



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Apr 10, 2017 – 02:10 PM EDT

PDB ID : 5L35
EMDB ID: : EMD-8314
Title : Cryo-EM structure of bacteriophage Sf6 at 2.9 Angstrom resolution
Authors : Zhao, H.; Tang, L.
Deposited on : 2016-08-03
Resolution : 2.89 Å(reported)

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

A user guide is available at

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

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) : rb-20029077

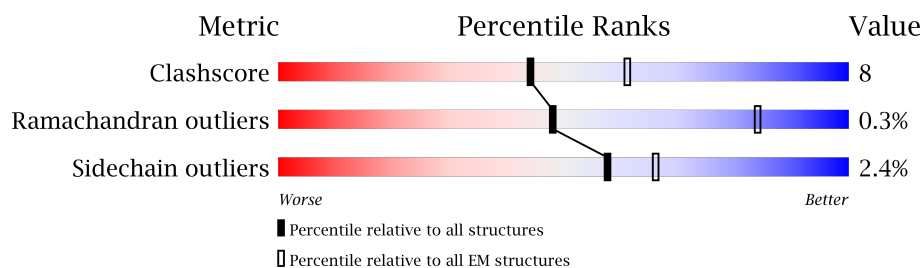
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.89 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 ≥ 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	422	
1	B	422	
1	C	422	
1	D	422	
1	E	422	
1	F	422	
1	G	422	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 22464 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 Gene 5 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		
1	B	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		
1	C	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		
1	D	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		
1	E	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		
1	F	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		
1	G	422	Total	C	N	O	S	0	0
			3209	2018	550	631	10		

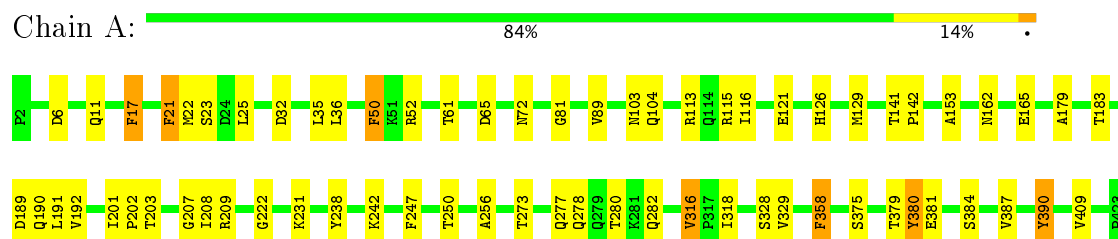
- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
2	E	1	Total	Cl	0
			1	1	

