	2.17	0.44
1:C:398:THR:O	1:C:402:GLU:HG2	2.18	0.44
1:C:423:LYS:HD3	1:C:426:GLY:CA	2.44	0.44
1:D:213:SER:HB2	2:D:642:HOH:O	2.17	0.44
1:D:91:GLY:HA3	1:D:125:ALA:O	2.18	0.44
1:F:409:LEU:O	1:F:413:VAL:HG23	2.17	0.44
1:A:423:LYS:HD3	1:A:426:GLY:CA	2.44	0.43
1:C:91:GLY:HA3	1:C:125:ALA:O	2.18	0.43
1:C:408:HIS:HB3	1:E:436:PHE:CG	2.53	0.43
1:C:417:LEU:HD12	1:C:429:PRO:HG2	1.99	0.43
1:C:421:PHE:CD2	1:C:423:LYS:HE2	2.52	0.43
1:D:436:PHE:HB2	1:E:408:HIS:CD2	2.53	0.43
1:E:409:LEU:O	1:E:413:VAL:HG23	2.17	0.43
1:B:466:ARG:HG3	2:B:717:HOH:O	2.18	0.43
1:D:466:ARG:HG3	2:D:716:HOH:O	2.18	0.43
1:F:385:TRP:CZ2	1:F:389:LEU:HD11	2.54	0.43
1:F:400:LYS:HA	1:F:403:ARG:HG2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:ILE:HD11	2:B:714:HOH:O	2.18	0.43
1:E:118:VAL:HG23	1:E:120:VAL:HG23	2.00	0.43
1:E:142:GLU:O	1:E:146:ARG:CG	2.50	0.43
1:E:385:TRP:CZ2	1:E:389:LEU:HD11	2.54	0.43
1:E:400:LYS:HA	1:E:403:ARG:HG2	1.99	0.43
1:E:398:THR:O	1:E:402:GLU:HG2	2.18	0.43
1:E:466:ARG:HG3	2:E:716:HOH:O	2.19	0.43
1:F:466:ARG:HG3	2:F:716:HOH:O	2.18	0.43
1:D:429:PRO:HA	1:E:416:SER:CB	2.48	0.43
1:F:118:VAL:HG23	1:F:120:VAL:HG23	2.00	0.43
1:C:385:TRP:CZ2	1:C:389:LEU:HD11	2.54	0.43
1:C:436:PHE:CG	1:D:408:HIS:HB3	2.54	0.43
1:D:417:LEU:HD12	1:D:429:PRO:HG2	1.99	0.43
1:E:93:ILE:HD11	2:E:713:HOH:O	2.18	0.43
1:F:398:THR:O	1:F:402:GLU:HG2	2.18	0.43
1:A:93:ILE:HG12	1:A:127:ALA:HB3	2.01	0.43
1:A:385:TRP:CZ2	1:A:389:LEU:HD11	2.54	0.43
1:A:67:ARG:HB2	1:A:71:SER:HB3	2.01	0.43
1:B:403:ARG:NH2	2:B:616:HOH:O	2.51	0.43
1:A:436:PHE:CD1	1:B:408:HIS:HB3	2.54	0.43
1:C:67:ARG:HB2	1:C:71:SER:HB3	2.01	0.43
1:C:93:ILE:HG12	1:C:127:ALA:HB3	2.01	0.43
1:D:385:TRP:CZ2	1:D:389:LEU:HD11	2.54	0.43
1:D:93:ILE:HD11	2:D:713:HOH:O	2.18	0.43
1:E:403:ARG:NH2	2:E:616:HOH:O	2.51	0.43
1:A:93:ILE:HD11	2:A:713:HOH:O	2.18	0.43
1:B:385:TRP:CZ2	1:B:389:LEU:HD11	2.54	0.43
1:B:417:LEU:HD12	1:B:429:PRO:HG2	1.99	0.43
1:C:93:ILE:HD11	2:C:711:HOH:O	2.18	0.43
1:A:66:ARG:NH1	1:A:70:GLY:O	2.52	0.43
1:C:66:ARG:NH1	1:C:70:GLY:O	2.52	0.43
1:F:403:ARG:NH2	2:F:616:HOH:O	2.51	0.43
1:F:93:ILE:HD11	2:F:713:HOH:O	2.18	0.43
1:D:118:VAL:HG23	1:D:120:VAL:HG23	2.00	0.43
1:D:403:ARG:NH2	2:D:616:HOH:O	2.51	0.43
1:D:436:PHE:CG	1:E:408:HIS:HB3	2.54	0.43
1:D:67:ARG:HB2	1:D:71:SER:HB3	2.01	0.43
1:B:66:ARG:NH1	1:B:70:GLY:O	2.52	0.42
1:B:67:ARG:HB2	1:B:71:SER:HB3	2.01	0.42
