Full wwPDB EM Validation Report ⓘ

Mar 3, 2025 – 03:05 pm GMT

PDB ID	:	8S7H
EMDB ID	:	EMD-19772
Title	:	Fructose 6-phosphate aldolase (FSA) from Escherichia coli
Authors	:	Hebert, H.; Widersten, M.
Deposited on	:	2024-03-01
Resolution	:	2.80 Å(reported)
Based on initial model	:	1L6W

This is a Full wwPDB EM 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/EMValidationReportHelp
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:

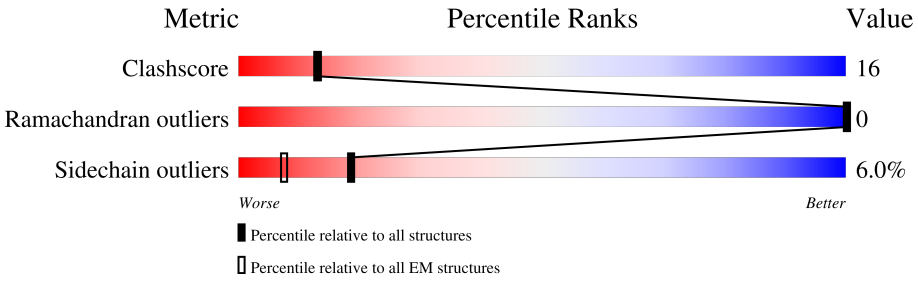
EMDB validation analysis	:	FAILED
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41

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 2.80 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	227	60% 33%
1	B	227	65% 30%
1	C	227	65% 30%
1	D	227	60% 33%
1	E	227	66% 28%
1	F	227	65% 29%
1	G	227	67% 27%
1	H	227	62% 32%
1	I	227	66% 30%

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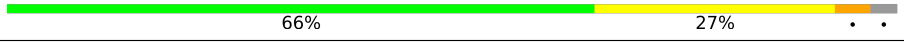
Mol	Chain	Length	Quality of chain
1	J	227	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 16120 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 Fructose-6-phosphate aldolase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	220	Total	C	N	O	S	0	0
			1612	1029	272	302	9		
1	B	220	Total	C	N	O	S	0	0
			1612	1029	272	302	9		
1	C	220	Total	C	N	O	S	0	0
			1612	1029	272	302	9		
1	D	220	Total	C	N	O	S	0	0
			1612	1029	272	302	9		
1	E	220	Total	C	N	O	S	0	0
			1612	1029	272	302	9		
1	F	220	Total	C	N	O	S	0	0
			1612	1029	272	302	9		
1	G	220	Total	C	N	O	S	0	0
			1612	1029	272	302	9		
1	H	220	Total	C	N	O	S	0	0
			1612	1029	272	302	9		
1	I	220	Total	C	N	O	S	0	0
			1612	1029	272	302	9		
1	J	220	Total	C	N	O	S	0	0
			1612	1029	272	302	9		

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	221	THR	-	expression tag	UNP P78055
A	222	SER	-	expression tag	UNP P78055
A	223	HIS	-	expression tag	UNP P78055
A	224	HIS	-	expression tag	UNP P78055
A	225	HIS	-	expression tag	UNP P78055
A	226	HIS	-	expression tag	UNP P78055
A	227	HIS	-	expression tag	UNP P78055
B	221	THR	-	expression tag	UNP P78055
B	222	SER	-	expression tag	UNP P78055
B	223	HIS	-	expression tag	UNP P78055

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Chain	Residue	Modelled	Actual	Comment	Reference
B	224	HIS	-	expression tag	UNP P78055
B	225	HIS	-	expression tag	UNP P78055
B	226	HIS	-	expression tag	UNP P78055
B	227	HIS	-	expression tag	UNP P78055
C	221	THR	-	expression tag	UNP P78055
C	222	SER	-	expression tag	UNP P78055
C	223	HIS	-	expression tag	UNP P78055
C	224	HIS	-	expression tag	UNP P78055
C	225	HIS	-	expression tag	UNP P78055
C	226	HIS	-	expression tag	UNP P78055
C	227	HIS	-	expression tag	UNP P78055
D	221	THR	-	expression tag	UNP P78055
D	222	SER	-	expression tag	UNP P78055
D	223	HIS	-	expression tag	UNP P78055
D	224	HIS	-	expression tag	UNP P78055
D	225	HIS	-	expression tag	UNP P78055
D	226	HIS	-	expression tag	UNP P78055
D	227	HIS	-	expression tag	UNP P78055
E	221	THR	-	expression tag	UNP P78055
E	222	SER	-	expression tag	UNP P78055
E	223	HIS	-	expression tag	UNP P78055
E	224	HIS	-	expression tag	UNP P78055
E	225	HIS	-	expression tag	UNP P78055
E	226	HIS	-	expression tag	UNP P78055
E	227	HIS	-	expression tag	UNP P78055
F	221	THR	-	expression tag	UNP P78055
F	222	SER	-	expression tag	UNP P78055
F	223	HIS	-	expression tag	UNP P78055
F	224	HIS	-	expression tag	UNP P78055
F	225	HIS	-	expression tag	UNP P78055
F	226	HIS	-	expression tag	UNP P78055
F	227	HIS	-	expression tag	UNP P78055
G	221	THR	-	expression tag	UNP P78055
G	222	SER	-	expression tag	UNP P78055
G	223	HIS	-	expression tag	UNP P78055
G	224	HIS	-	expression tag	UNP P78055
G	225	HIS	-	expression tag	UNP P78055
G	226	HIS	-	expression tag	UNP P78055
G	227	HIS	-	expression tag	UNP P78055
H	221	THR	-	expression tag	UNP P78055
H	222	SER	-	expression tag	UNP P78055
H	223	HIS	-	expression tag	UNP P78055

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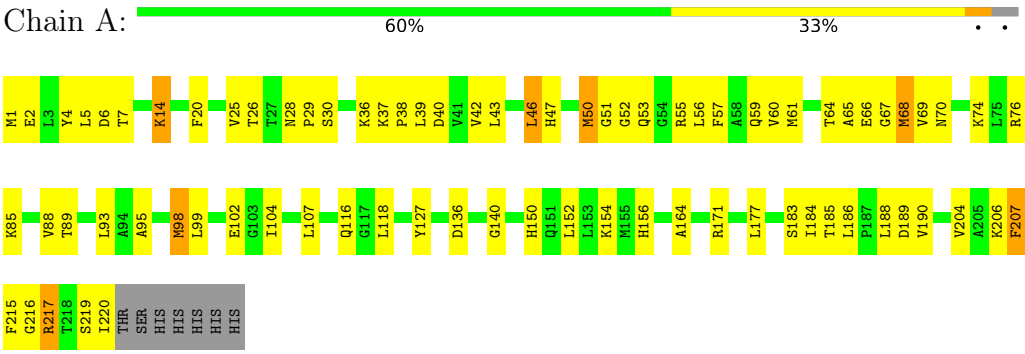
Chain	Residue	Modelled	Actual	Comment	Reference
H	224	HIS	-	expression tag	UNP P78055
H	225	HIS	-	expression tag	UNP P78055
H	226	HIS	-	expression tag	UNP P78055
H	227	HIS	-	expression tag	UNP P78055
I	221	THR	-	expression tag	UNP P78055
I	222	SER	-	expression tag	UNP P78055
I	223	HIS	-	expression tag	UNP P78055
I	224	HIS	-	expression tag	UNP P78055
I	225	HIS	-	expression tag	UNP P78055
I	226	HIS	-	expression tag	UNP P78055
I	227	HIS	-	expression tag	UNP P78055
J	221	THR	-	expression tag	UNP P78055
J	222	SER	-	expression tag	UNP P78055
J	223	HIS	-	expression tag	UNP P78055
J	224	HIS	-	expression tag	UNP P78055
J	225	HIS	-	expression tag	UNP P78055
J	226	HIS	-	expression tag	UNP P78055
J	227	HIS	-	expression tag	UNP P78055

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. 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.

