Full wwPDB X-ray Structure Validation Report ⓘ

May 19, 2022 – 02:44 pm BST

PDB ID	:	7PDJ
Title	:	R12E vFLIP mutant
Authors	:	Barrett, T.E.
Deposited on	:	2021-08-05
Resolution	:	4.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

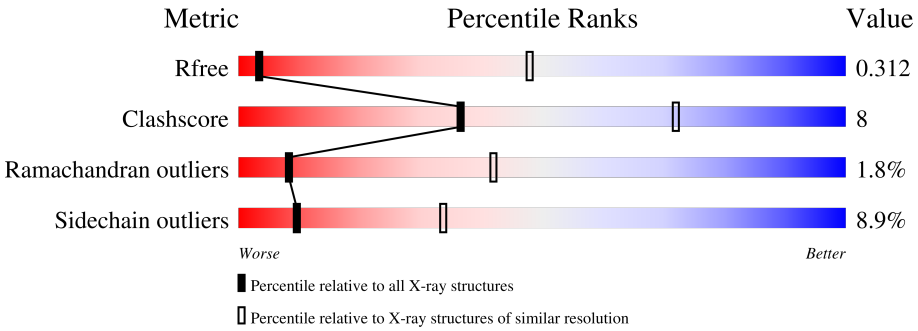
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.28.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 4.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1005 (4.62-3.78)
Clashscore	141614	1044 (4.60-3.80)
Ramachandran outliers	138981	1000 (4.60-3.80)
Sidechain outliers	138945	1007 (4.62-3.78)

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

Mol	Chain	Length	Quality of chain
1	A	193	65% 19% • 14%
1	B	193	62% 18% • 19%
1	C	193	67% 16% • 15%
1	D	193	67% 17% • 15%
1	E	193	64% 17% • 18%
1	F	193	66% 14% • 18%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 7092 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called FLICE inhibitory protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	166	Total	C	N	O	S	0	0	0
			1239	797	202	232	8			
1	B	157	Total	C	N	O	S	0	0	0
			1159	745	188	219	7			
1	C	164	Total	C	N	O	S	0	0	0
			1208	780	199	221	8			
1	D	165	Total	C	N	O	S	0	0	0
			1216	782	201	225	8			
1	E	159	Total	C	N	O	S	0	0	0
			1139	734	183	215	7			
1	F	159	Total	C	N	O	S	0	0	0
			1131	716	191	216	8			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP Q76RF1
A	-3	ALA	-	expression tag	UNP Q76RF1
A	-2	MET	-	expression tag	UNP Q76RF1
A	-1	GLY	-	expression tag	UNP Q76RF1
A	0	SER	-	expression tag	UNP Q76RF1
A	12	GLU	ARG	engineered mutation	UNP Q76RF1
B	-4	GLY	-	expression tag	UNP Q76RF1
B	-3	ALA	-	expression tag	UNP Q76RF1
B	-2	MET	-	expression tag	UNP Q76RF1
B	-1	GLY	-	expression tag	UNP Q76RF1
B	0	SER	-	expression tag	UNP Q76RF1
B	12	GLU	ARG	engineered mutation	UNP Q76RF1
C	-4	GLY	-	expression tag	UNP Q76RF1
C	-3	ALA	-	expression tag	UNP Q76RF1
C	-2	MET	-	expression tag	UNP Q76RF1
C	-1	GLY	-	expression tag	UNP Q76RF1
C	0	SER	-	expression tag	UNP Q76RF1

