wwPDB EM Map/Model Validation Report (i)

Jun 20, 2016 – 12:49 PM EDT

PDB ID	:	5K12
EMDB ID:	:	EMD-8194
Title	:	Cryo-EM structure of glutamate dehydrogenase at 1.8 A 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 wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

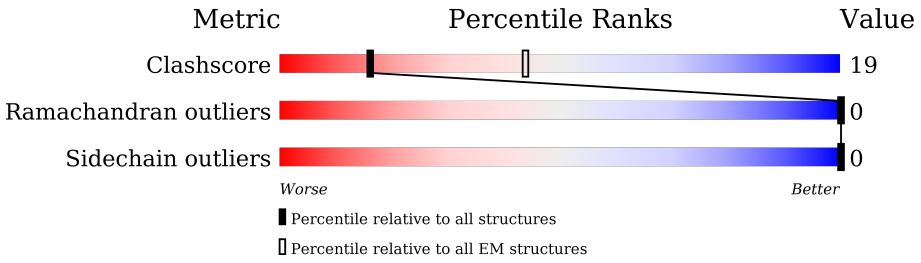
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027790

1 Overall quality at a glance (i)

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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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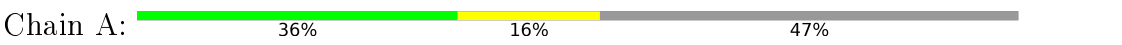
Mol	Chain	Residues	Atoms	AltConf
2	E	181	Total O 181 181	0
2	F	181	Total O 181 181	0

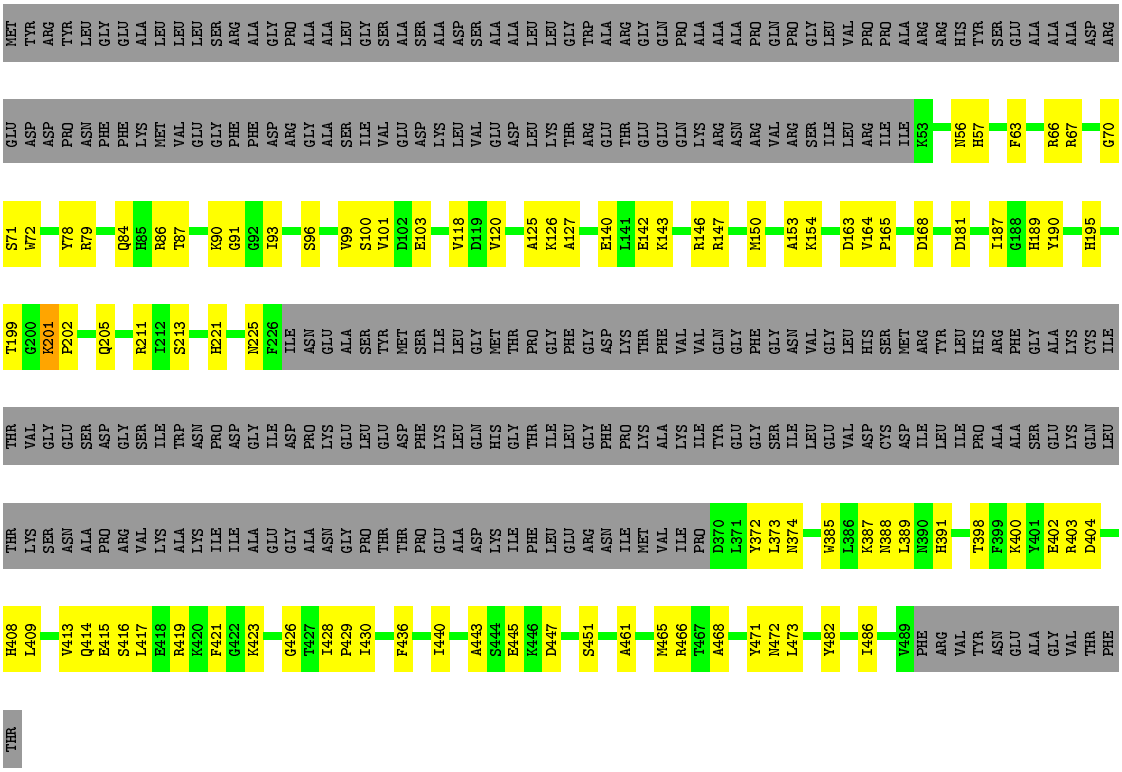
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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 1, mitochondrial