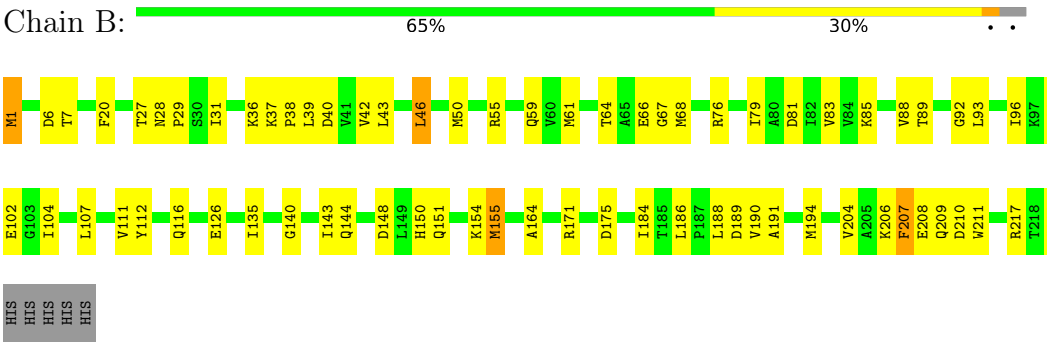
• Molecule 1: Fructose-6-phosphate aldolase 1

Chain A:



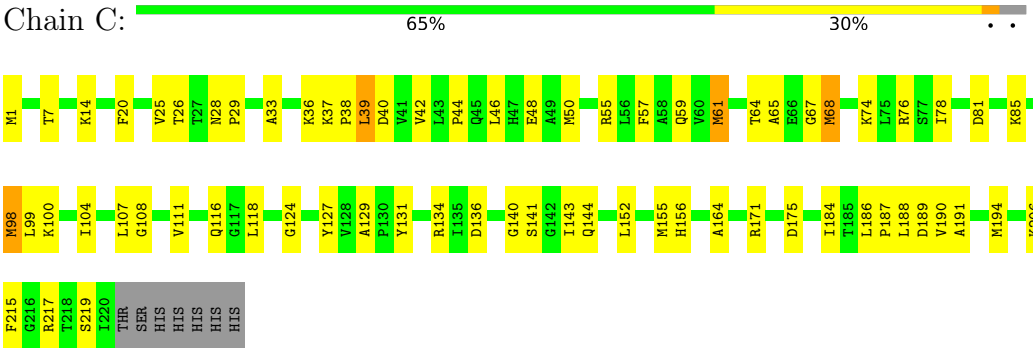
• Molecule 1: Fructose-6-phosphate aldolase 1

Chain B:



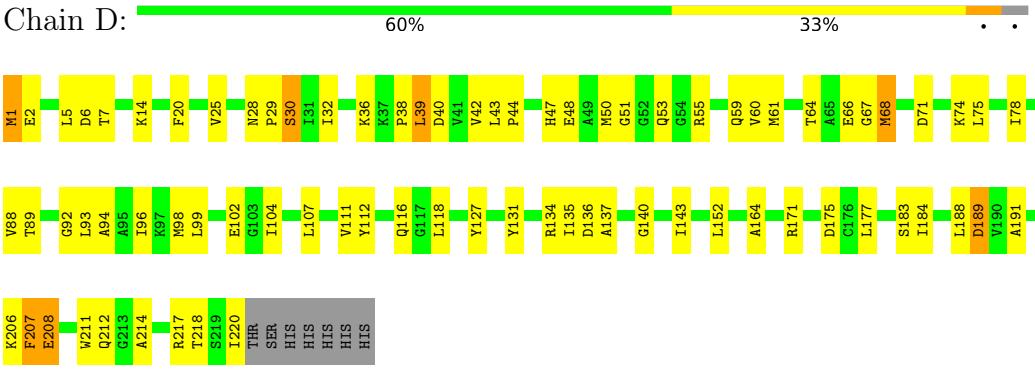
• Molecule 1: Fructose-6-phosphate aldolase 1

Chain C:



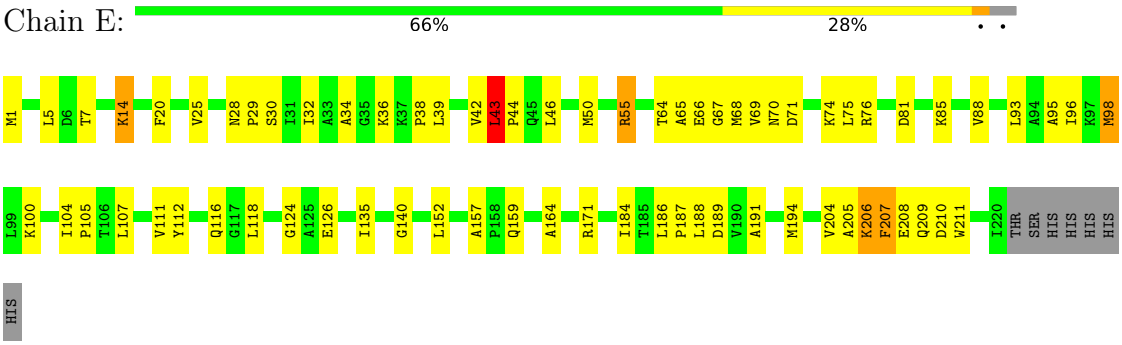
• Molecule 1: Fructose-6-phosphate aldolase 1

Chain D:



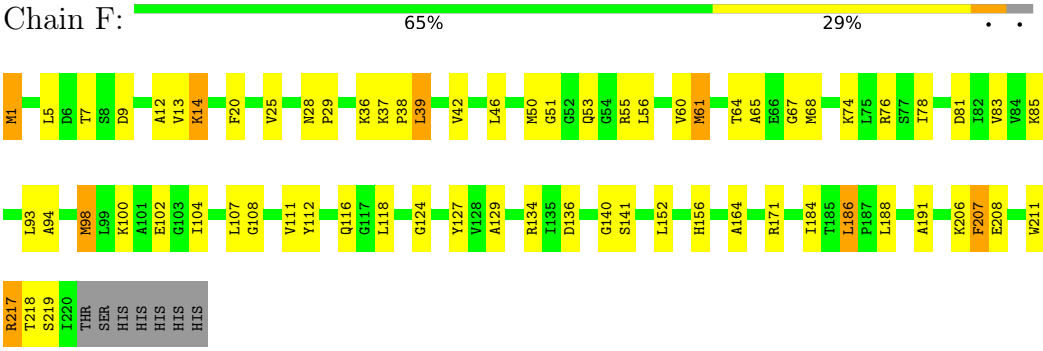
• Molecule 1: Fructose-6-phosphate aldolase 1

Chain E:



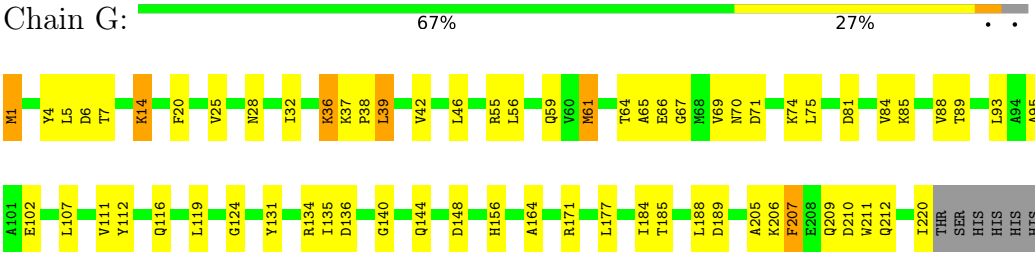
• Molecule 1: Fructose-6-phosphate aldolase 1

Chain F:



• Molecule 1: Fructose-6-phosphate aldolase 1

Chain G:

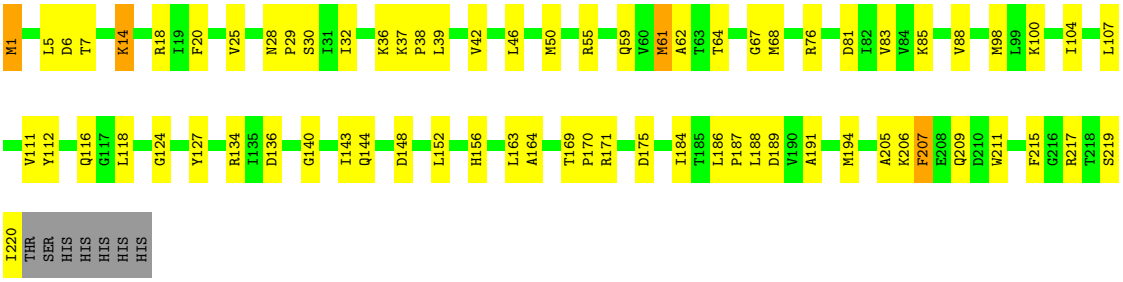


• Molecule 1: Fructose-6-phosphate aldolase 1

Chain H:

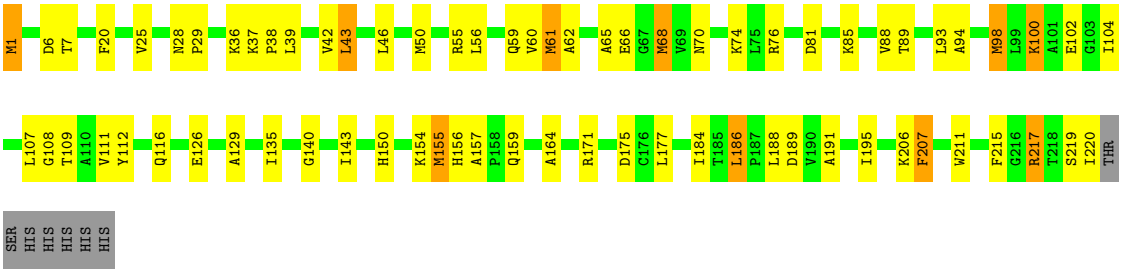
• Molecule 1: Fructose-6-phosphate aldolase 1

Chain I:



• Molecule 1: Fructose-6-phosphate aldolase 1

Chain J:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D5	Depositor
Number of particles used	162766	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	48.64	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	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	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.29	0/1637	0.63	1/2227 (0.0%)
1	B	0.29	0/1637	0.61	0/2227
1	C	0.29	0/1637	0.61	0/2227
1	D	0.28	0/1637	0.60	1/2227 (0.0%)
1	E	0.29	0/1637	0.62	1/2227 (0.0%)
1	F	0.29	0/1637	0.59	0/2227
1	G	0.29	0/1637	0.62	2/2227 (0.1%)
1	H	0.28	0/1637	0.61	2/2227 (0.1%)
1	I	0.29	0/1637	0.61	0/2227
1	J	0.28	0/1637	0.61	2/2227 (0.1%)
All	All	0.29	0/16370	0.61	9/22270 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	43	LEU	CA-CB-CG	7.97	133.64	115.30
1	H	43	LEU	CA-CB-CG	6.78	130.90	115.30
1	G	99	LEU	CA-CB-CG	6.17	129.49	115.30
1	H	194	MET	CA-CB-CG	5.78	123.12	113.30
1	A	46	LEU	CA-CB-CG	5.63	128.26	115.30
1	J	43	LEU	CA-CB-CG	5.31	127.51	115.30
1	D	194	MET	CA-CB-CG	5.28	122.27	113.30
1	J	155	MET	CA-CB-CG	5.25	122.23	113.30
1	G	98	MET	CA-CB-CG	5.06	121.90	113.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1612	0	1676	72	0
1	B	1612	0	1676	54	0
1	C	1612	0	1676	55	0
1	D	1612	0	1676	62	0
1	E	1612	0	1676	58	0
1	F	1612	0	1676	59	0
1	G	1612	0	1676	54	0
1	H	1612	0	1676	73	0
1	I	1612	0	1676	63	0
1	J	1612	0	1676	64	0
All	All	16120	0	16760	534	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 16.