1:C:416:SER:CB	1:E:429:PRO:HA	2.48	0.42
1:C:429:PRO:HA	1:D:416:SER:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:ARG:NH1	1:D:70:GLY:O	2.52	0.42
1:B:118:VAL:HG23	1:B:120:VAL:HG23	2.00	0.42
1:B:96:SER:HB3	1:B:99:VAL:HG13	2.02	0.42
1:D:96:SER:HB3	1:D:99:VAL:HG13	2.02	0.42
1:E:66:ARG:NH1	1:E:70:GLY:O	2.52	0.42
1:D:443:ALA:HA	1:D:447:ASP:OD2	2.20	0.42
1:F:66:ARG:NH1	1:F:70:GLY:O	2.52	0.42
1:B:443:ALA:HA	1:B:447:ASP:OD2	2.20	0.42
1:C:436:PHE:HB2	1:D:408:HIS:CD2	2.53	0.42
1:E:443:ALA:HA	1:E:447:ASP:OD2	2.20	0.42
1:D:374:ASN:O	2:D:604:HOH:O	2.22	0.42
1:F:443:ALA:HA	1:F:447:ASP:OD2	2.20	0.42
1:A:96:SER:HB3	1:A:99:VAL:HG13	2.02	0.42
1:A:96:SER:O	1:A:99:VAL:HG22	2.20	0.42
1:C:96:SER:HB3	1:C:99:VAL:HG13	2.02	0.42
1:D:150:MET:HG2	1:D:154:LYS:NZ	2.35	0.42
1:B:150:MET:HG2	1:B:154:LYS:NZ	2.35	0.42
1:C:96:SER:O	1:C:99:VAL:HG22	2.20	0.42
1:B:429:PRO:HA	1:F:416:SER:HB3	2.01	0.42
1:A:466:ARG:HG3	2:A:716:HOH:O	2.19	0.42
1:A:468:ALA:O	1:A:472:ASN:HA	2.20	0.42
1:C:466:ARG:HG3	2:C:715:HOH:O	2.19	0.42
1:C:468:ALA:O	1:C:472:ASN:HA	2.20	0.42
1:E:150:MET:HG2	1:E:154:LYS:NZ	2.35	0.42
1:A:414:GLN:O	1:A:417:LEU:N	2.53	0.42
1:B:374:ASN:O	2:B:604:HOH:O	2.22	0.42
1:E:67:ARG:HB2	1:E:71:SER:HB3	2.01	0.42
1:E:96:SER:O	1:E:99:VAL:HG22	2.20	0.42
1:F:150:MET:HG2	1:F:154:LYS:NZ	2.35	0.42
1:F:67:ARG:HB2	1:F:71:SER:HB3	2.01	0.42
1:B:93:ILE:HG12	1:B:127:ALA:HB3	2.01	0.41
1:A:154:LYS:HE2	1:E:84:GLN:HE22	1.84	0.41
1:C:414:GLN:O	1:C:417:LEU:N	2.53	0.41
1:D:414:GLN:O	1:D:417:LEU:N	2.53	0.41
1:B:414:GLN:O	1:B:417:LEU:N	2.53	0.41
1:D:93:ILE:HG12	1:D:127:ALA:HB3	2.01	0.41
1:E:404:ASP:O	1:E:408:HIS:ND1	2.32	0.41
1:E:468:ALA:O	1:E:472:ASN:HA	2.20	0.41
1:F:468:ALA:O	1:F:472:ASN:HA	2.20	0.41
1:F:96:SER:O	1:F:99:VAL:HG22	2.20	0.41
1:A:443:ALA:HA	1:A:447:ASP:OD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:468:ALA:O	1:D:472:ASN:HA	2.20	0.41
1:E:89:CYS:HB3	1:E:125:ALA:HB2	2.02	0.41
1:F:89:CYS:HB3	1:F:125:ALA:HB2	2.03	0.41
1:B:86:ARG:HD3	2:B:681:HOH:O	2.21	0.41
1:D:96:SER:O	1:D:99:VAL:HG22	2.20	0.41
1:E:93:ILE:HG12	1:E:127:ALA:HB3	2.01	0.41
1:C:84:GLN:HE22	1:F:154:LYS:HE2	1.84	0.41
1:B:468:ALA:O	1:B:472:ASN:HA	2.20	0.41
1:B:96:SER:O	1:B:99:VAL:HG22	2.20	0.41
1:C:374:ASN:O	2:C:604:HOH:O	2.22	0.41
1:C:443:ALA:HA	1:C:447:ASP:OD2	2.20	0.41
1:D:86:ARG:HD3	2:D:680:HOH:O	2.21	0.41