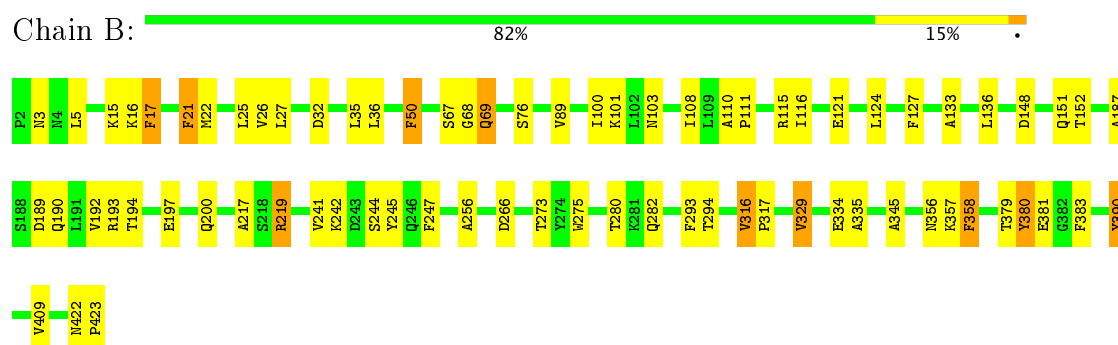
3 Residue-property plots

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

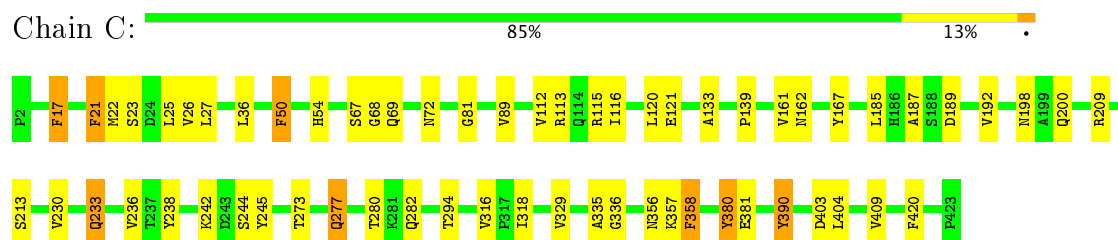
• Molecule 1: Gene 5 protein



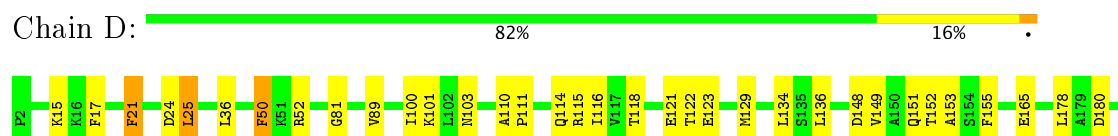
• Molecule 1: Gene 5 protein



• Molecule 1: Gene 5 protein



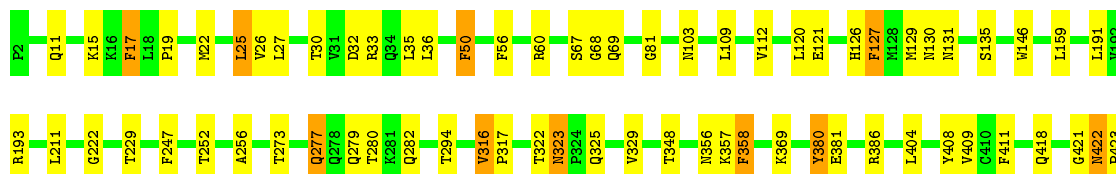
• Molecule 1: Gene 5 protein





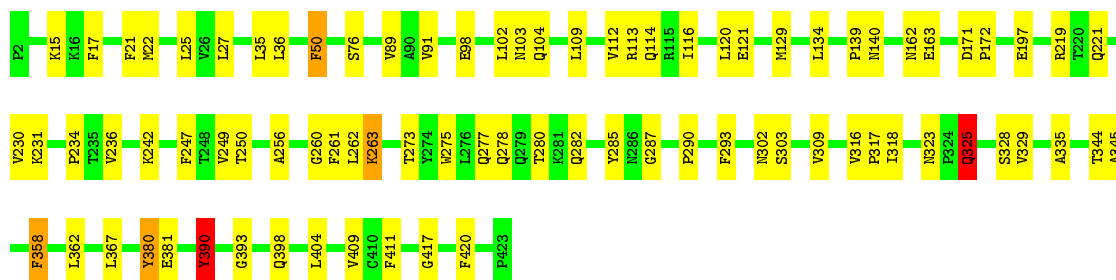
- Molecule 1: Gene 5 protein

Chain E: 84% 14%



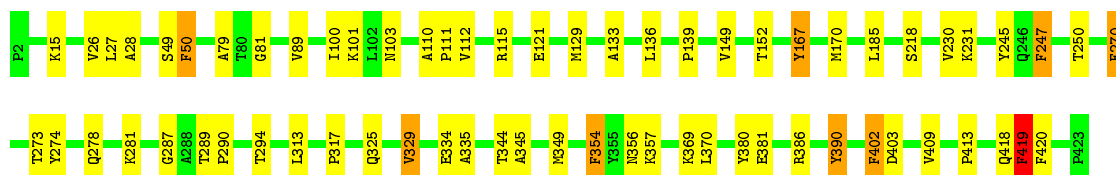
- Molecule 1: Gene 5 protein

Chain F: 80% 18%



- Molecule 1: Gene 5 protein

Chain G: 84% 14%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	68000	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)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.54	0/3274	0.78	3/4455 (0.1%)
1	B	0.52	0/3274	0.75	1/4455 (0.0%)
1	C	0.52	0/3274	0.78	2/4455 (0.0%)
1	D	0.52	0/3274	0.76	3/4455 (0.1%)
1	E	0.54	0/3274	0.81	7/4455 (0.2%)
1	F	0.55	1/3274 (0.0%)	0.79	3/4455 (0.1%)
1	G	0.50	0/3274	0.75	3/4455 (0.1%)
All	All	0.53	1/22918 (0.0%)	0.78	22/31185 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	E	0	1
1	F	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	325	GLN	CB-CG	6.18	1.69	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	193	ARG	NE-CZ-NH2	7.82	124.21	120.30
1	E	159	LEU	CA-CB-CG	7.67	132.95	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	25	LEU	CA-CB-CG	7.17	131.80	115.30
1	A	115	ARG	NE-CZ-NH1	-6.77	116.92	120.30
1	G	419	PHE	CB-CG-CD2	-6.70	116.11	120.80
1	E	193	ARG	CG-CD-NE	6.11	124.63	111.80
1	E	193	ARG	NE-CZ-NH1	-6.01	117.29	120.30
1	A	191	LEU	CA-CB-CG	5.93	128.93	115.30
1	F	390	TYR	CB-CG-CD2	-5.87	117.48	121.00
1	E	325	GLN	CG-CD-OE1	-5.84	109.91	121.60
1	F	325	GLN	CA-CB-CG	5.82	126.21	113.40
1	C	185	LEU	CB-CG-CD2	-5.80	101.14	111.00
1	A	115	ARG	NE-CZ-NH2	5.72	123.16	120.30
1	E	191	LEU	CA-CB-CG	5.63	128.24	115.30
1	E	25	LEU	CB-CG-CD2	-5.62	101.45	111.00
1	D	36	LEU	CA-CB-CG	5.50	127.94	115.30
1	G	287	GLY	N-CA-C	-5.39	99.63	113.10
1	C	233	GLN	CG-CD-OE1	-5.34	110.92	121.60
1	F	316	VAL	C-N-CD	5.13	139.18	128.40
1	D	316	VAL	C-N-CD	5.06	139.03	128.40
1	G	419	PHE	CB-CG-CD1	5.05	124.34	120.80
1	B	219	ARG	NE-CZ-NH1	-5.01	117.80	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	222	GLY	Peptide
1	E	222	GLY	Peptide
1	F	328	SER	Peptide

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	3209	0	3149	48	0
1	B	3209	0	3149	52	0
1	C	3209	0	3149	57	0
1	D	3209	0	3149	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3209	0	3149	52	0
1	F	3209	0	3149	63	0
1	G	3209	0	3149	51	0
2	E	1	0	0	0	0
All	All	22464	0	22043	350	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 8.