All (534) 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:E:43:LEU:HD12	1:E:44:PRO:HD3	1.49	0.94
1:I:37:LYS:HE3	1:I:37:LYS:HA	1.58	0.82
1:J:126:GLU:N	1:J:126:GLU:OE2	2.17	0.78
1:B:126:GLU:OE2	1:B:126:GLU:N	2.18	0.76
1:H:43:LEU:HD12	1:H:44:PRO:HD3	1.66	0.76
1:J:157:ALA:HB1	1:J:159:GLN:HE22	1.52	0.74
1:G:5:LEU:HB2	1:G:25:VAL:HG22	1.70	0.74
1:D:29:PRO:HD3	1:D:59:GLN:HB3	1.70	0.73
1:D:140:GLY:O	1:I:171:ARG:NH2	2.21	0.73
1:H:5:LEU:HB2	1:H:25:VAL:HG22	1.70	0.73
1:J:59:GLN:HB2	1:J:85:LYS:HE3	1.69	0.72
1:F:207:PHE:HZ	1:G:28:ASN:HB2	1.54	0.72
1:B:208:GLU:OE1	1:B:209:GLN:NE2	2.22	0.72
1:B:140:GLY:O	1:G:171:ARG:NH2	2.23	0.72
1:H:76:ARG:NH1	1:H:80:ALA:O	2.21	0.71
1:E:5:LEU:HB2	1:E:25:VAL:HG22	1.72	0.71
1:C:39:LEU:HA	1:C:42:VAL:HG22	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:LEU:HA	1:A:42:VAL:HG22	1.73	0.70
1:E:76:ARG:HH12	1:E:105:PRO:HD2	1.56	0.70
1:J:186:LEU:HD13	1:J:191:ALA:HB2	1.73	0.69
1:G:37:LYS:HE3	1:G:38:PRO:HD2	1.73	0.69
1:C:171:ARG:NH2	1:H:140:GLY:O	2.24	0.69
1:G:39:LEU:HA	1:G:42:VAL:HG22	1.72	0.69
1:F:29:PRO:HB3	1:J:211:TRP:HD1	1.58	0.69
1:D:5:LEU:HB2	1:D:25:VAL:HG22	1.73	0.69
1:H:107:LEU:HD23	1:H:127:TYR:HB2	1.74	0.69
1:J:39:LEU:HA	1:J:42:VAL:HG22	1.75	0.69
1:D:39:LEU:HA	1:D:42:VAL:HG22	1.75	0.68
1:F:39:LEU:HA	1:F:42:VAL:HG22	1.75	0.68
1:E:34:ALA:O	1:E:36:LYS:NZ	2.25	0.68
1:E:171:ARG:NH2	1:J:140:GLY:O	2.27	0.67
1:F:65:ALA:HB1	1:F:98:MET:HE1	1.75	0.67
1:H:88:VAL:HB	1:H:116:GLN:HE21	1.58	0.67
1:I:39:LEU:HA	1:I:42:VAL:HG22	1.76	0.67
1:F:37:LYS:HE2	1:F:37:LYS:HA	1.76	0.67
1:H:211:TRP:NE1	1:H:219:SER:O	2.28	0.67
1:J:29:PRO:HD3	1:J:59:GLN:HB3	1.75	0.67
1:D:88:VAL:HB	1:D:116:GLN:HE21	1.60	0.67
1:I:5:LEU:HB2	1:I:25:VAL:HG22	1.76	0.67
1:C:55:ARG:NH2	1:C:81:ASP:O	2.28	0.66
1:H:55:ARG:NH2	1:H:81:ASP:O	2.28	0.66
1:F:215:PHE:HB3	1:F:217:ARG:HH21	1.61	0.66
1:D:85:LYS:HA	1:D:107:LEU:HB3	1.78	0.66
1:C:164:ALA:HB3	1:C:184:ILE:HG22	1.78	0.66
1:D:118:LEU:HD12	1:D:152:LEU:HB3	1.78	0.66
1:F:55:ARG:NH2	1:F:81:ASP:O	2.29	0.66
1:H:217:ARG:NH1	1:H:217:ARG:HB2	2.11	0.65
1:A:140:GLY:O	1:F:171:ARG:NH2	2.28	0.65
1:E:140:GLY:O	1:J:171:ARG:NH2	2.26	0.65
1:G:66:GLU:OE1	1:G:66:GLU:N	2.29	0.65
1:A:215:PHE:O	1:A:217:ARG:NH2	2.30	0.65
1:B:55:ARG:NH2	1:B:81:ASP:O	2.30	0.65
1:I:55:ARG:NH2	1:I:81:ASP:O	2.31	0.64
1:C:100:LYS:HG3	1:C:124:GLY:HA3	1.80	0.64
1:F:46:LEU:HD22	1:F:56:LEU:HD21	1.80	0.64
1:B:55:ARG:HH21	1:B:83:VAL:HG23	1.63	0.63
1:E:39:LEU:HA	1:E:42:VAL:HG22	1.81	0.63
1:A:207:PHE:HZ	1:E:28:ASN:HB2	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:25:VAL:HG11	1:J:46:LEU:HD11	1.81	0.63
1:H:55:ARG:HH21	1:H:83:VAL:HG23	1.64	0.63
1:H:164:ALA:HB3	1:H:184:ILE:HG22	1.79	0.63
1:G:112:TYR:HA	1:G:135:ILE:HD11	1.81	0.63
1:D:164:ALA:HB3	1:D:184:ILE:HG22	1.80	0.63
1:C:37:LYS:HA	1:C:37:LYS:HE2	1.80	0.63
1:H:66:GLU:OE1	1:H:66:GLU:N	2.21	0.63
1:F:60:VAL:HA	1:J:220:ILE:HD11	1.80	0.62
1:A:68:MET:HE3	1:A:68:MET:H	1.65	0.62
1:D:55:ARG:NH2	1:D:81:ASP:O	2.31	0.62
1:H:43:LEU:HA	1:H:46:LEU:HD12	1.81	0.62
1:D:66:GLU:N	1:D:66:GLU:OE2	2.32	0.62
1:E:100:LYS:HG3	1:E:124:GLY:HA3	1.81	0.61
1:F:28:ASN:HB2	1:J:207:PHE:HZ	1.65	0.61
1:F:100:LYS:HG3	1:F:124:GLY:HA3	1.80	0.61
1:H:207:PHE:HE1	1:I:30:SER:H	1.48	0.61
1:A:46:LEU:HD22	1:A:56:LEU:HD21	1.81	0.61
1:A:55:ARG:NH2	1:A:81:ASP:O	2.34	0.61
1:D:99:LEU:HD12	1:D:104:ILE:HB	1.81	0.61
1:B:28:ASN:HB2	1:C:207:PHE:HZ	1.65	0.61
1:D:171:ARG:NH2	1:I:140:GLY:O	2.34	0.61
1:I:100:LYS:HG3	1:I:124:GLY:HA3	1.82	0.61
1:C:141:SER:HB3	1:C:144:GLN:HE21	1.65	0.61
1:A:88:VAL:HB	1:A:116:GLN:HE21	1.66	0.60
1:D:189:ASP:N	1:D:189:ASP:OD2	2.33	0.60
1:C:140:GLY:O	1:H:171:ARG:NH2	2.32	0.60
1:C:186:LEU:HG	1:C:191:ALA:HB2	1.84	0.60
1:I:207:PHE:HZ	1:J:28:ASN:HB2	1.65	0.60
1:G:211:TRP:CE3	1:H:29:PRO:HB3	2.36	0.59
1:J:37:LYS:HE2	1:J:38:PRO:HD2	1.84	0.59
1:A:5:LEU:HB2	1:A:25:VAL:HG22	1.83	0.59
1:I:85:LYS:HG2	1:I:107:LEU:HB3	1.84	0.59
1:E:7:THR:HG21	1:E:188:LEU:HD21	1.84	0.59
1:F:29:PRO:HB3	1:J:211:TRP:CD1	2.37	0.59
1:J:76:ARG:HG3	1:J:104:ILE:HD13	1.84	0.59
1:G:100:LYS:HG3	1:G:124:GLY:HA3	1.84	0.59
1:F:219:SER:HA	1:G:61:MET:HE3	1.85	0.59
1:J:189:ASP:OD2	1:J:189:ASP:N	2.35	0.59
1:B:36:LYS:O	1:B:36:LYS:NZ	2.29	0.59
1:B:76:ARG:HG3	1:B:104:ILE:HD13	1.85	0.58
1:G:164:ALA:HB3	1:G:184:ILE:HG22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:220:ILE:HG13	1:H:61:MET:HG3	1.85	0.58
1:D:71:ASP:O	1:D:75:LEU:HD13	2.03	0.58
1:F:88:VAL:HB	1:F:116:GLN:HE21	1.68	0.58
1:E:171:ARG:HH11	1:E:171:ARG:HA	1.67	0.58
1:E:189:ASP:N	1:E:189:ASP:OD1	2.36	0.58
1:G:189:ASP:OD2	1:G:189:ASP:N	2.36	0.58
1:B:171:ARG:HA	1:B:171:ARG:HH11	1.69	0.58
1:J:112:TYR:HA	1:J:135:ILE:HD11	1.86	0.58
1:I:189:ASP:OD1	1:I:189:ASP:N	2.33	0.58
1:J:38:PRO:O	1:J:42:VAL:HG13	2.04	0.58
1:I:25:VAL:HB	1:I:50:MET:HE1	1.86	0.58
1:A:25:VAL:HB	1:A:46:LEU:HD21	1.85	0.58
1:E:186:LEU:HD12	1:E:187:PRO:HD2	1.85	0.58
1:E:85:LYS:HD2	1:E:107:LEU:HD22	1.86	0.57
1:J:171:ARG:HH11	1:J:171:ARG:HA	1.68	0.57
1:J:88:VAL:HB	1:J:116:GLN:HE21	1.69	0.57
1:B:171:ARG:NH2	1:G:140:GLY:O	2.32	0.57
1:H:207:PHE:HZ	1:I:28:ASN:HB2	1.68	0.57
1:G:88:VAL:HB	1:G:116:GLN:HE21	1.70	0.57
1:H:177:LEU:HD21	1:H:184:ILE:HG12	1.87	0.57
1:F:7:THR:HG21	1:F:188:LEU:HD21	1.87	0.57
1:I:211:TRP:NE1	1:I:219:SER:O	2.33	0.57
1:D:36:LYS:O	1:D:36:LYS:NZ	2.27	0.57
1:D:136:ASP:OD1	1:I:169:THR:OG1	2.20	0.56
1:H:39:LEU:HA	1:H:42:VAL:HG22	1.87	0.56
1:H:189:ASP:OD2	1:H:189:ASP:N	2.36	0.56
1:A:98:MET:SD	1:A:99:LEU:HD22	2.46	0.56
1:I:88:VAL:HB	1:I:116:GLN:HE21	1.70	0.56
1:D:38:PRO:O	1:D:42:VAL:HG13	2.05	0.56
1:A:164:ALA:HB3	1:A:184:ILE:HG22	1.86	0.56
1:I:171:ARG:HA	1:I:171:ARG:HH11	1.70	0.56
1:G:85:LYS:HD2	1:G:107:LEU:HD22	1.87	0.56
1:A:189:ASP:OD2	1:A:189:ASP:N	2.35	0.56
1:A:211:TRP:CD1	1:E:29:PRO:HB3	2.40	0.56
1:J:164:ALA:HB3	1:J:184:ILE:HG22	1.87	0.56
1:B:46:LEU:O	1:B:50:MET:HG2	2.06	0.56
1:A:66:GLU:OE1	1:A:66:GLU:N	2.24	0.56
1:E:88:VAL:HB	1:E:116:GLN:HE21	1.71	0.56
1:J:7:THR:HG21	1:J:188:LEU:HD21	1.86	0.56
1:B:189:ASP:N	1:B:189:ASP:OD2	2.38	0.55