1:E:96:SER:HB3	1:E:99:VAL:HG13	2.02	0.41
1:C:154:LYS:HE2	1:F:84:GLN:HE22	1.84	0.41
1:F:96:SER:HB3	1:F:99:VAL:HG13	2.02	0.41
1:C:150:MET:HG2	1:C:154:LYS:NZ	2.35	0.41
1:C:86:ARG:HD3	2:C:679:HOH:O	2.21	0.41
1:D:89:CYS:HB3	1:D:125:ALA:HB2	2.03	0.41
1:A:86:ARG:HD3	2:A:680:HOH:O	2.21	0.41
1:B:403:ARG:CZ	2:B:616:HOH:O	2.69	0.41
1:D:403:ARG:CZ	2:D:616:HOH:O	2.69	0.41
1:F:93:ILE:HG12	1:F:127:ALA:HB3	2.01	0.41
1:A:90:LYS:NZ	1:A:164:VAL:HG12	2.36	0.41
1:B:89:CYS:HB3	1:B:125:ALA:HB2	2.03	0.41
1:C:90:LYS:NZ	1:C:164:VAL:HG12	2.36	0.41
1:F:404:ASP:O	1:F:408:HIS:ND1	2.32	0.41
1:A:150:MET:HG2	1:A:154:LYS:NZ	2.35	0.41
1:A:408:HIS:HD2	1:F:436:PHE:HB2	1.86	0.41
1:A:374:ASN:O	2:A:604:HOH:O	2.22	0.40
1:B:90:LYS:NZ	1:B:164:VAL:HG12	2.36	0.40
1:D:90:LYS:NZ	1:D:164:VAL:HG12	2.36	0.40
1:E:414:GLN:O	1:E:417:LEU:N	2.53	0.40
1:A:78:TYR:CE1	1:A:101:VAL:HG22	2.57	0.40
1:C:78:TYR:CE1	1:C:101:VAL:HG22	2.57	0.40
1:B:436:PHE:CD1	1:F:408:HIS:HB3	2.56	0.40
1:F:414:GLN:O	1:F:417:LEU:N	2.53	0.40
1:E:424:HIS:ND1	1:E:424:HIS:O	2.55	0.40
1:F:424:HIS:ND1	1:F:424:HIS:O	2.55	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	290/558 (52%)	279 (96%)	11 (4%)	0	100	100
1	B	290/558 (52%)	279 (96%)	11 (4%)	0	100	100
1	C	290/558 (52%)	279 (96%)	11 (4%)	0	100	100
1	D	290/558 (52%)	279 (96%)	11 (4%)	0	100	100
1	E	290/558 (52%)	279 (96%)	11 (4%)	0	100	100
1	F	290/558 (52%)	279 (96%)	11 (4%)	0	100	100
All	All	1740/3348 (52%)	1674 (96%)	66 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	244/456 (54%)	244 (100%)	0	100	100
1	B	244/456 (54%)	244 (100%)	0	100	100
1	C	244/456 (54%)	244 (100%)	0	100	100
1	D	244/456 (54%)	244 (100%)	0	100	100
1	E	244/456 (54%)	244 (100%)	0	100	100
1	F	244/456 (54%)	244 (100%)	0	100	100
All	All	1464/2736 (54%)	1464 (100%)	0	100	100



There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	189	HIS
1	A	195	HIS
1	A	209	HIS
1	A	388	ASN
1	A	414	GLN
1	B	189	HIS
1	B	195	HIS
1	B	209	HIS
1	B	388	ASN
1	B	414	GLN
1	C	189	HIS
1	C	195	HIS
1	C	209	HIS
1	C	388	ASN
1	C	414	GLN
1	D	189	HIS
1	D	195	HIS
1	D	209	HIS
1	D	388	ASN
1	D	414	GLN
1	E	189	HIS
1	E	195	HIS
1	E	209	HIS
1	E	388	ASN
1	E	414	GLN
1	F	189	HIS
1	F	195	HIS
1	F	209	HIS
1	F	388	ASN
1	F	414	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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.