All (350) 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:422:ASN:N	1:E:422:ASN:HD22	1.71	0.87
1:C:390:TYR:HD1	1:C:390:TYR:H	1.21	0.85
1:G:390:TYR:H	1:G:390:TYR:HD1	1.24	0.80
1:F:398:GLN:HE21	1:G:370:LEU:HD23	1.47	0.79
1:C:26:VAL:HG21	1:C:213:SER:HB2	1.64	0.79
1:E:127:PHE:HE2	1:E:131:ASN:HD21	1.31	0.79
1:B:390:TYR:H	1:B:390:TYR:HD1	1.30	0.79
1:C:113:ARG:HH11	1:C:380:TYR:HD2	1.30	0.79
1:C:236:VAL:HG12	1:C:318:ILE:HA	1.65	0.78
1:G:15:LYS:HE3	1:G:103:ASN:HD22	1.49	0.77
1:F:280:THR:HG22	1:F:282:GLN:HG2	1.65	0.76
1:A:390:TYR:HD1	1:A:390:TYR:H	1.35	0.74
1:E:127:PHE:CE2	1:E:131:ASN:ND2	2.57	0.72
1:E:280:THR:HG22	1:E:282:GLN:HG2	1.72	0.70
1:A:89:VAL:HG12	1:A:116:ILE:HD11	1.73	0.70
1:A:81:GLY:HA3	1:A:409:VAL:HG22	1.75	0.69
1:A:162:ASN:OD1	1:F:22:MET:HB3	1.94	0.68
1:D:280:THR:HG22	1:D:282:GLN:HG2	1.74	0.68
1:A:380:TYR:CE1	1:A:381:GLU:HG2	2.29	0.67
1:G:89:VAL:HG21	1:G:112:VAL:HG13	1.77	0.66
1:B:280:THR:HG22	1:B:282:GLN:HG2	1.78	0.66
1:D:371:HIS:O	1:D:372:SER:HB2	1.95	0.66
1:G:390:TYR:HD1	1:G:390:TYR:N	1.93	0.65
1:F:15:LYS:HE3	1:F:103:ASN:HD22	1.61	0.65
1:E:380:TYR:CD1	1:E:381:GLU:HG2	2.31	0.65
1:F:303:SER:HB3	1:F:309:VAL:HG22	1.79	0.65
1:G:344:THR:HG22	1:G:345:ALA:H	1.63	0.64
1:C:356:ASN:OD1	1:C:357:LYS:N	2.30	0.64
1:A:113:ARG:HB3	1:A:380:TYR:HD2	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:390:TYR:H	1:F:390:TYR:HD1	1.45	0.63
1:G:419:PHE:H	1:G:419:PHE:HD1	1.46	0.63
1:C:68:GLY:O	1:C:69:GLN:HG3	1.98	0.63
1:E:380:TYR:CE1	1:E:381:GLU:HG2	2.33	0.63
1:E:277:GLN:HG2	1:E:280:THR:H	1.63	0.63
1:C:189:ASP:HB2	1:D:188:SER:HA	1.81	0.63
1:D:377:VAL:HG22	1:D:386:ARG:HD3	1.79	0.63
1:G:390:TYR:CD1	1:G:390:TYR:N	2.67	0.62
1:E:277:GLN:HG3	1:E:279:GLN:H	1.64	0.62
1:B:89:VAL:HG12	1:B:116:ILE:HD11	1.82	0.62
1:B:15:LYS:HE3	1:B:103:ASN:HD22	1.64	0.62
1:E:126:HIS:O	1:E:130:ASN:HB2	1.98	0.62
1:D:118:THR:O	1:D:121:GLU:HG2	1.99	0.62
1:F:113:ARG:HB3	1:F:380:TYR:HD2	1.66	0.61
1:E:127:PHE:CE1	1:E:408:TYR:HB3	2.36	0.60
1:E:127:PHE:HE1	1:E:408:TYR:HB3	1.64	0.60
1:F:273:THR:HG22	1:F:329:VAL:HG22	1.83	0.60
1:B:217:ALA:HA	1:C:282:GLN:HE21	1.67	0.60
1:F:25:LEU:HA	1:F:121:GLU:OE1	2.01	0.60
1:G:278:GLN:O	1:G:281:LYS:NZ	2.35	0.60
1:D:231:LYS:HB3	1:D:250:THR:HG23	1.82	0.60
1:C:273:THR:HG22	1:C:329:VAL:HG22	1.83	0.60
1:C:238:TYR:O	1:C:242:LYS:HB2	2.02	0.59
1:C:380:TYR:CD1	1:C:381:GLU:HG2	2.37	0.59
1:F:89:VAL:HG12	1:F:116:ILE:HD11	1.84	0.59
1:C:26:VAL:HG23	1:C:27:LEU:H	1.66	0.59
1:G:274:TYR:CZ	1:G:290:PRO:HG3	2.38	0.58
1:D:273:THR:HG22	1:D:329:VAL:HG22	1.84	0.58
1:E:120:LEU:HD12	1:E:404:LEU:HD21	1.85	0.58
1:G:245:TYR:HD2	1:G:413:PRO:HD2	1.67	0.58
1:D:123:GLU:OE1	1:E:60:ARG:NH1	2.28	0.58
1:A:6:ASP:N	1:A:6:ASP:OD1	2.35	0.58
1:B:136:LEU:HD12	1:B:152:THR:HG22	1.86	0.58
1:B:22:MET:HG3	1:C:162:ASN:ND2	2.20	0.57
1:B:192:VAL:HG21	1:C:187:ALA:HB3	1.87	0.57
1:B:25:LEU:HA	1:B:121:GLU:OE1	2.04	0.57
1:E:421:GLY:C	1:E:422:ASN:HD22	2.07	0.57
1:C:236:VAL:CG1	1:C:318:ILE:HA	2.32	0.57
1:E:422:ASN:N	1:E:422:ASN:ND2	2.48	0.57
1:D:136:LEU:HD12	1:D:152:THR:HG22	1.88	0.56
1:F:398:GLN:NE2	1:G:370:LEU:HA	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:LEU:HD22	1:C:409:VAL:HG23	1.86	0.56