1:H:43:LEU:HD12	1:H:44:PRO:CD	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:LYS:O	1:A:78:ILE:HG12	2.05	0.55
1:F:5:LEU:HB2	1:F:25:VAL:HG22	1.87	0.55
1:H:39:LEU:O	1:H:43:LEU:HG	2.06	0.55
1:E:71:ASP:O	1:E:75:LEU:HD13	2.07	0.55
1:G:171:ARG:HH11	1:G:171:ARG:HA	1.70	0.55
1:I:7:THR:HG21	1:I:188:LEU:HD21	1.89	0.55
1:I:76:ARG:HG3	1:I:104:ILE:HD13	1.88	0.55
1:G:144:GLN:NE2	1:G:148:ASP:OD1	2.38	0.55
1:H:171:ARG:HH11	1:H:171:ARG:HA	1.71	0.55
1:A:38:PRO:O	1:A:42:VAL:HG13	2.07	0.55
1:C:171:ARG:HH11	1:C:171:ARG:HA	1.70	0.55
1:D:81:ASP:N	1:D:81:ASP:OD1	2.39	0.55
1:F:171:ARG:HA	1:F:171:ARG:HH11	1.71	0.55
1:A:59:GLN:HB2	1:A:85:LYS:HE2	1.88	0.55
1:C:28:ASN:HB2	1:D:207:PHE:HZ	1.72	0.55
1:G:207:PHE:HZ	1:H:28:ASN:HB2	1.72	0.55
1:J:55:ARG:NH2	1:J:81:ASP:O	2.40	0.55
1:G:55:ARG:NH2	1:G:81:ASP:O	2.40	0.55
1:H:81:ASP:OD2	1:H:81:ASP:N	2.33	0.55
1:J:39:LEU:O	1:J:43:LEU:HD12	2.07	0.55
1:E:81:ASP:OD1	1:E:81:ASP:N	2.38	0.54
1:C:85:LYS:HD2	1:C:107:LEU:HD22	1.88	0.54
1:E:157:ALA:HB1	1:E:159:GLN:HE22	1.71	0.54
1:C:74:LYS:O	1:C:78:ILE:HG12	2.07	0.54
1:C:118:LEU:HD12	1:C:152:LEU:HB3	1.88	0.54
1:G:7:THR:HG21	1:G:188:LEU:HD21	1.89	0.54
1:H:85:LYS:HB3	1:H:107:LEU:HD12	1.89	0.54
1:E:95:ALA:HA	1:E:98:MET:SD	2.48	0.54
1:F:186:LEU:HD13	1:F:191:ALA:HB2	1.90	0.54
1:B:81:ASP:OD2	1:B:81:ASP:N	2.41	0.54
1:B:59:GLN:HB2	1:B:85:LYS:NZ	2.23	0.54
1:D:171:ARG:HA	1:D:171:ARG:HH11	1.71	0.54
1:F:25:VAL:HB	1:F:46:LEU:HD21	1.88	0.54
1:H:38:PRO:O	1:H:42:VAL:HG13	2.08	0.54
1:A:28:ASN:HB2	1:B:207:PHE:HZ	1.73	0.53
1:B:85:LYS:HB3	1:B:107:LEU:HB3	1.89	0.53
1:G:65:ALA:O	1:G:69:VAL:HG23	2.08	0.53
1:H:39:LEU:HD23	1:H:40:ASP:H	1.73	0.53
1:I:191:ALA:HA	1:I:194:MET:HG2	1.89	0.53
1:B:186:LEU:HD13	1:B:191:ALA:HB2	1.90	0.53
1:H:57:PHE:HB3	1:H:85:LYS:HD3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:76:ARG:HH21	1:H:104:ILE:HG12	1.72	0.53
1:J:66:GLU:OE2	1:J:66:GLU:N	2.40	0.53
1:C:217:ARG:NH1	1:C:219:SER:OG	2.41	0.53
1:D:107:LEU:HD22	1:D:127:TYR:HB2	1.90	0.53
1:I:144:GLN:NE2	1:I:148:ASP:OD1	2.41	0.53
1:G:64:THR:O	1:G:67:GLY:N	2.42	0.53
1:I:81:ASP:OD2	1:I:81:ASP:N	2.42	0.53
1:D:74:LYS:O	1:D:78:ILE:HG12	2.08	0.53
1:B:211:TRP:NE1	1:B:219:SER:O	2.27	0.53
1:G:207:PHE:HE2	1:H:29:PRO:HB2	1.74	0.53
1:E:64:THR:O	1:E:67:GLY:N	2.42	0.52
1:E:55:ARG:NH2	1:E:81:ASP:O	2.43	0.52
1:B:164:ALA:HB3	1:B:184:ILE:HG22	1.91	0.52
1:C:36:LYS:O	1:C:36:LYS:NZ	2.26	0.52
1:H:74:LYS:O	1:H:78:ILE:HG12	2.10	0.52
1:J:60:VAL:HG21	1:J:68:MET:HB3	1.92	0.52
1:A:207:PHE:HE2	1:E:30:SER:H	1.57	0.52
1:A:211:TRP:HD1	1:E:29:PRO:HB3	1.74	0.52
1:C:88:VAL:HB	1:C:116:GLN:HE21	1.75	0.52
1:C:7:THR:HG21	1:C:188:LEU:HD21	1.90	0.52
1:G:36:LYS:HD2	1:G:36:LYS:O	2.10	0.52
1:I:36:LYS:HD2	1:I:36:LYS:N	2.24	0.52
1:B:7:THR:HG21	1:B:188:LEU:HD21	1.91	0.52
1:C:190:VAL:HG12	1:C:194:MET:HE1	1.92	0.52
1:A:64:THR:O	1:A:67:GLY:N	2.43	0.51
1:A:68:MET:HE3	1:A:68:MET:N	2.24	0.51
1:E:76:ARG:HH12	1:E:104:ILE:HA	1.75	0.51
1:I:38:PRO:O	1:I:42:VAL:HG13	2.10	0.51
1:A:212:GLN:NE2	1:A:216:GLY:HA2	2.25	0.51
1:A:39:LEU:HD23	1:A:40:ASP:H	1.74	0.51
1:D:59:GLN:HB2	1:D:85:LYS:HE2	1.91	0.51
1:F:171:ARG:HA	1:F:171:ARG:NH1	2.25	0.51
1:A:7:THR:HG21	1:A:188:LEU:HD21	1.92	0.51
1:A:81:ASP:OD2	1:A:81:ASP:N	2.44	0.51
1:F:25:VAL:HG11	1:F:46:LEU:HD11	1.93	0.51
1:H:1:MET:HB2	1:I:156:HIS:HB3	1.92	0.51
1:C:136:ASP:O	1:H:171:ARG:NH2	2.43	0.51
1:I:1:MET:HB2	1:J:156:HIS:CD2	2.46	0.51
1:I:107:LEU:HG	1:I:127:TYR:HB2	1.91	0.51
1:D:204:VAL:O	1:D:208:GLU:HG3	2.11	0.51
1:H:217:ARG:HB2	1:H:217:ARG:HH11	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:212:GLN:HE21	1:F:218:THR:HG23	1.75	0.50
1:A:171:ARG:HH12	1:F:141:SER:HA	1.76	0.50
1:B:66:GLU:CD	1:B:66:GLU:H	2.11	0.50
1:D:51:GLY:O	1:D:53:GLN:NE2	2.40	0.50
1:H:171:ARG:HA	1:H:171:ARG:NH1	2.26	0.50
1:C:171:ARG:HA	1:C:171:ARG:NH1	2.26	0.50
1:A:65:ALA:HA	1:A:68:MET:SD	2.52	0.50
1:G:38:PRO:O	1:G:42:VAL:HG13	2.12	0.50
1:H:211:TRP:CE3	1:I:29:PRO:HB3	2.47	0.50
1:C:131:TYR:HB3	1:C:134:ARG:HG2	1.94	0.50
1:E:186:LEU:HG	1:E:191:ALA:HB2	1.93	0.50
1:F:74:LYS:O	1:F:78:ILE:HG12	2.12	0.50
1:I:220:ILE:HG13	1:J:61:MET:SD	2.52	0.49
1:H:98:MET:O	1:H:102:GLU:HG2	2.12	0.49
1:F:36:LYS:O	1:F:36:LYS:NZ	2.26	0.49
1:E:46:LEU:O	1:E:50:MET:HG2	2.12	0.49
1:F:64:THR:O	1:F:67:GLY:N	2.45	0.49
1:A:37:LYS:HE2	1:A:37:LYS:HA	1.93	0.49
1:E:70:ASN:O	1:E:74:LYS:HG3	2.12	0.49
1:F:118:LEU:HD22	1:F:152:LEU:HB3	1.94	0.49
1:H:143:ILE:HD12	1:H:175:ASP:HB2	1.95	0.49
1:J:85:LYS:HB3	1:J:107:LEU:HB3	1.95	0.49
1:C:99:LEU:HD12	1:C:104:ILE:HB	1.95	0.49
1:F:55:ARG:HH21	1:F:83:VAL:HG23	1.77	0.49
1:F:212:GLN:HB2	1:F:218:THR:HG22	1.95	0.49
1:G:207:PHE:CE2	1:H:29:PRO:HB2	2.48	0.49
1:J:36:LYS:O	1:J:36:LYS:NZ	2.27	0.48
1:A:60:VAL:HG11	1:A:68:MET:HB2	1.95	0.48
1:F:107:LEU:HG	1:F:127:TYR:HB2	1.93	0.48
1:D:32:ILE:HD12	1:D:42:VAL:HG21	1.95	0.48
1:H:144:GLN:NE2	1:H:148:ASP:OD1	2.45	0.48
1:G:4:TYR:HB2	1:G:185:THR:HB	1.95	0.48
1:A:85:LYS:HB3	1:A:107:LEU:HB3	1.93	0.48
1:D:28:ASN:HB2	1:E:207:PHE:HZ	1.78	0.48
1:D:39:LEU:O	1:D:43:LEU:HD22	2.13	0.48
1:E:38:PRO:O	1:E:42:VAL:HG13	2.13	0.48
1:J:177:LEU:HD21	1:J:184:ILE:HG12	1.95	0.48
1:D:7:THR:HG21	1:D:188:LEU:HD21	1.96	0.48
1:E:171:ARG:HA	1:E:171:ARG:NH1	2.28	0.48
1:B:37:LYS:HE2	1:B:38:PRO:HD2	1.96	0.48
1:H:85:LYS:HZ3	1:H:85:LYS:HB2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:171:ARG:HA	1:J:171:ARG:NH1	2.28	0.48
1:B:39:LEU:HA	1:B:42:VAL:HG22	1.95	0.48
1:C:206:LYS:O	1:C:206:LYS:HD3	2.14	0.48
1:D:39:LEU:HD23	1:D:40:ASP:H	1.78	0.48
1:J:46:LEU:HD22	1:J:56:LEU:HD21	1.94	0.48
1:A:55:ARG:HA	1:A:55:ARG:CZ	2.44	0.48
1:A:207:PHE:HE2	1:E:30:SER:N	2.12	0.48
1:E:164:ALA:HB3	1:E:184:ILE:HG22	1.96	0.48
1:J:55:ARG:CZ	1:J:55:ARG:HA	2.44	0.48
1:G:98:MET:O	1:G:102:GLU:HG2	2.13	0.48
1:H:4:TYR:HB2	1:H:185:THR:HB	1.95	0.47
1:D:29:PRO:HB3	1:E:211:TRP:CE3	2.49	0.47
1:D:47:HIS:O	1:D:50:MET:HB2	2.13	0.47
1:E:112:TYR:HA	1:E:135:ILE:HD11	1.95	0.47
1:I:29:PRO:HD3	1:I:59:GLN:HB3	1.96	0.47
1:A:204:VAL:O	1:A:208:GLU:HG3	2.14	0.47