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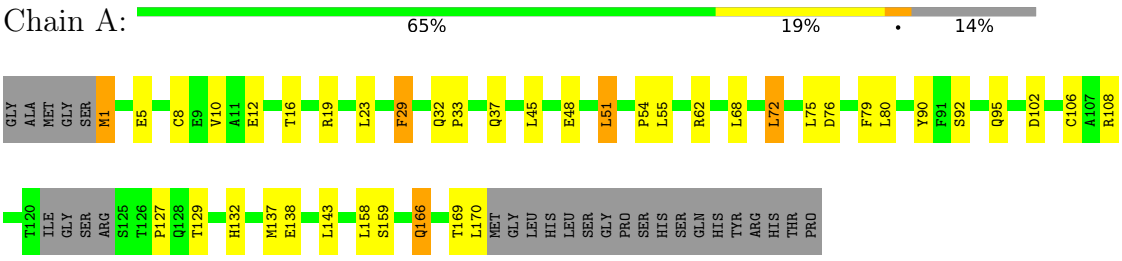
Chain	Residue	Modelled	Actual	Comment	Reference
C	12	GLU	ARG	engineered mutation	UNP Q76RF1
D	-4	GLY	-	expression tag	UNP Q76RF1
D	-3	ALA	-	expression tag	UNP Q76RF1
D	-2	MET	-	expression tag	UNP Q76RF1
D	-1	GLY	-	expression tag	UNP Q76RF1
D	0	SER	-	expression tag	UNP Q76RF1
D	12	GLU	ARG	engineered mutation	UNP Q76RF1
E	-4	GLY	-	expression tag	UNP Q76RF1
E	-3	ALA	-	expression tag	UNP Q76RF1
E	-2	MET	-	expression tag	UNP Q76RF1
E	-1	GLY	-	expression tag	UNP Q76RF1
E	0	SER	-	expression tag	UNP Q76RF1
E	12	GLU	ARG	engineered mutation	UNP Q76RF1
F	-4	GLY	-	expression tag	UNP Q76RF1
F	-3	ALA	-	expression tag	UNP Q76RF1
F	-2	MET	-	expression tag	UNP Q76RF1
F	-1	GLY	-	expression tag	UNP Q76RF1
F	0	SER	-	expression tag	UNP Q76RF1
F	12	GLU	ARG	engineered mutation	UNP Q76RF1

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.

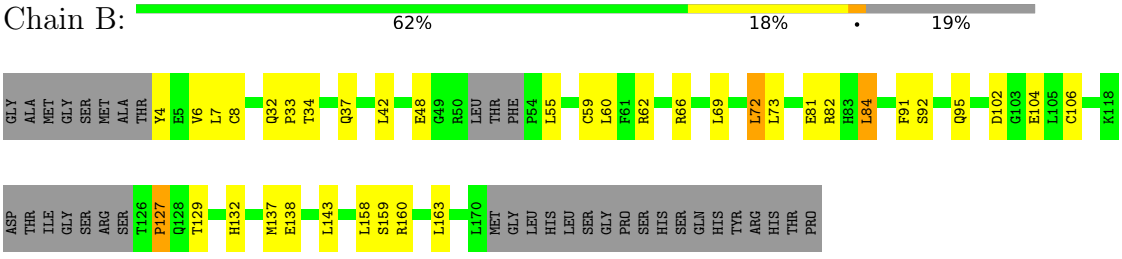
• Molecule 1: FLICE inhibitory protein

Chain A:



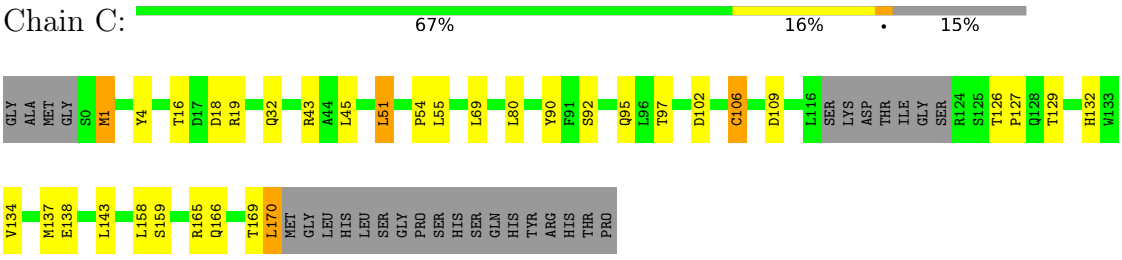
• Molecule 1: FLICE inhibitory protein

Chain B:



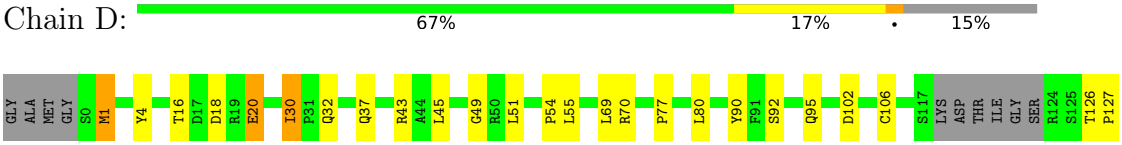
• Molecule 1: FLICE inhibitory protein

Chain C:



• Molecule 1: FLICE inhibitory protein

Chain D:

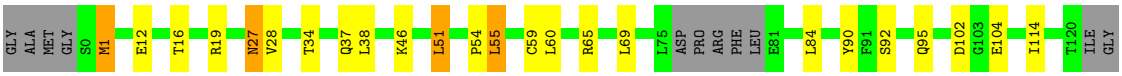


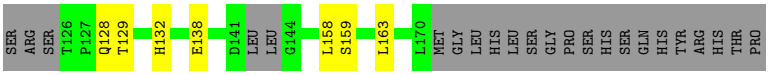
• Molecule 1: FLICE inhibitory protein

Chain E:

• Molecule 1: FLICE inhibitory protein

Chain F:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	119.40Å 69.32Å 131.89Å 90.00° 89.85° 90.00°	Depositor
Resolution (Å)	65.94 – 4.20 65.94 – 4.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (65.94-4.20) 98.3 (65.94-4.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.48 (at 4.14Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.223 , 0.273 0.263 , 0.312	Depositor DCC
R_{free} test set	790 reflections (9.78%)	wwPDB-VP
Wilson B-factor (Å^2)	105.2	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.075 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.068 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.259 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.259 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.079 for -h,-k,l	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	7092	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.12% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.34	0/1261	0.53	0/1724
1	B	0.35	0/1179	0.53	0/1612
1	C	0.37	0/1230	0.52	0/1683
1	D	0.35	0/1237	0.57	0/1692
1	E	0.35	0/1161	0.52	0/1593
1	F	0.34	0/1145	0.54	0/1564
All	All	0.35	0/7213	0.54	0/9868

There are no bond length outliers.

There are no bond angle outliers.