1:D:369:LYS:HB2	1:D:386:ARG:NH2	2.20	0.56
1:F:129:MET:HE3	1:F:219:ARG:HB3	1.86	0.56
1:G:149:VAL:HG13	1:G:170:MET:HE1	1.87	0.56
1:E:22:MET:SD	1:F:162:ASN:ND2	2.78	0.56
1:F:98:GLU:HA	1:F:102:LEU:HB2	1.87	0.56
1:D:244:SER:O	1:D:245:TYR:HB2	2.06	0.56
1:D:285:TYR:CE1	1:D:290:PRO:HG3	2.40	0.56
1:F:390:TYR:N	1:F:390:TYR:HD1	2.04	0.56
1:D:238:TYR:O	1:D:242:LYS:HB3	2.06	0.56
1:E:32:ASP:OD1	1:E:33:ARG:N	2.40	0.55
1:C:277:GLN:HG2	1:C:280:THR:HB	1.87	0.55
1:C:403:ASP:OD1	1:C:403:ASP:N	2.39	0.55
1:D:100:ILE:HG13	1:D:101:LYS:HG3	1.86	0.55
1:B:241:VAL:HG11	1:B:316:VAL:HG11	1.88	0.55
1:C:380:TYR:CE1	1:C:381:GLU:HG2	2.42	0.55
1:F:261:PHE:CD2	1:F:262:LEU:HD13	2.42	0.55
1:D:153:ALA:HB2	1:D:208:ILE:HB	1.88	0.54
1:A:179:ALA:O	1:A:183:THR:HG23	2.07	0.54
1:A:25:LEU:HA	1:A:121:GLU:OE1	2.06	0.54
1:E:129:MET:HG3	1:E:418:GLN:HE21	1.73	0.54
1:D:148:ASP:O	1:D:151:GLN:HG2	2.08	0.54
1:B:133:ALA:O	1:B:294:THR:HG23	2.08	0.54
1:B:32:ASP:OD2	1:B:35:LEU:HB2	2.07	0.54
1:D:358:PHE:N	1:D:358:PHE:CD1	2.76	0.54
1:F:260:GLY:H	1:F:302:ASN:HB3	1.73	0.53
1:B:390:TYR:N	1:B:390:TYR:CD1	2.74	0.53
1:F:234:PRO:HG3	1:F:249:VAL:HG23	1.89	0.53
1:F:76:SER:O	1:F:242:LYS:HD2	2.07	0.53
1:C:89:VAL:HG12	1:C:116:ILE:HD11	1.89	0.53
1:G:380:TYR:CD2	1:G:381:GLU:HG2	2.43	0.53
1:G:81:GLY:HA3	1:G:409:VAL:HG22	1.91	0.53
1:D:193:ARG:O	1:D:197:GLU:HG2	2.09	0.53
1:C:244:SER:O	1:C:245:TYR:HB2	2.08	0.53
1:F:393:GLY:HA3	1:G:390:TYR:CE2	2.43	0.53
1:C:26:VAL:HG23	1:C:27:LEU:N	2.24	0.53
1:G:129:MET:HG3	1:G:418:GLN:HE21	1.73	0.53
1:E:273:THR:HG22	1:E:329:VAL:HG22	1.89	0.53
1:B:217:ALA:HA	1:C:282:GLN:NE2	2.24	0.53
1:D:110:ALA:H	1:D:111:PRO:HD2	1.72	0.53
1:G:354:PHE:H	1:G:354:PHE:HD1	1.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:129:MET:HG3	1:D:418:GLN:HE21	1.73	0.52
1:G:334:GLU:HG2	1:G:335:ALA:N	2.24	0.52
1:B:76:SER:O	1:B:242:LYS:HD2	2.10	0.52
1:B:15:LYS:HE3	1:B:103:ASN:ND2	2.25	0.52
1:D:129:MET:HG3	1:D:418:GLN:NE2	2.24	0.52
1:A:22:MET:HG3	1:A:23:SER:H	1.75	0.52
1:C:25:LEU:HA	1:C:121:GLU:OE1	2.10	0.52
1:E:135:SER:HB3	1:E:294:THR:HG21	1.91	0.52
1:E:273:THR:HG22	1:E:329:VAL:CG2	2.39	0.52
1:B:36:LEU:HD22	1:B:409:VAL:HG23	1.92	0.52
1:F:380:TYR:CE1	1:F:381:GLU:HG2	2.44	0.52
1:C:22:MET:HG2	1:C:23:SER:H	1.75	0.52
1:E:36:LEU:HD22	1:E:409:VAL:HG23	1.92	0.52
1:F:36:LEU:HD22	1:F:409:VAL:HG23	1.92	0.52
1:B:380:TYR:CE1	1:B:381:GLU:HG2	2.44	0.51
1:E:348:THR:HG23	1:F:290:PRO:HG2	1.92	0.51
1:D:89:VAL:HG12	1:D:116:ILE:HD11	1.93	0.51
1:G:356:ASN:OD1	1:G:357:LYS:N	2.42	0.51
1:D:134:LEU:HD13	1:D:155:PHE:HE2	1.76	0.51
1:F:390:TYR:N	1:F:390:TYR:CD1	2.77	0.51
1:G:369:LYS:HB3	1:G:386:ARG:NH2	2.25	0.51
1:A:390:TYR:N	1:A:390:TYR:CD1	2.74	0.51
1:A:50:PHE:CD1	1:A:50:PHE:N	2.79	0.51
1:B:15:LYS:O	1:B:16:LYS:HG3	2.11	0.51
1:A:247:PHE:CD2	1:A:316:VAL:HG12	2.46	0.51
1:D:409:VAL:HG21	1:D:411:PHE:CZ	2.46	0.51
1:A:192:VAL:HG21	1:B:187:ALA:HB3	1.93	0.51
1:B:193:ARG:O	1:B:197:GLU:HG2	2.11	0.50
1:E:25:LEU:HA	1:E:121:GLU:OE1	2.11	0.50
1:F:236:VAL:HG12	1:F:318:ILE:HA	1.92	0.50
1:G:369:LYS:HB3	1:G:386:ARG:HH21	1.77	0.50