1:A:26:THR:HB	1:A:57:PHE:HD2	1.78	0.47
1:B:99:LEU:HD12	1:B:104:ILE:HB	1.97	0.47
1:D:212:GLN:HB2	1:D:218:THR:HG22	1.96	0.47
1:C:186:LEU:HD12	1:C:187:PRO:HD2	1.96	0.47
1:C:55:ARG:CZ	1:C:55:ARG:HA	2.44	0.47
1:C:59:GLN:HB2	1:C:85:LYS:NZ	2.29	0.47
1:E:205:ALA:O	1:E:209:GLN:HG2	2.15	0.47
1:D:194:MET:O	1:D:194:MET:HE3	2.15	0.47
1:E:126:GLU:N	1:E:126:GLU:OE1	2.47	0.47
1:G:81:ASP:OD2	1:G:81:ASP:N	2.43	0.47
1:G:171:ARG:HA	1:G:171:ARG:NH1	2.29	0.47
1:H:207:PHE:HE1	1:I:30:SER:N	2.10	0.47
1:I:164:ALA:HB3	1:I:184:ILE:HG22	1.96	0.47
1:A:98:MET:O	1:A:102:GLU:HG2	2.15	0.47
1:C:108:GLY:O	1:C:129:ALA:N	2.43	0.47
1:G:70:ASN:O	1:G:74:LYS:HG2	2.14	0.47
1:J:98:MET:O	1:J:102:GLU:HG2	2.15	0.47
1:D:171:ARG:HA	1:D:171:ARG:NH1	2.29	0.47
1:D:177:LEU:HD21	1:D:184:ILE:HG12	1.97	0.47
1:H:212:GLN:HB2	1:H:218:THR:HG22	1.96	0.47
1:I:55:ARG:HH21	1:I:83:VAL:HG23	1.80	0.47
1:F:61:MET:HE3	1:J:219:SER:HA	1.97	0.47
1:G:55:ARG:CZ	1:G:55:ARG:HA	2.45	0.47
1:H:78:ILE:O	1:H:79:ILE:HD13	2.16	0.46
1:H:219:SER:HA	1:I:61:MET:HE3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:143:ILE:HD12	1:I:175:ASP:HB2	1.97	0.46
1:C:190:VAL:HG12	1:C:194:MET:CE	2.44	0.46
1:D:206:LYS:HD3	1:D:206:LYS:O	2.15	0.46
1:G:131:TYR:HB3	1:G:134:ARG:HG2	1.97	0.46
1:I:118:LEU:HD23	1:I:152:LEU:HB3	1.97	0.46
1:A:207:PHE:CZ	1:E:29:PRO:HD2	2.50	0.46
1:J:62:ALA:HB3	1:J:68:MET:HG3	1.97	0.46
1:J:206:LYS:O	1:J:206:LYS:HD3	2.16	0.46
1:A:51:GLY:O	1:A:53:GLN:NE2	2.39	0.46
1:D:143:ILE:HD12	1:D:175:ASP:HB2	1.98	0.46
1:E:76:ARG:NH1	1:E:105:PRO:HD2	2.28	0.46
1:B:206:LYS:O	1:B:206:LYS:HD3	2.15	0.46
1:F:108:GLY:O	1:F:129:ALA:N	2.42	0.46
1:G:59:GLN:HB2	1:G:85:LYS:NZ	2.30	0.46
1:I:18:ARG:HB2	1:I:18:ARG:CZ	2.45	0.46
1:A:220:ILE:HG12	1:E:75:LEU:HD11	1.98	0.46
1:C:29:PRO:HB3	1:D:211:TRP:CE3	2.50	0.46
1:D:89:THR:O	1:D:93:LEU:HD23	2.16	0.46
1:B:88:VAL:HB	1:B:116:GLN:HE21	1.79	0.46
1:D:55:ARG:CZ	1:D:55:ARG:HA	2.46	0.46
1:I:32:ILE:HD12	1:I:42:VAL:HG21	1.98	0.46
1:G:98:MET:SD	1:G:99:LEU:HD22	2.56	0.46
1:F:111:VAL:HA	1:F:116:GLN:NE2	2.31	0.46
1:H:186:LEU:HD12	1:H:190:VAL:HG12	1.98	0.46
1:I:186:LEU:HG	1:I:191:ALA:HB2	1.98	0.46
1:H:68:MET:HE3	1:H:95:ALA:HB2	1.97	0.45
1:A:70:ASN:O	1:A:74:LYS:HG2	2.15	0.45
1:E:65:ALA:HA	1:E:68:MET:HE2	1.98	0.45
1:G:98:MET:C	1:G:98:MET:HE2	2.37	0.45
1:I:55:ARG:CZ	1:I:55:ARG:HA	2.46	0.45
1:B:55:ARG:HA	1:B:55:ARG:NH1	2.31	0.45
1:C:61:MET:HG3	1:D:220:ILE:HG13	1.97	0.45
1:D:94:ALA:O	1:D:98:MET:HG2	2.16	0.45
1:G:205:ALA:O	1:G:209:GLN:HG2	2.16	0.45
1:H:205:ALA:HA	1:H:208:GLU:OE1	2.16	0.45
1:J:29:PRO:CD	1:J:59:GLN:HB3	2.46	0.45
1:A:206:LYS:O	1:A:206:LYS:HD3	2.16	0.45
1:C:33:ALA:HB1	1:D:214:ALA:HB2	1.99	0.45
1:G:210:ASP:OD2	1:H:30:SER:HA	2.16	0.45
1:H:29:PRO:HA	1:H:32:ILE:HB	1.98	0.45
1:I:171:ARG:HA	1:I:171:ARG:NH1	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:MET:O	1:B:102:GLU:HG2	2.17	0.45
1:H:206:LYS:O	1:H:206:LYS:HD3	2.16	0.45
1:A:206:LYS:HA	1:A:206:LYS:HE2	1.99	0.45
1:D:136:ASP:OD2	1:I:171:ARG:HB2	2.17	0.45
1:A:150:HIS:O	1:A:154:LYS:HG2	2.17	0.45
1:B:27:THR:HB	1:B:31:ILE:HD11	1.98	0.45
1:B:89:THR:O	1:B:93:LEU:HD23	2.16	0.45
1:F:94:ALA:O	1:F:98:MET:SD	2.75	0.45
1:A:65:ALA:O	1:A:69:VAL:HG23	2.16	0.45
1:C:85:LYS:HG2	1:C:107:LEU:HB3	1.99	0.45
1:H:59:GLN:HB2	1:H:85:LYS:NZ	2.32	0.45
1:A:4:TYR:HB2	1:A:185:THR:HB	1.99	0.45
1:A:66:GLU:HA	1:A:69:VAL:HB	1.99	0.45
1:B:29:PRO:HD2	1:C:207:PHE:CZ	2.52	0.45
1:C:26:THR:HB	1:C:57:PHE:HD2	1.81	0.45
1:I:1:MET:HB2	1:J:156:HIS:CG	2.52	0.45
1:J:70:ASN:O	1:J:74:LYS:HG2	2.16	0.45
1:J:100:LYS:HE3	1:J:100:LYS:HB3	1.68	0.45
1:H:150:HIS:O	1:H:154:LYS:HG2	2.16	0.45
1:A:37:LYS:HE2	1:A:38:PRO:HD2	1.99	0.44
1:B:29:PRO:HB3	1:C:211:TRP:CE3	2.52	0.44
1:D:217:ARG:CZ	1:D:217:ARG:HB2	2.46	0.44
1:B:217:ARG:HB2	1:B:217:ARG:CZ	2.46	0.44
1:C:143:ILE:HD12	1:C:175:ASP:HB2	1.98	0.44
1:D:98:MET:O	1:D:102:GLU:HG2	2.18	0.44
1:G:14:LYS:HE3	1:G:14:LYS:HB3	1.65	0.44
1:J:81:ASP:OD2	1:J:81:ASP:N	2.50	0.44
1:B:112:TYR:HA	1:B:135:ILE:HD11	1.98	0.44
1:D:112:TYR:HA	1:D:135:ILE:HD11	1.99	0.44
1:B:151:GLN:O	1:B:155:MET:HG3	2.18	0.44
1:F:76:ARG:HG3	1:F:104:ILE:HD13	1.99	0.44
1:A:89:THR:O	1:A:93:LEU:HD23	2.18	0.44
1:A:219:SER:OG	1:E:71:ASP:OD1	2.36	0.44
1:B:171:ARG:NH2	1:G:136:ASP:O	2.50	0.44
1:E:85:LYS:HG2	1:E:107:LEU:HB3	1.98	0.44
1:F:206:LYS:O	1:F:206:LYS:HD3	2.17	0.44
1:H:85:LYS:HD2	1:H:107:LEU:HD12	1.99	0.44
1:J:143:ILE:HD12	1:J:175:ASP:HB2	2.00	0.44
1:C:107:LEU:HG	1:C:127:TYR:HB2	2.00	0.44
1:G:89:THR:O	1:G:93:LEU:HD23	2.17	0.44
1:A:14:LYS:HB3	1:A:14:LYS:HE3	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:VAL:HA	1:D:116:GLN:NE2	2.33	0.44
1:E:66:GLU:HA	1:E:69:VAL:HB	2.00	0.44
1:E:118:LEU:HD23	1:E:152:LEU:HB3	1.98	0.44
1:F:55:ARG:NH1	1:F:55:ARG:HA	2.32	0.44
1:F:90:ALA:HB2	1:J:195:ILE:HD12	1.99	0.44
1:H:194:MET:HE2	1:H:194:MET:O	2.17	0.44
1:E:55:ARG:CZ	1:E:55:ARG:HA	2.47	0.44
1:H:47:HIS:O	1:H:50:MET:HB2	2.18	0.44
1:A:220:ILE:HD13	1:E:71:ASP:HB3	1.99	0.44
1:C:25:VAL:HB	1:C:50:MET:HE2	2.00	0.44
1:F:9:ASP:O	1:F:13:VAL:HG13	2.18	0.44
1:G:6:ASP:OD2	1:G:6:ASP:N	2.46	0.44
1:I:14:LYS:HE3	1:I:14:LYS:HB3	1.58	0.44
1:I:107:LEU:HD11	1:I:163:LEU:HD23	2.00	0.44
1:B:39:LEU:HD23	1:B:40:ASP:H	1.82	0.43
1:C:29:PRO:HD2	1:D:207:PHE:CE1	2.53	0.43
1:G:177:LEU:HD21	1:G:184:ILE:HG12	2.00	0.43
1:H:7:THR:HG21	1:H:188:LEU:HD21	1.99	0.43
1:B:171:ARG:HA	1:B:171:ARG:NH1	2.31	0.43
1:D:64:THR:O	1:D:67:GLY:N	2.51	0.43
1:I:25:VAL:HB	1:I:46:LEU:HD21	1.99	0.43
1:E:159:GLN:OE1	1:E:159:GLN:N	2.40	0.43
1:G:95:ALA:HA	1:G:98:MET:SD	2.58	0.43
1:H:36:LYS:O	1:H:36:LYS:NZ	2.26	0.43
1:I:111:VAL:HA	1:I:116:GLN:NE2	2.33	0.43
1:I:205:ALA:O	1:I:209:GLN:HG2	2.18	0.43
1:A:107:LEU:HG	1:A:127:TYR:HB2	2.00	0.43
1:A:171:ARG:NH1	1:F:136:ASP:OD1	2.52	0.43
1:B:38:PRO:O	1:B:42:VAL:HG13	2.18	0.43
1:B:64:THR:O	1:B:67:GLY:N	2.51	0.43
1:D:2:GLU:HB2	1:D:183:SER:HB3	2.01	0.43
1:E:14:LYS:HE3	1:E:14:LYS:HB3	1.64	0.43
1:H:191:ALA:O	1:H:194:MET:HB3	2.19	0.43
1:I:55:ARG:HA	1:I:55:ARG:NH1	2.33	0.43
1:I:64:THR:O	1:I:67:GLY:N	2.52	0.43
