WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 28, 2018 – 12:32 PM EST

PDB ID : 3DOS

Title : Crystal structure of the complex of the Caf1M chaperone with the mini-fiber of two Caf1 subunits (Caf1:Caf1), carrying the Thr7Phe and Ala9Val mutations in the Gd donor strand

Authors : Fooks, L.J.; Yu, X.; Moslehi-Mohebi, E.; Tischenko, V.; Knight, S.D.; MacIntyre, S.; Zavialov, A.V.

Deposited on : 2008-07-06

Resolution : 2.40 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

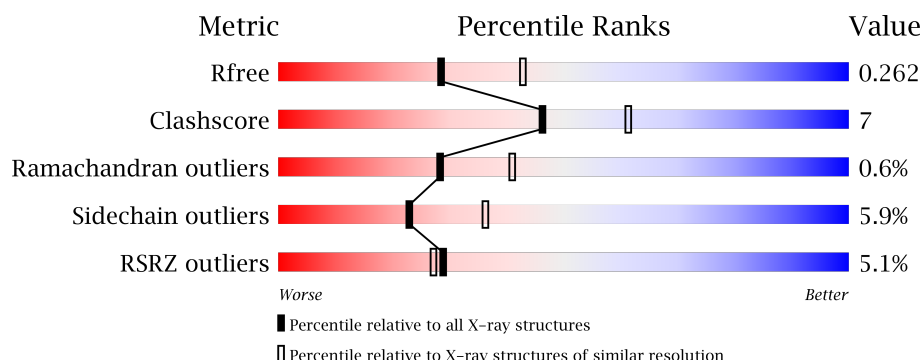|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030736

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 2.40 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	Percentile Ranks	Value
Rfree		0.262
Clashscore		7
Ramachandran outliers		0.6%
Sidechain outliers		5.9%
RSRZ outliers		5.1%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

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 on the lower 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	235	3% / 72% 13% • 14%
1	D	235	6% / 63% 17% • 19%
2	B	149	11% / 80% 17% •••
2	C	149	2% / 74% 16% • 9%
2	E	149	3% / 83% 15% •

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Mol	Chain	Length	Quality of chain
2	F	149	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7373 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 Chaperone protein caf1M.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	203	Total	C	N	O	S	0	0	2
			1550	998	265	283	4			
1	D	191	Total	C	N	O	S	0	0	0
			1481	956	251	270	4			

- Molecule 2 is a protein called F1 capsule antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	148	Total	C	N	O	S	0	0	1
			1085	677	178	228	2			
2	C	135	Total	C	N	O	S	0	0	0
			996	619	165	210	2			
2	E	149	Total	C	N	O	S	0	0	0
			1096	683	180	231	2			
2	F	132	Total	C	N	O	S	0	0	1
			973	602	162	207	2			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	7	PHE	THR	ENGINEERED	UNP P26948
B	9	VAL	ALA	ENGINEERED	UNP P26948
C	7	PHE	THR	ENGINEERED	UNP P26948
C	9	VAL	ALA	ENGINEERED	UNP P26948
E	7	PHE	THR	ENGINEERED	UNP P26948
E	9	VAL	ALA	ENGINEERED	UNP P26948
F	7	PHE	THR	ENGINEERED	UNP P26948
F	9	VAL	ALA	ENGINEERED	UNP P26948

- Molecule 3 is water.

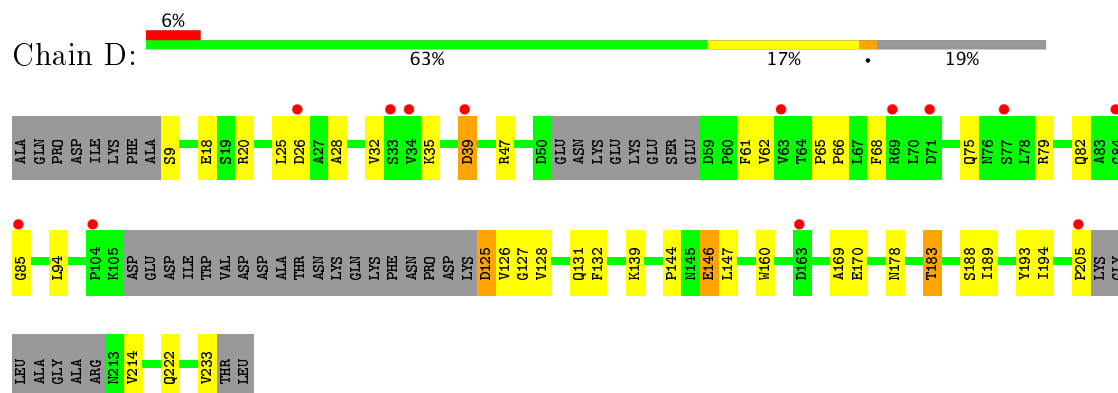| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	59	Total 59	O 59	0	0
3	B	10	Total 10	O 10	0	0
3	C	42	Total 42	O 42	0	0
3	D	22	Total 22	O 22	0	0
3	E	29	Total 29	O 29	0	0
3	F	30	Total 30	O 30	0	0