1:B:244:SER:O	1:B:245:TYR:HB2	2.12	0.50
1:A:318:ILE:HD12	1:A:328:SER:OG	2.12	0.50
1:E:129:MET:HG3	1:E:418:GLN:NE2	2.25	0.50
1:A:273:THR:HG22	1:A:329:VAL:HG22	1.94	0.50
1:B:247:PHE:CE2	1:B:317:PRO:HD3	2.47	0.50
1:C:89:VAL:HG11	1:C:112:VAL:HG13	1.94	0.50
1:F:114:GLN:HG2	1:F:380:TYR:OH	2.12	0.50
1:B:219:ARG:NH1	1:B:266:ASP:OD1	2.44	0.49
1:E:322:THR:C	1:E:323:ASN:HD22	2.14	0.49
1:F:140:ASN:OD1	1:F:140:ASN:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:MET:HG2	1:C:23:SER:N	2.27	0.49
1:C:390:TYR:N	1:C:390:TYR:CD1	2.71	0.49
1:E:50:PHE:CD1	1:E:50:PHE:N	2.79	0.49
1:C:192:VAL:HG21	1:D:187:ALA:HB3	1.94	0.49
1:D:121:GLU:HG3	1:D:122:THR:N	2.27	0.49
1:E:109:LEU:O	1:E:112:VAL:HG22	2.13	0.49
1:C:230:VAL:HG23	1:C:336:GLY:H	1.78	0.49
1:A:238:TYR:O	1:A:242:LYS:HB3	2.12	0.49
1:D:50:PHE:N	1:D:50:PHE:CD1	2.80	0.49
1:E:68:GLY:O	1:E:69:GLN:HG3	2.13	0.49
1:F:120:LEU:HD21	1:F:362:LEU:HD21	1.95	0.49
1:C:50:PHE:N	1:C:50:PHE:CD1	2.79	0.48
1:B:194:THR:HG22	1:B:200:GLN:HB2	1.95	0.48
1:B:21:PHE:CD1	1:B:21:PHE:N	2.82	0.48
1:C:113:ARG:NH1	1:C:380:TYR:HD2	2.04	0.48
1:D:230:VAL:HG23	1:D:335:ALA:HA	1.95	0.48
1:F:261:PHE:HD2	1:F:262:LEU:HD13	1.78	0.48
1:A:22:MET:HG3	1:A:23:SER:N	2.28	0.48
1:D:81:GLY:CA	1:D:409:VAL:HG12	2.44	0.48
1:G:50:PHE:N	1:G:50:PHE:CD1	2.82	0.48
1:A:61:THR:HG21	1:A:65:ASP:H	1.79	0.48
1:C:161:VAL:CG1	1:C:356:ASN:HD22	2.26	0.48
1:G:100:ILE:HG13	1:G:101:LYS:HG2	1.94	0.48
1:G:402:PHE:CD1	1:G:402:PHE:N	2.81	0.48
1:A:231:LYS:HB3	1:A:250:THR:HG23	1.96	0.48
1:E:30:THR:HG21	1:E:211:LEU:HD11	1.95	0.48
1:F:98:GLU:HA	1:F:102:LEU:HD12	1.95	0.48
1:D:15:LYS:HE3	1:D:103:ASN:ND2	2.28	0.48
1:F:50:PHE:N	1:F:50:PHE:CD1	2.81	0.47
1:A:358:PHE:N	1:A:358:PHE:CD1	2.82	0.47
1:C:273:THR:HG22	1:C:329:VAL:CG2	2.43	0.47
1:G:152:THR:HB	1:G:354:PHE:CD2	2.49	0.47
1:A:11:GLN:OE1	1:A:11:GLN:N	2.47	0.47
1:B:108:ILE:HG23	1:C:54:HIS:CD2	2.50	0.47
1:E:229:THR:O	1:E:252:THR:HG22	2.14	0.47
1:F:120:LEU:HD12	1:F:404:LEU:HD21	1.97	0.47
1:F:323:ASN:O	1:F:325:GLN:N	2.47	0.47
1:B:89:VAL:HG23	1:C:72:ASN:ND2	2.30	0.47
1:A:201:ILE:HB	1:A:202:PRO:HD2	1.96	0.47
1:A:273:THR:HG22	1:A:329:VAL:CG2	2.45	0.47
1:B:50:PHE:CD1	1:B:50:PHE:N	2.83	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:209:ARG:HH12	1:D:211:LEU:HD21	1.79	0.47
1:F:358:PHE:CD1	1:F:358:PHE:N	2.82	0.47
1:F:139:PRO:HA	1:F:420:PHE:CD1	2.49	0.47
1:A:72:ASN:HB2	1:F:91:VAL:HG12	1.96	0.47
1:D:24:ASP:O	1:D:25:LEU:HG	2.14	0.47
1:B:273:THR:HG22	1:B:329:VAL:HG22	1.97	0.46
1:E:356:ASN:OD1	1:E:357:LYS:N	2.48	0.46
1:G:231:LYS:HB3	1:G:250:THR:HG23	1.97	0.46
1:B:68:GLY:O	1:B:69:GLN:HG3	2.15	0.46
1:C:17:PHE:CD1	1:C:17:PHE:N	2.83	0.46
1:A:277:GLN:HG3	1:A:278:GLN:N	2.29	0.46
1:C:139:PRO:HA	1:C:420:PHE:CD1	2.51	0.46
1:G:230:VAL:HG23	1:G:335:ALA:HA	1.98	0.46
1:C:233:GLN:HG2	1:C:233:GLN:O	2.14	0.46
1:D:273:THR:HG22	1:D:329:VAL:CG2	2.45	0.46
1:D:236:VAL:HG11	1:D:317:PRO:HD2	1.97	0.46
1:D:180:ASP:HB3	1:E:146:TRP:CZ3	2.51	0.46
1:F:221:GLN:O	1:F:263:LYS:HG3	2.16	0.46
1:F:380:TYR:CD1	1:F:381:GLU:HG2	2.50	0.46
1:A:103:ASN:O	1:A:104:GLN:HB2	2.14	0.46
1:G:115:ARG:HD2	1:G:115:ARG:HA	1.53	0.46
1:G:273:THR:HG22	1:G:329:VAL:HG22	1.97	0.46