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	1239	0	1189	23	0
1	B	1159	0	1090	20	0
1	C	1208	0	1152	19	0
1	D	1216	0	1168	18	0
1	E	1139	0	1035	20	0
1	F	1131	0	1045	13	0
All	All	7092	0	6679	109	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 (109) 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:C:129:THR:HB	1:C:132:HIS:HB2	1.49	0.95
1:B:59:CYS:HG	1:B:91:PHE:HZ	0.96	0.94
1:D:129:THR:HB	1:D:132:HIS:HB2	1.48	0.94
1:A:129:THR:HB	1:A:132:HIS:HB2	1.48	0.93
1:E:129:THR:HB	1:E:132:HIS:HB2	1.53	0.90
1:D:129:THR:HB	1:D:132:HIS:CB	2.17	0.75
1:C:129:THR:HB	1:C:132:HIS:CB	2.17	0.74
1:A:129:THR:HB	1:A:132:HIS:CB	2.16	0.74
1:E:129:THR:HB	1:E:132:HIS:CB	2.20	0.72
1:F:129:THR:HB	1:F:132:HIS:CB	2.20	0.71
1:A:10:VAL:HG22	1:A:72:LEU:HD13	1.73	0.69
1:E:69:LEU:HD23	1:E:73:LEU:HD12	1.77	0.65
1:F:60:LEU:HB2	1:F:69:LEU:HD21	1.78	0.65
1:B:69:LEU:HA	1:B:73:LEU:HB2	1.78	0.65
1:D:4:TYR:HD1	1:D:43:ARG:NH1	1.99	0.61
1:C:4:TYR:HD1	1:C:43:ARG:NH1	1.99	0.61
1:E:26:LEU:HD12	1:E:45:LEU:HD13	1.82	0.60
1:F:55:LEU:O	1:F:59:CYS:HB2	2.01	0.60
1:D:69:LEU:HD12	1:D:77:PRO:HB3	1.83	0.60
1:B:62:ARG:HH21	1:B:84:LEU:HD22	1.66	0.60
1:A:92:SER:H	1:A:95:GLN:HE21	1.51	0.59
1:A:23:LEU:HB3	1:A:29:PHE:HA	1.86	0.58
1:C:137:MET:HB2	1:C:143:LEU:HB2	1.86	0.57
1:E:69:LEU:HB3	1:E:75:LEU:HD11	1.85	0.57
1:C:92:SER:H	1:C:95:GLN:HE21	1.52	0.56
1:F:92:SER:H	1:F:95:GLN:HE21	1.53	0.56
1:D:92:SER:H	1:D:95:GLN:HE21	1.54	0.55
1:B:92:SER:H	1:B:95:GLN:HE21	1.53	0.55
1:B:32:GLN:HE22	1:B:132:HIS:HD2	1.53	0.55
1:E:32:GLN:HE22	1:E:132:HIS:HD2	1.54	0.54
1:B:60:LEU:HB2	1:B:69:LEU:HD21	1.88	0.54
1:E:92:SER:H	1:E:95:GLN:HE21	1.54	0.54
1:E:137:MET:HB3	1:E:143:LEU:HB2	1.88	0.54
1:C:32:GLN:HE22	1:C:132:HIS:HD2	1.57	0.53
1:A:32:GLN:HE22	1:A:132:HIS:HD2	1.56	0.52
1:D:32:GLN:HE22	1:D:132:HIS:HD2	1.57	0.52
1:C:165:ARG:O	1:C:169:THR:HG23	2.09	0.52
1:D:4:TYR:CD1	1:D:43:ARG:NH1	2.77	0.52
1:C:16:THR:HA	1:C:19:ARG:HD2	1.92	0.52
1:B:137:MET:HB2	1:B:143:LEU:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:137:MET:HB2	1:D:143:LEU:HB2	1.91	0.51
1:B:4:TYR:CE2	1:B:8:CYS:SG	3.04	0.51
1:C:97:THR:HG21	1:C:170:LEU:HD22	1.92	0.51
1:F:16:THR:HA	1:F:19:ARG:HD2	1.93	0.51
1:C:4:TYR:CD1	1:C:43:ARG:NH1	2.78	0.50
1:A:137:MET:HB2	1:A:143:LEU:HB2	1.93	0.50
1:A:62:ARG:NH1	1:E:86:GLY:HA2	2.28	0.49
1:A:16:THR:HA	1:A:19:ARG:HD2	1.94	0.49
1:D:1:MET:SD	1:D:51:LEU:O	2.71	0.49
1:B:127:PRO:HD2	1:B:132:HIS:CD2	2.48	0.48
1:F:19:ARG:HG2	1:F:38:LEU:HD22	1.95	0.48
1:C:1:MET:SD	1:C:51:LEU:O	2.73	0.47
1:D:20:GLU:OE2	1:D:129:THR:HG21	2.14	0.47
1:B:106:CYS:HB2	1:E:106:CYS:HB2	1.95	0.47
1:D:127:PRO:HD2	1:D:132:HIS:CD2	2.50	0.47