1:C:76:ARG:HG3	1:C:104:ILE:HD13	2.01	0.43
1:H:109:THR:HG1	1:H:131:TYR:HH	1.67	0.43
1:A:85:LYS:HB3	1:A:107:LEU:HD22	2.01	0.43
1:F:211:TRP:NE1	1:F:219:SER:O	2.52	0.43
1:J:111:VAL:HA	1:J:116:GLN:NE2	2.34	0.43
1:A:171:ARG:NH2	1:F:140:GLY:O	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:137:ALA:HA	1:I:170:PRO:HG2	2.01	0.43
1:H:55:ARG:NH1	1:H:55:ARG:HA	2.33	0.43
1:A:39:LEU:O	1:A:43:LEU:HD22	2.19	0.43
1:A:76:ARG:HG3	1:A:104:ILE:HD13	2.01	0.43
1:F:29:PRO:HD2	1:J:207:PHE:CZ	2.54	0.43
1:F:156:HIS:HB3	1:J:1:MET:HB2	2.00	0.43
1:B:150:HIS:O	1:B:154:LYS:HG2	2.19	0.42
1:B:190:VAL:O	1:B:194:MET:HB2	2.19	0.42
1:C:64:THR:O	1:C:67:GLY:N	2.52	0.42
1:C:111:VAL:HA	1:C:116:GLN:NE2	2.34	0.42
1:J:59:GLN:OE1	1:J:60:VAL:N	2.53	0.42
1:B:92:GLY:O	1:B:96:ILE:HD13	2.19	0.42
1:D:171:ARG:HB2	1:I:136:ASP:HB3	2.02	0.42
1:E:111:VAL:HA	1:E:116:GLN:NE2	2.35	0.42
1:H:37:LYS:HE3	1:H:38:PRO:HD2	2.02	0.42
1:H:76:ARG:NH2	1:H:104:ILE:HG23	2.34	0.42
1:H:210:ASP:OD2	1:I:30:SER:HA	2.19	0.42
1:A:55:ARG:HA	1:A:55:ARG:NH1	2.34	0.42
1:C:189:ASP:OD1	1:C:189:ASP:N	2.53	0.42
1:E:96:ILE:O	1:E:100:LYS:HG2	2.20	0.42
1:H:111:VAL:HA	1:H:116:GLN:NE2	2.34	0.42
1:B:143:ILE:HD12	1:B:175:ASP:HB2	2.01	0.42
1:C:95:ALA:HA	1:C:98:MET:CE	2.50	0.42
1:F:38:PRO:O	1:F:42:VAL:HG13	2.20	0.42
1:H:59:GLN:HB2	1:H:85:LYS:HZ3	1.84	0.42
1:A:156:HIS:HB3	1:B:1:MET:HB2	2.01	0.42
1:C:29:PRO:HD3	1:C:59:GLN:HB3	2.02	0.42
1:F:65:ALA:HA	1:F:68:MET:HE2	2.00	0.42
1:I:207:PHE:CZ	1:J:29:PRO:HD2	2.54	0.42
1:B:43:LEU:HD11	1:B:79:ILE:HG21	2.02	0.42
1:C:44:PRO:O	1:C:48:GLU:HG2	2.20	0.42
1:D:131:TYR:HB3	1:D:134:ARG:HG2	2.02	0.42
1:D:191:ALA:O	1:D:194:MET:HB3	2.20	0.42
1:G:46:LEU:HD22	1:G:56:LEU:HD21	2.01	0.42
1:H:207:PHE:CZ	1:I:29:PRO:HD2	2.55	0.42
1:I:61:MET:HE1	1:I:62:ALA:HA	2.02	0.42
1:I:217:ARG:CZ	1:I:217:ARG:HB2	2.49	0.42
1:I:219:SER:HA	1:J:61:MET:HE3	2.01	0.42
1:A:2:GLU:HB2	1:A:183:SER:HB3	2.01	0.42
1:D:92:GLY:O	1:D:96:ILE:HG12	2.20	0.42
1:F:29:PRO:HB2	1:J:207:PHE:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:29:PRO:HB2	1:J:207:PHE:HE1	1.85	0.42
1:B:204:VAL:O	1:B:208:GLU:OE2	2.37	0.41
1:D:205:ALA:HA	1:D:208:GLU:OE2	2.20	0.41
1:F:217:ARG:CZ	1:F:217:ARG:HB2	2.50	0.41
1:I:207:PHE:HE2	1:J:29:PRO:HB2	1.85	0.41
1:G:119:LEU:HD23	1:G:119:LEU:HA	1.89	0.41
1:A:118:LEU:HD23	1:A:152:LEU:HB3	2.01	0.41
1:C:100:LYS:HD2	1:C:100:LYS:HA	1.84	0.41
1:F:14:LYS:HE3	1:F:14:LYS:HB3	1.75	0.41
1:F:89:THR:O	1:F:93:LEU:HD23	2.19	0.41
1:G:85:LYS:HG2	1:G:107:LEU:HB3	2.01	0.41
1:I:112:TYR:OH	1:I:134:ARG:HG2	2.20	0.41
1:I:206:LYS:O	1:I:206:LYS:HD3	2.20	0.41
1:A:186:LEU:HD12	1:A:190:VAL:HG12	2.02	0.41
1:C:42:VAL:O	1:C:46:LEU:HG	2.20	0.41
1:C:55:ARG:HA	1:C:55:ARG:NH1	2.35	0.41
1:D:44:PRO:O	1:D:48:GLU:HG2	2.21	0.41
1:E:65:ALA:O	1:E:69:VAL:HG23	2.21	0.41
1:G:111:VAL:HA	1:G:116:GLN:NE2	2.35	0.41
1:I:186:LEU:HD12	1:I:187:PRO:HD2	2.01	0.41
1:J:108:GLY:O	1:J:129:ALA:N	2.41	0.41
1:G:71:ASP:O	1:G:75:LEU:HG	2.19	0.41
1:J:59:GLN:NE2	1:J:109:THR:HG21	2.35	0.41
1:J:89:THR:O	1:J:93:LEU:HD23	2.20	0.41
1:J:150:HIS:O	1:J:154:LYS:HG2	2.21	0.41
1:A:36:LYS:O	1:A:36:LYS:NZ	2.26	0.41
1:C:65:ALA:HA	1:C:68:MET:CE	2.51	0.41
1:E:28:ASN:O	1:E:32:ILE:HG12	2.20	0.41
1:G:75:LEU:HD12	1:G:84:VAL:HG22	2.02	0.41
1:J:65:ALA:HB1	1:J:98:MET:HE1	2.02	0.41
1:A:177:LEU:HD21	1:A:184:ILE:HG12	2.03	0.41
1:B:111:VAL:HA	1:B:116:GLN:NE2	2.36	0.41
1:B:144:GLN:NE2	1:B:148:ASP:OD2	2.53	0.41
1:C:38:PRO:O	1:C:42:VAL:HG13	2.20	0.41
1:D:60:VAL:HG21	1:D:68:MET:HB3	2.03	0.41
1:F:51:GLY:O	1:F:53:GLN:NE2	2.37	0.41
1:A:95:ALA:HA	1:A:98:MET:SD	2.60	0.41
1:C:39:LEU:HD23	1:C:40:ASP:H	1.86	0.41
1:E:68:MET:SD	1:E:68:MET:N	2.94	0.41
1:A:47:HIS:CD2	1:A:52:GLY:HA2	2.55	0.41
1:F:112:TYR:OH	1:F:134:ARG:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:28:ASN:O	1:G:32:ILE:HG12	2.21	0.41
1:H:26:THR:HA	1:H:57:PHE:HB2	2.02	0.41
1:J:94:ALA:O	1:J:98:MET:SD	2.79	0.41
1:J:217:ARG:N	1:J:217:ARG:HE	2.18	0.41
1:A:46:LEU:HD23	1:A:50:MET:HE1	2.02	0.41
1:B:29:PRO:HD3	1:B:59:GLN:HB3	2.03	0.41
1:A:30:SER:HA	1:B:210:ASP:OD2	2.22	0.40
1:B:100:LYS:HE3	1:B:100:LYS:HB3	1.81	0.40
1:C:156:HIS:CD2	1:D:1:MET:HB2	2.56	0.40
1:D:30:SER:HA	1:E:210:ASP:OD2	2.21	0.40
1:A:29:PRO:HB2	1:B:207:PHE:CE2	2.56	0.40
1:A:29:PRO:HB2	1:B:207:PHE:HE2	1.86	0.40
1:F:1:MET:HB2	1:G:156:HIS:HB3	2.03	0.40
1:J:46:LEU:O	1:J:50:MET:HG2	2.22	0.40
1:F:9:ASP:HB3	1:F:12:ALA:HB3	2.04	0.40
1:F:215:PHE:HB3	1:F:217:ARG:NH2	2.34	0.40
1:G:1:MET:HB2	1:H:156:HIS:HB3	2.02	0.40
1:H:65:ALA:HA	1:H:68:MET:HE2	2.04	0.40
1:A:136:ASP:HB3	1:F:171:ARG:HB2	2.04	0.40
1:E:157:ALA:HB1	1:E:159:GLN:NE2	2.36	0.40
1:E:204:VAL:O	1:E:208:GLU:HG2	2.21	0.40
1:E:206:LYS:HD2	1:E:206:LYS:C	2.42	0.40
1:F:164:ALA:HB3	1:F:184:ILE:HG22	2.03	0.40
1:I:59:GLN:HB2	1:I:85:LYS:NZ	2.37	0.40
1:J:211:TRP:CD2	1:J:215:PHE:HD2	2.40	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 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	218/227 (96%)	213 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	218/227 (96%)	215 (99%)	3 (1%)	0	100	100
1	C	218/227 (96%)	213 (98%)	5 (2%)	0	100	100
1	D	218/227 (96%)	212 (97%)	6 (3%)	0	100	100
1	E	218/227 (96%)	211 (97%)	7 (3%)	0	100	100
1	F	218/227 (96%)	213 (98%)	5 (2%)	0	100	100
1	G	218/227 (96%)	213 (98%)	5 (2%)	0	100	100
1	H	218/227 (96%)	214 (98%)	4 (2%)	0	100	100
1	I	218/227 (96%)	214 (98%)	4 (2%)	0	100	100
1	J	218/227 (96%)	211 (97%)	7 (3%)	0	100	100
All	All	2180/2270 (96%)	2129 (98%)	51 (2%)	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	167/174 (96%)	157 (94%)	10 (6%)	16	44
1	B	167/174 (96%)	158 (95%)	9 (5%)	18	48
1	C	167/174 (96%)	157 (94%)	10 (6%)	16	44
1	D	167/174 (96%)	156 (93%)	11 (7%)	14	39
1	E	167/174 (96%)	157 (94%)	10 (6%)	16	44
1	F	167/174 (96%)	154 (92%)	13 (8%)	10	31
1	G	167/174 (96%)	157 (94%)	10 (6%)	16	44
1	H	167/174 (96%)	159 (95%)	8 (5%)	21	53
1	I	167/174 (96%)	158 (95%)	9 (5%)	18	48
1	J	167/174 (96%)	156 (93%)	11 (7%)	14	39
All	All	1670/1740 (96%)	1569 (94%)	101 (6%)	18	44