1:A:126:HIS:HA	1:A:129:MET:HE2	1.98	0.46
1:B:334:GLU:HG2	1:B:335:ALA:H	1.81	0.46
1:E:15:LYS:HE3	1:E:103:ASN:HD22	1.80	0.46
1:A:165:GLU:OE2	1:A:209:ARG:HD3	2.15	0.46
1:D:277:GLN:HG3	1:D:278:GLN:N	2.31	0.46
1:D:52:ARG:HH11	1:D:52:ARG:HG3	1.82	0.45
1:E:358:PHE:N	1:E:358:PHE:CD1	2.84	0.45
1:A:21:PHE:N	1:A:21:PHE:CD1	2.84	0.45
1:C:50:PHE:N	1:C:50:PHE:HD1	2.14	0.45
1:D:358:PHE:N	1:D:358:PHE:HD1	2.14	0.45
1:B:380:TYR:CD1	1:B:381:GLU:HG2	2.52	0.45
1:F:273:THR:HG22	1:F:329:VAL:CG2	2.47	0.45
1:B:100:ILE:HG13	1:B:101:LYS:HG2	1.97	0.45
1:E:11:GLN:N	1:E:11:GLN:OE1	2.50	0.45
1:B:189:ASP:OD1	1:B:190:GLN:N	2.50	0.45
1:E:247:PHE:CD2	1:E:316:VAL:HG12	2.52	0.45
1:G:185:LEU:HD12	1:G:185:LEU:O	2.16	0.45
1:A:17:PHE:CD1	1:A:17:PHE:N	2.85	0.45
1:C:21:PHE:N	1:C:21:PHE:CD1	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:369:LYS:HB3	1:E:386:ARG:NH2	2.32	0.45
1:G:247:PHE:HE1	1:G:313:LEU:HB2	1.81	0.45
1:A:375:SER:HB2	1:A:387:VAL:O	2.16	0.45
1:B:26:VAL:HG23	1:B:27:LEU:N	2.32	0.45
1:G:247:PHE:CE1	1:G:313:LEU:HB2	2.52	0.45
1:A:380:TYR:CD1	1:A:381:GLU:HG2	2.52	0.44
1:B:3:ASN:HB3	1:B:5:LEU:HD22	1.98	0.44
1:C:167:TYR:CE1	1:C:209:ARG:HD2	2.53	0.44
1:G:218:SER:HB2	1:G:349:MET:O	2.17	0.44
1:G:49:SER:HA	1:G:79:ALA:O	2.17	0.44
1:B:89:VAL:HG23	1:C:72:ASN:HD21	1.83	0.44
1:F:275:TRP:NE1	1:F:293:PHE:HA	2.32	0.44
1:A:203:THR:HG23	1:A:209:ARG:NH1	2.32	0.44
1:A:52:ARG:HG3	1:A:52:ARG:HH11	1.83	0.44
1:B:124:LEU:O	1:B:127:PHE:N	2.51	0.44
1:F:109:LEU:O	1:F:112:VAL:HG22	2.17	0.44
1:G:110:ALA:HB3	1:G:111:PRO:HD3	1.98	0.44
1:B:275:TRP:NE1	1:B:293:PHE:HA	2.33	0.44
1:F:27:LEU:N	1:F:121:GLU:OE2	2.49	0.44
1:G:136:LEU:HD12	1:G:152:THR:HG22	1.98	0.44
1:C:358:PHE:CD1	1:C:358:PHE:N	2.86	0.44
1:G:289:THR:O	1:G:289:THR:HG23	2.17	0.44
1:G:334:GLU:HG2	1:G:335:ALA:H	1.82	0.44
1:B:115:ARG:HA	1:B:115:ARG:HD2	1.50	0.44
1:B:356:ASN:OD1	1:B:357:LYS:N	2.50	0.44
1:C:139:PRO:HA	1:C:420:PHE:CG	2.53	0.44
1:A:153:ALA:HB2	1:A:208:ILE:HB	1.99	0.43
1:C:280:THR:HG22	1:C:282:GLN:CG	2.48	0.43
1:F:231:LYS:HB3	1:F:250:THR:HG23	2.00	0.43
1:G:247:PHE:CE2	1:G:317:PRO:CD	3.01	0.43
1:C:380:TYR:HD1	1:C:381:GLU:N	2.17	0.43
1:F:280:THR:CG2	1:F:282:GLN:HG2	2.41	0.43
1:G:270:PHE:N	1:G:270:PHE:HD1	2.16	0.43
1:B:21:PHE:HD1	1:B:21:PHE:N	2.16	0.43
1:B:358:PHE:N	1:B:358:PHE:CD1	2.87	0.43
1:C:198:ASN:HB3	1:C:200:GLN:HG2	2.00	0.43
1:D:15:LYS:HE3	1:D:103:ASN:HD22	1.83	0.43
1:A:32:ASP:OD2	1:A:35:LEU:HB2	2.18	0.43
1:A:50:PHE:HD1	1:A:50:PHE:N	2.16	0.43
1:B:17:PHE:N	1:B:17:PHE:CD1	2.86	0.43
1:C:81:GLY:HA3	1:C:409:VAL:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:81:GLY:HA3	1:E:409:VAL:HG22	1.99	0.43
1:E:17:PHE:CD1	1:E:17:PHE:N	2.86	0.43
1:A:17:PHE:HD1	1:A:17:PHE:N	2.16	0.43
1:F:277:GLN:HG3	1:F:278:GLN:N	2.33	0.43
1:G:270:PHE:N	1:G:270:PHE:CD1	2.86	0.43
1:G:26:VAL:HG23	1:G:27:LEU:N	2.33	0.43
1:B:280:THR:CG2	1:B:282:GLN:HG2	2.46	0.43
1:D:149:VAL:HG21	1:D:178:LEU:HD11	2.01	0.43
1:D:344:THR:HB	1:D:347:GLN:CG	2.49	0.43
1:E:422:ASN:HA	1:E:423:PRO:HD3	1.63	0.43
1:F:102:LEU:HA	1:F:102:LEU:HD23	1.78	0.43
1:G:139:PRO:HA	1:G:420:PHE:CD1	2.54	0.43
1:G:167:TYR:N	1:G:167:TYR:CD1	2.87	0.43