1:E:84:LEU:HD23	1:E:87:THR:HB	1.98	0.46
1:D:30:ILE:HD12	1:D:37:GLN:HB3	1.98	0.46
1:B:160:ARG:NH1	1:E:106:CYS:SG	2.89	0.46
1:A:127:PRO:HD2	1:A:132:HIS:CD2	2.51	0.45
1:F:1:MET:SD	1:F:51:LEU:O	2.74	0.45
1:B:7:LEU:HD23	1:B:42:LEU:HB3	1.97	0.45
1:B:33:PRO:HA	1:B:37:GLN:HE21	1.82	0.45
1:B:34:THR:OG1	1:B:37:GLN:HG3	2.17	0.45
1:E:33:PRO:HA	1:E:37:GLN:HE21	1.82	0.45
1:A:1:MET:SD	1:A:51:LEU:O	2.75	0.45
1:F:114:ILE:HD11	1:F:128:GLN:HA	1.99	0.45
1:B:106:CYS:SG	1:E:160:ARG:NH2	2.88	0.45
1:D:127:PRO:HD2	1:D:132:HIS:NE2	2.32	0.44
1:E:28:VAL:HG11	1:E:41:ALA:HB1	1.99	0.44
1:C:127:PRO:HD2	1:C:132:HIS:CD2	2.52	0.44
1:A:92:SER:H	1:A:95:GLN:NE2	2.15	0.44
1:D:137:MET:CB	1:D:143:LEU:HB2	2.48	0.44
1:C:134:VAL:O	1:C:138:GLU:OE1	2.36	0.43
1:A:54:PRO:HB2	1:A:90:TYR:CE2	2.53	0.43
1:A:166:GLN:H	1:A:166:GLN:HG2	1.64	0.43
1:B:92:SER:H	1:B:95:GLN:NE2	2.16	0.43
1:C:54:PRO:HB2	1:C:90:TYR:CE2	2.54	0.43
1:A:33:PRO:HA	1:A:37:GLN:HE21	1.84	0.42
1:A:169:THR:HB	1:A:170:LEU:HD22	2.01	0.42
1:B:137:MET:CB	1:B:143:LEU:HB2	2.49	0.42
1:E:54:PRO:HB2	1:E:90:TYR:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:27:ASN:HD22	1:F:27:ASN:HA	1.74	0.42
1:C:92:SER:H	1:C:95:GLN:NE2	2.16	0.42
1:E:92:SER:H	1:E:95:GLN:NE2	2.17	0.42
1:F:92:SER:H	1:F:95:GLN:NE2	2.17	0.42
1:A:45:LEU:HB2	1:A:51:LEU:HD12	2.00	0.42
1:E:84:LEU:HA	1:E:87:THR:HB	2.01	0.42
1:B:104:GLU:HG2	1:B:163:LEU:HD21	2.02	0.42
1:D:54:PRO:HB2	1:D:90:TYR:CE2	2.55	0.42
1:F:34:THR:HG23	1:F:37:GLN:HE21	1.85	0.42
1:A:8:CYS:O	1:A:12:GLU:HG3	2.20	0.42
1:C:106:CYS:SG	1:C:109:ASP:OD2	2.76	0.42
1:F:54:PRO:HB2	1:F:90:TYR:CE2	2.55	0.42
1:C:127:PRO:HD2	1:C:132:HIS:NE2	2.35	0.41
1:B:6:VAL:HG13	1:B:72:LEU:HB3	2.02	0.41
1:C:45:LEU:HB2	1:C:51:LEU:HD12	2.03	0.41
1:A:76:ASP:HB3	1:A:79:PHE:HB2	2.02	0.41
1:F:104:GLU:HG2	1:F:163:LEU:HD21	2.03	0.41
1:A:137:MET:CB	1:A:143:LEU:HB2	2.50	0.41
1:B:66:ARG:HH21	1:B:81:GLU:HB2	1.85	0.41
1:A:68:LEU:HD22	1:A:72:LEU:HD11	2.02	0.41
1:C:54:PRO:HB2	1:C:90:TYR:HE2	1.86	0.41
1:D:169:THR:HB	1:D:170:LEU:HD22	2.02	0.41
1:A:127:PRO:HD2	1:A:132:HIS:NE2	2.35	0.40
1:D:45:LEU:HB3	1:D:51:LEU:HG	2.03	0.40
1:A:54:PRO:HB2	1:A:90:TYR:HE2	1.86	0.40
1:D:133:TRP:O	1:D:137:MET:HG2	2.21	0.40
1:E:93:PRO:O	1:E:97:THR:OG1	2.30	0.40
1:E:54:PRO:HB2	1:E:90:TYR:HE2	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	162/193 (84%)	147 (91%)	13 (8%)	2 (1%)	13 50
1	B	151/193 (78%)	137 (91%)	11 (7%)	3 (2%)	7 40
1	C	160/193 (83%)	146 (91%)	12 (8%)	2 (1%)	12 48
1	D	161/193 (83%)	146 (91%)	12 (8%)	3 (2%)	8 41
1	E	155/193 (80%)	138 (89%)	13 (8%)	4 (3%)	5 35
1	F	151/193 (78%)	139 (92%)	9 (6%)	3 (2%)	7 40
All	All	940/1158 (81%)	853 (91%)	70 (7%)	17 (2%)	8 42