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	6	ASP
1	A	14	LYS
1	A	20	PHE
1	A	50	MET
1	A	61	MET
1	A	68	MET
1	A	98	MET
1	A	207	PHE
1	A	217	ARG
1	B	1	MET
1	B	6	ASP
1	B	20	PHE
1	B	46	LEU
1	B	61	MET
1	B	68	MET
1	B	100	LYS
1	B	155	MET
1	B	207	PHE
1	C	1	MET
1	C	14	LYS
1	C	20	PHE
1	C	39	LEU
1	C	61	MET
1	C	68	MET
1	C	98	MET
1	C	155	MET
1	C	207	PHE
1	C	215	PHE
1	D	1	MET
1	D	6	ASP
1	D	14	LYS
1	D	20	PHE
1	D	30	SER
1	D	39	LEU
1	D	61	MET
1	D	68	MET
1	D	189	ASP
1	D	207	PHE
1	D	208	GLU
1	E	1	MET
1	E	14	LYS

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Mol	Chain	Res	Type
1	E	20	PHE
1	E	43	LEU
1	E	55	ARG
1	E	93	LEU
1	E	98	MET
1	E	194	MET
1	E	206	LYS
1	E	207	PHE
1	F	1	MET
1	F	14	LYS
1	F	20	PHE
1	F	39	LEU
1	F	50	MET
1	F	61	MET
1	F	85	LYS
1	F	98	MET
1	F	102	GLU
1	F	186	LEU
1	F	207	PHE
1	F	208	GLU
1	F	217	ARG
1	G	1	MET
1	G	14	LYS
1	G	20	PHE
1	G	36	LYS
1	G	39	LEU
1	G	61	MET
1	G	98	MET
1	G	206	LYS
1	G	207	PHE
1	G	212	GLN
1	H	1	MET
1	H	6	ASP
1	H	20	PHE
1	H	61	MET
1	H	98	MET
1	H	100	LYS
1	H	207	PHE
1	H	208	GLU
1	I	1	MET
1	I	6	ASP
1	I	14	LYS

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Mol	Chain	Res	Type
1	I	20	PHE
1	I	61	MET
1	I	68	MET
1	I	98	MET
1	I	207	PHE
1	I	215	PHE
1	J	1	MET
1	J	6	ASP
1	J	20	PHE
1	J	61	MET
1	J	68	MET
1	J	98	MET
1	J	100	LYS
1	J	155	MET
1	J	186	LEU
1	J	207	PHE
1	J	217	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	212	GLN
1	B	209	GLN
1	C	144	GLN
1	E	156	HIS

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)

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.