1:D:241:VAL:HG11	1:D:316:VAL:HG11	2.01	0.42
1:A:113:ARG:HB3	1:A:380:TYR:CD2	2.48	0.42
1:C:133:ALA:O	1:C:294:THR:HG23	2.19	0.42
1:D:110:ALA:N	1:D:111:PRO:HD2	2.34	0.42
1:E:15:LYS:HE3	1:E:103:ASN:ND2	2.34	0.42
1:A:358:PHE:HD1	1:A:358:PHE:N	2.17	0.42
1:C:17:PHE:HD1	1:C:17:PHE:N	2.16	0.42
1:F:221:GLN:HG3	1:F:344:THR:O	2.19	0.42
1:E:19:PRO:HB3	1:F:163:GLU:HG3	2.02	0.42
1:F:249:VAL:HG22	1:F:250:THR:H	1.84	0.42
1:G:28:ALA:N	1:G:121:GLU:OE2	2.50	0.42
1:G:325:GLN:H	1:G:325:GLN:HG2	1.55	0.42
1:G:419:PHE:CD1	1:G:419:PHE:N	2.88	0.42
1:B:379:THR:HA	1:B:383:PHE:O	2.20	0.42
1:E:369:LYS:HB2	1:E:369:LYS:HE3	1.91	0.42
1:A:379:THR:HG22	1:A:384:SER:HA	2.01	0.42
1:C:115:ARG:HA	1:C:115:ARG:HD2	1.70	0.42
1:F:15:LYS:HB3	1:F:104:GLN:NE2	2.35	0.42
1:G:369:LYS:HB2	1:G:369:LYS:HE3	1.79	0.42
1:A:189:ASP:OD1	1:A:190:GLN:N	2.53	0.42
1:B:108:ILE:HD12	1:C:54:HIS:NE2	2.34	0.42
1:D:221:GLN:HB2	1:D:345:ALA:O	2.20	0.42
1:D:277:GLN:HG2	1:D:280:THR:H	1.85	0.42
1:B:247:PHE:CD2	1:B:316:VAL:HG13	2.54	0.41
1:C:120:LEU:HD12	1:C:404:LEU:HD21	2.02	0.41
1:E:348:THR:HG23	1:F:290:PRO:CG	2.49	0.41
1:F:285:TYR:CE2	1:F:287:GLY:HA2	2.55	0.41
1:F:236:VAL:CG1	1:F:318:ILE:HA	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:ALA:N	1:B:111:PRO:CD	2.83	0.41
1:F:230:VAL:HG23	1:F:335:ALA:HA	2.02	0.41
1:E:247:PHE:CE2	1:E:317:PRO:HD3	2.55	0.41
1:F:247:PHE:CE2	1:F:317:PRO:HD3	2.56	0.41
1:B:422:ASN:HA	1:B:423:PRO:HD3	1.86	0.41
1:D:386:ARG:HA	1:D:386:ARG:HD2	1.79	0.41
1:F:221:GLN:HB2	1:F:345:ALA:O	2.21	0.41
1:F:113:ARG:CB	1:F:380:TYR:HD2	2.33	0.41
1:E:17:PHE:HD1	1:E:17:PHE:N	2.19	0.41
1:E:35:LEU:HD23	1:E:411:PHE:CZ	2.55	0.41
1:A:61:THR:HG21	1:A:65:ASP:N	2.35	0.41
1:B:148:ASP:O	1:B:151:GLN:HG2	2.21	0.41
1:D:21:PHE:N	1:D:21:PHE:CD1	2.88	0.41
1:D:111:PRO:HG2	1:E:56:PHE:HE2	1.84	0.41
1:F:171:ASP:HB2	1:F:172:PRO:CD	2.50	0.41
1:G:133:ALA:O	1:G:294:THR:HG23	2.20	0.41
1:E:358:PHE:N	1:E:358:PHE:HD1	2.18	0.41
1:F:113:ARG:HB3	1:F:380:TYR:CD2	2.51	0.41
1:F:35:LEU:HD23	1:F:411:PHE:CZ	2.56	0.41
1:F:367:LEU:HA	1:F:367:LEU:HD23	1.84	0.41
1:D:114:GLN:HB3	1:D:380:TYR:CE2	2.56	0.40
1:E:380:TYR:C	1:E:380:TYR:CD1	2.95	0.40
1:F:134:LEU:O	1:F:417:GLY:HA3	2.21	0.40
1:G:403:ASP:N	1:G:403:ASP:OD1	2.53	0.40
1:A:141:THR:HG22	1:A:142:PRO:O	2.21	0.40
1:A:36:LEU:HD22	1:A:409:VAL:HG23	2.04	0.40
1:A:280:THR:HG22	1:A:282:GLN:HG2	2.04	0.40
1:C:242:LYS:HE2	1:C:242:LYS:HB3	1.91	0.40
1:C:230:VAL:HG23	1:C:335:ALA:HA	2.02	0.40
1:D:165:GLU:OE2	1:D:209:ARG:HD2	2.21	0.40
1:C:380:TYR:CD1	1:C:380:TYR:C	2.95	0.40
1:D:115:ARG:HD2	1:D:115:ARG:HA	1.54	0.40
1:A:207:GLY:N	1:F:197:GLU:O	2.50	0.40
1:E:26:VAL:HG23	1:E:27:LEU:N	2.36	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	420/422 (100%)	408 (97%)	11 (3%)	1 (0%)	51	82
1	B	420/422 (100%)	399 (95%)	17 (4%)	4 (1%)	18	51
1	C	420/422 (100%)	404 (96%)	15 (4%)	1 (0%)	51	82
1	D	420/422 (100%)	396 (94%)	23 (6%)	1 (0%)	51	82
1	E	420/422 (100%)	400 (95%)	18 (4%)	2 (0%)	32	68
1	F	420/422 (100%)	405 (96%)	14 (3%)	1 (0%)	51	82
1	G	420/422 (100%)	401 (96%)	19 (4%)	0	100	100
All	All	2940/2954 (100%)	2813 (96%)	117 (4%)	10 (0%)	48	77