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	PHE
1	A	159	SER
1	B	159	SER
1	C	159	SER
1	D	159	SER
1	E	15	GLY
1	E	29	PHE
1	E	76	ASP
1	E	159	SER
1	F	159	SER
1	B	127	PRO
1	F	28	VAL
1	B	129	THR
1	D	49	GLY
1	F	84	LEU
1	D	126	THR
1	C	126	THR

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	128/170 (75%)	114 (89%)	14 (11%)	6 26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	118/170 (69%)	110 (93%)	8 (7%)	16 43
1	C	121/170 (71%)	110 (91%)	11 (9%)	9 32
1	D	124/170 (73%)	112 (90%)	12 (10%)	8 29
1	E	110/170 (65%)	102 (93%)	8 (7%)	14 41
1	F	109/170 (64%)	99 (91%)	10 (9%)	9 31
All	All	710/1020 (70%)	647 (91%)	63 (9%)	9 34

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	5	GLU
1	A	48	GLU
1	A	51	LEU
1	A	55	LEU
1	A	72	LEU
1	A	75	LEU
1	A	80	LEU
1	A	102	ASP
1	A	106	CYS
1	A	108	ARG
1	A	138	GLU
1	A	158	LEU
1	A	166	GLN
1	B	48	GLU
1	B	55	LEU
1	B	72	LEU
1	B	82	ARG
1	B	84	LEU
1	B	102	ASP
1	B	138	GLU
1	B	158	LEU
1	C	1	MET
1	C	18	ASP
1	C	51	LEU
1	C	55	LEU
1	C	69	LEU
1	C	80	LEU
1	C	102	ASP
1	C	106	CYS

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Mol	Chain	Res	Type
1	C	158	LEU
1	C	166	GLN
1	C	170	LEU
1	D	1	MET
1	D	16	THR
1	D	18	ASP
1	D	20	GLU
1	D	30	ILE
1	D	55	LEU
1	D	70	ARG
1	D	80	LEU
1	D	102	ASP
1	D	106	CYS
1	D	138	GLU
1	D	158	LEU
1	E	17	ASP
1	E	51	LEU
1	E	55	LEU
1	E	69	LEU
1	E	75	LEU
1	E	102	ASP
1	E	158	LEU
1	E	162	ASP
1	F	1	MET
1	F	12	GLU
1	F	27	ASN
1	F	46	LYS
1	F	51	LEU
1	F	55	LEU
1	F	65	ARG
1	F	102	ASP
1	F	138	GLU
1	F	158	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	37	GLN
1	A	95	GLN
1	B	37	GLN
1	B	95	GLN

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Mol	Chain	Res	Type
1	B	132	HIS
1	C	32	GLN
1	C	37	GLN
1	C	95	GLN
1	D	32	GLN
1	D	37	GLN
1	D	95	GLN
1	E	32	GLN
1	E	37	GLN
1	E	95	GLN
1	F	27	ASN
1	F	32	GLN
1	F	37	GLN
1	F	95	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 monosaccharides 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.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.