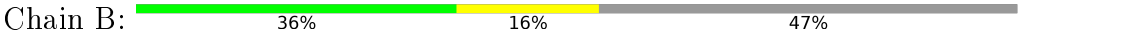
Chain A:

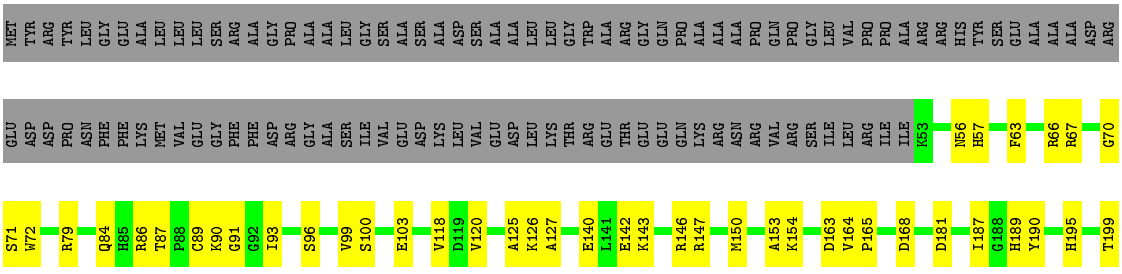


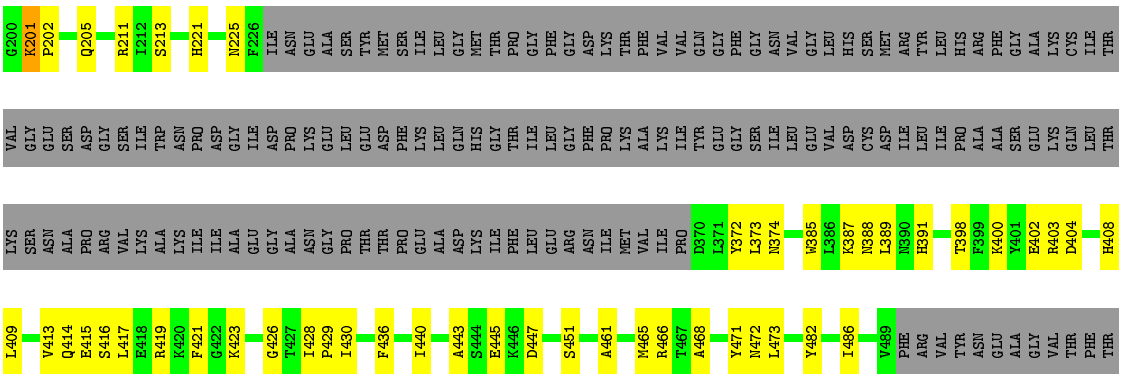


- Molecule 1: Glutamate dehydrogenase 1, mitochondrial

Chain B:

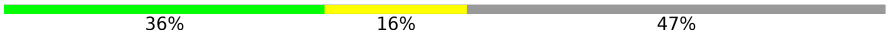


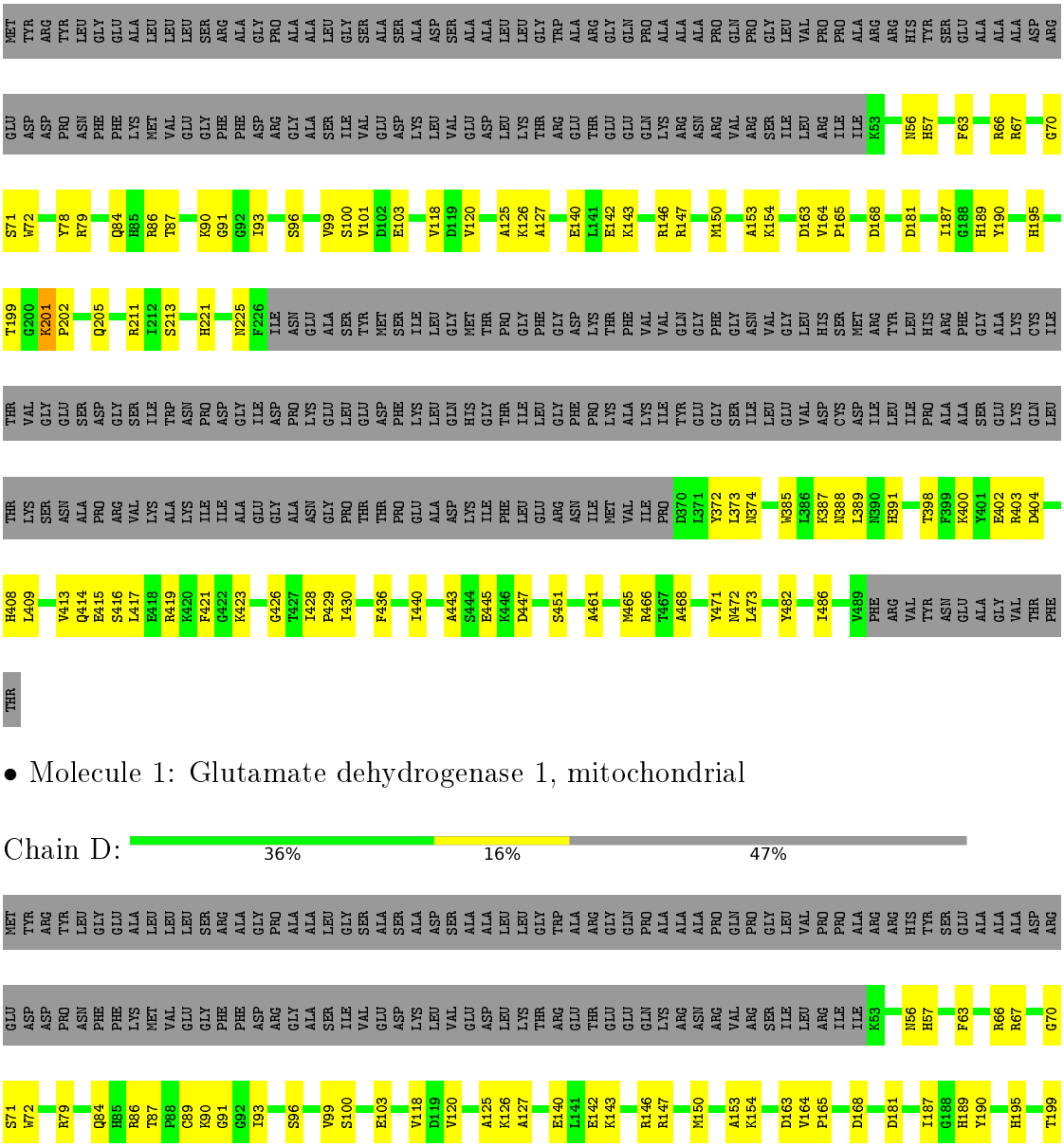




• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

Chain C:

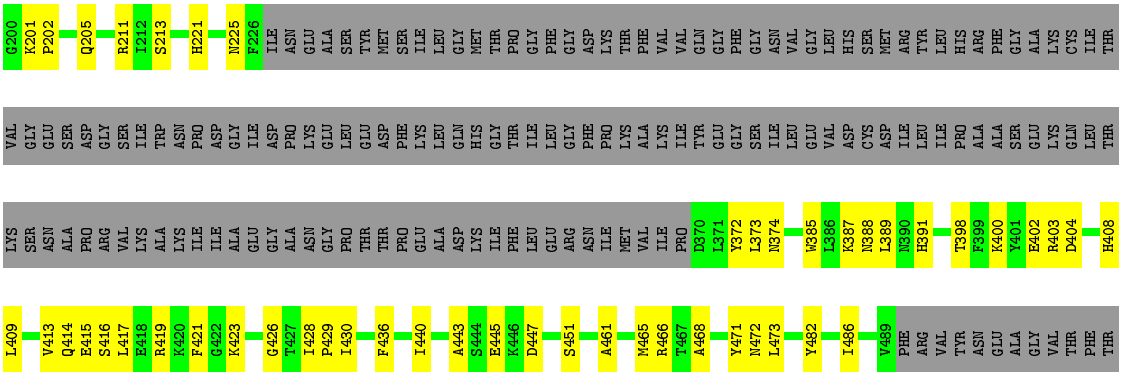




• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

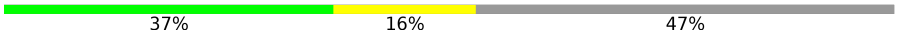
Chain D:

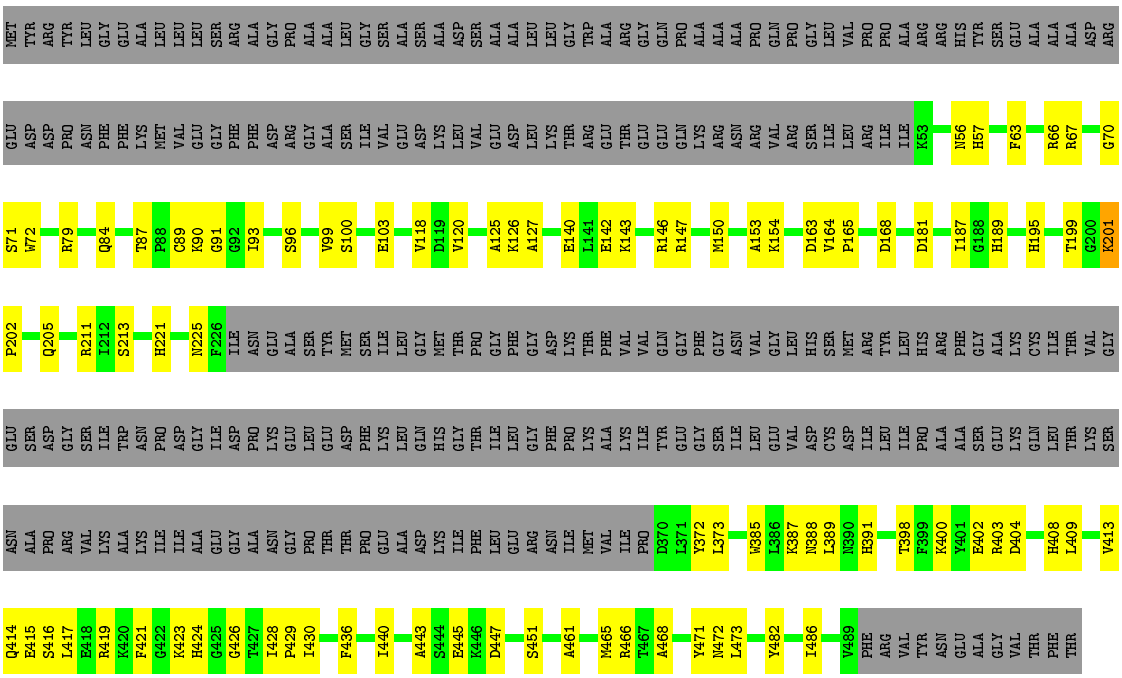
WORLDWIDE PDB PROTEIN DATA BANK
EMDataBank Unified Data Resource for 3DEM



• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

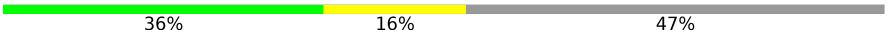
Chain E:

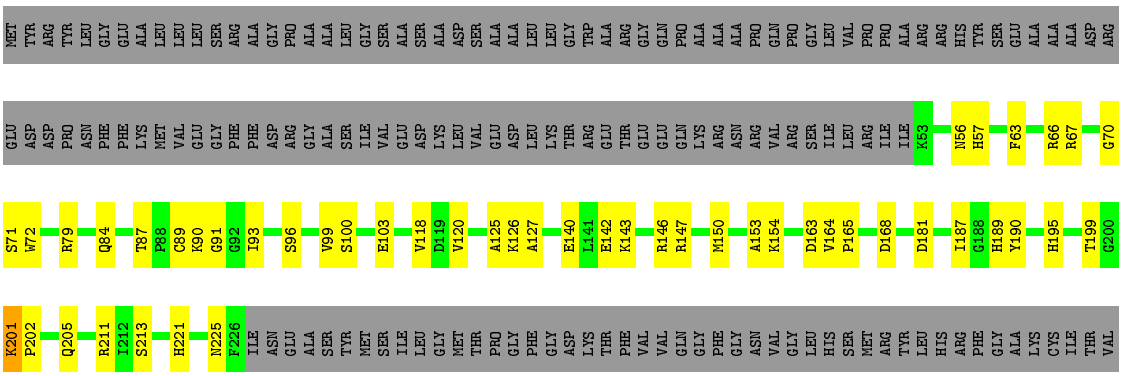


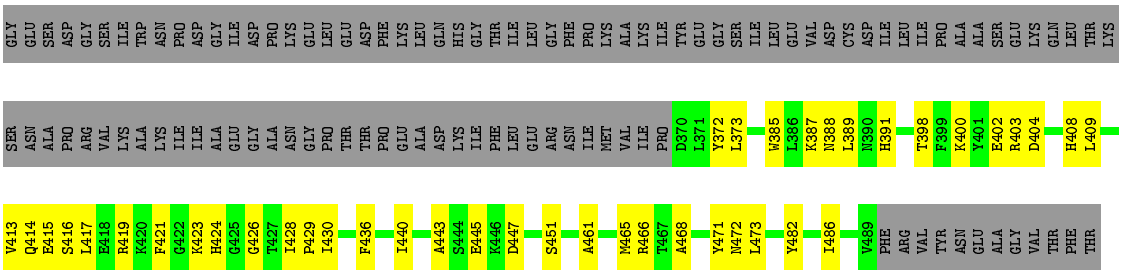


• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

Chain F:






GLY GLU SER ASP GLY SER ILE TRP ASN PRO ASP GLY ILE ASP PRO LYS GLU LEU GLU ASP PHE LYS LEU GLN HIS GLY THR ILE LEU GLY PHE PRO LYS ALA LYS ILE TYR GLU GLY SER ILE LEU GLU VAL ASP CYS ASP ILE LEU ILE PRO ALA ALA SER GLU LYS GLN LEU THR LYS
SER ASN ALA PRO ARG VAL LYS ALA LYS ILE ILE ALA GLU GLY ALA ASN GLY PRO THR THR PRO GLU ALA ASP LYS ILE PHE LEU GLU ARG ASN ILE MET VAL ILE PRO D370 L371 Y372 L373 W385 L386 K387 N388 L389 N390 H391 T398 F399 K400 Y401 E402 R403 D404 H408 L409
V413 Q414 E415 S416 L417 E418 R419 K420 F421 G422 K423 H424 G425 G426 T427 I428 P429 I430 F436 I440 A443 S444 E445 K446 D447 S451 A461 M465 R466 T467 A468 Y471 N472 L473 Y482 I486 V489 PHE ARG VAL TYR ASN GLU ALA GLY VAL THR PHE THR

4 Experimental information (i)

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 ($e^-/Å^2$)	Not provided	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	215000	Depositor
Image detector	Not provided	Depositor

5 Model quality

5.1 Standard geometry

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(^{o})	Ideal(^{o})
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

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:126:LYS:NZ	1:F:168:ASP:OD2	2.22	0.72
1:F:142:GLU:OE1	2:F:602:HOH:O	2.06	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:414:GLN:HG2	1:F:429:PRO:HD2	1.69	0.72
1:F:423:LYS:HD3	1:F:426:GLY:HA3	1.71	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:79:ARG:NE	1:B:163:ASP:OD2	2.20	0.70
1:B:126:LYS:NZ	1:B:168:ASP:OD2	2.22	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:146:ARG:NH1	1:B:181:ASP:OD2	2.32	0.63
1:B:150:MET:HE3	2:B:776:HOH:O	1.98	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:195:HIS:HE1	1:B:391:HIS:CD2	2.21	0.58
1:B:91:GLY:O	1:B:165:PRO:HA	2.03	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:C:451:SER:HB2	1:D:400:LYS:HB3	1.92	0.51
1:D:153:ALA:HB1	1:D:187:ILE:HG13	1.90	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:A:416:SER:HB3	1:F:429:PRO:HA	1.95	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: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:B:436:PHE:CG	1:F:408:HIS:HB3	2.49	0.48
1:C:430:ILE:HD12	2:C:709:HOH:O	2.13	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: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:C:416:SER:HB3	1:E:429:PRO:HA	1.97	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:B:398:THR:O	1:B:402:GLU:HG2	2.18	0.44
1:A:436:PHE:HB2	1:B:408:HIS:HD2	1.81	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:414:GLN:NE2	1:A:428:ILE:HA	2.31	0.44
1:A:91:GLY:HA3	1:A:125:ALA:O	2.18	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: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:408:HIS:HB3	1:F:436:PHE:CG	2.53	0.44
1:A:423:LYS:HD3	1:A:426:GLY:CA	2.44	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:91:GLY:HA3	1:C:125:ALA:O	2.18	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:398:THR:O	1:E:402:GLU:HG2	2.18	0.43
1:E:400:LYS:HA	1:E:403:ARG:HG2	1.99	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.