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	67	SER
1	E	67	SER
1	A	256	ALA
1	B	67	SER
1	D	256	ALA
1	F	256	ALA
1	B	69	GLN
1	E	256	ALA
1	B	256	ALA
1	B	345	ALA

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	350/350 (100%)	343 (98%)	7 (2%)	60	87
1	B	350/350 (100%)	342 (98%)	8 (2%)	56	85
1	C	350/350 (100%)	342 (98%)	8 (2%)	56	85
1	D	350/350 (100%)	340 (97%)	10 (3%)	48	81
1	E	350/350 (100%)	341 (97%)	9 (3%)	51	83
1	F	350/350 (100%)	342 (98%)	8 (2%)	56	85
1	G	350/350 (100%)	341 (97%)	9 (3%)	51	83
All	All	2450/2450 (100%)	2391 (98%)	59 (2%)	58	84

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	PHE
1	A	21	PHE
1	A	50	PHE
1	A	316	VAL
1	A	358	PHE
1	A	380	TYR
1	A	390	TYR
1	B	17	PHE
1	B	21	PHE
1	B	50	PHE
1	B	316	VAL
1	B	329	VAL
1	B	358	PHE
1	B	380	TYR
1	B	390	TYR
1	C	17	PHE
1	C	21	PHE
1	C	50	PHE
1	C	277	GLN
1	C	316	VAL
1	C	358	PHE
1	C	380	TYR
1	C	390	TYR
1	D	17	PHE
1	D	21	PHE
1	D	50	PHE
1	D	316	VAL
1	D	329	VAL
1	D	358	PHE

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Mol	Chain	Res	Type
1	D	371	HIS
1	D	372	SER
1	D	374	ASP
1	D	380	TYR
1	E	17	PHE
1	E	50	PHE
1	E	127	PHE
1	E	277	GLN
1	E	316	VAL
1	E	323	ASN
1	E	358	PHE
1	E	380	TYR
1	E	422	ASN
1	F	17	PHE
1	F	21	PHE
1	F	50	PHE
1	F	263	LYS
1	F	325	GLN
1	F	358	PHE
1	F	380	TYR
1	F	390	TYR
1	G	50	PHE
1	G	167	TYR
1	G	247	PHE
1	G	270	PHE
1	G	329	VAL
1	G	354	PHE
1	G	390	TYR
1	G	402	PHE
1	G	419	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	ASN
1	C	282	GLN
1	E	277	GLN
1	E	418	GLN
1	E	422	ASN
1	F	282	GLN
1	F	398	GLN
1	G	286	ASN

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 ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.