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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: Chaperone protein caf1M
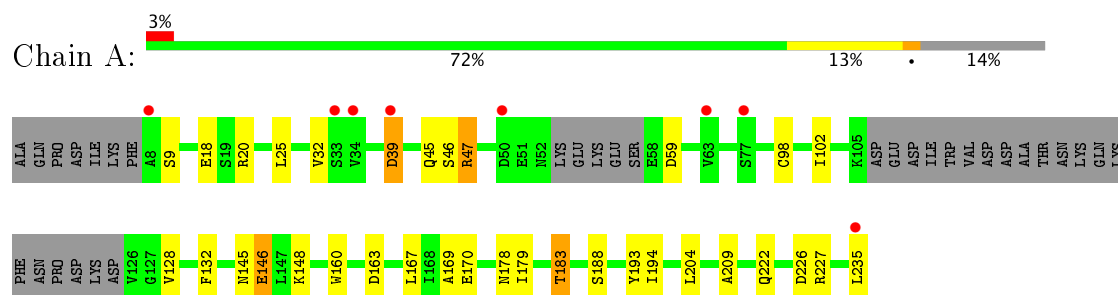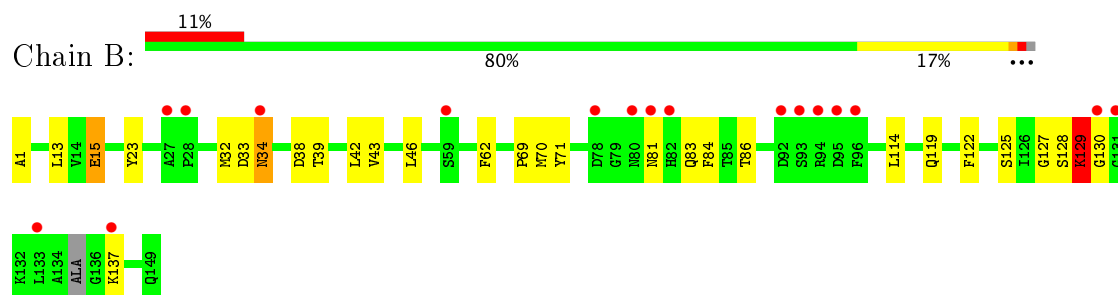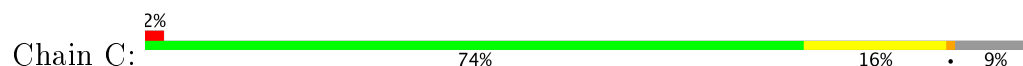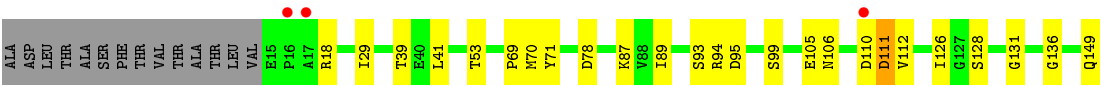
Chain A:

- Molecule 1: Chaperone protein caf1M

Chain D:

- Molecule 2: F1 capsule antigen

Chain B:

- Molecule 2: F1 capsule antigen

Chain C:

• Molecule 2: F1 capsule antigen

Chain E:

• Molecule 2: F1 capsule antigen

Chain F:
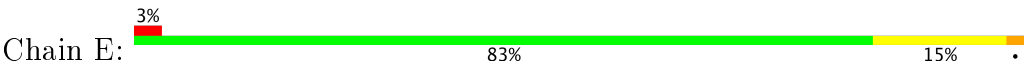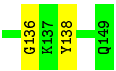
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	72.23Å　　91.18Å　　166.02Å 90.00°　　90.00°　　90.00°	Depositor
Resolution (Å)	31.64　–　2.40 31.63　–　2.40	Depositor EDS
% Data completeness (in resolution range)	91.1 (31.64-2.40) 91.2 (31.63-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.86 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.214　,　0.264 0.213　,　0.262	Depositor DCC
R_{free} test set	2008 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	25.9	Xtriage
Anisotropy	0.428	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 40.2	EDS
L-test for twinning[2]	$<|L|> = 0.49$, $<L^2> = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7373	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.27 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.2741e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[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 (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$>5	RMSZ	#$|Z|$>5
1	A	0.71	0/1587	0.76	0/2157
1	D	0.73	0/1517	0.76	0/2062
2	B	0.67	1/1099 (0.1%)	0.73	0/1491
2	C	0.73	0/1010	0.75	0/1370
2	E	0.63	0/1111	0.72	0/1510
2	F	0.78	0/985	0.74	0/1332
All	All	0.71	1/7309 (0.0%)	0.75	0/9922

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	15	GLU	CG-CD	5.38	1.60	1.51

There are no bond angle outliers.

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	1550	0	1540	22	0
1	D	1481	0	1464	34	0
2	B	1085	0	1068	22	0
2	C	996	0	973	16	0
2	E	1096	0	1079	16	0
2	F	973	0	945	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	59	0	0	6	0
3	B	10	0	0	0	0
3	C	42	0	0	0	0
3	D	22	0	0	2	0
3	E	29	0	0	1	0
3	F	30	0	0	2	0
All	All	7373	0	7069	103	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 7.

All (103) 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:D:189:ILE:CD1	1:D:205:PRO:HG3	1.91	1.00
1:D:144:PRO:HB2	1:D:146:GLU:HG2	1.46	0.97
1:D:189:ILE:HD11	1:D:205:PRO:HG3	1.52	0.90
2:E:13:LEU:HD22	2:F:29:ILE:HB	1.60	0.83
2:C:87:LYS:HE3	2:C:89:ILE:HD12	1.61	0.82
2:B:129:LYS:HE3	1:D:65:PRO:HD3	1.64	0.80
1:D:39:ASP:N	1:D:39:ASP:OD1	2.19	0.76
1:D:183:THR:HG22	3:D:255:HOH:O	1.87	0.74
1:D:189:ILE:HD11	1:D:205:PRO:CG	2.18	0.72
2:E:16:PRO:HG2	2:E:18:ARG:CZ	2.21	0.71
1:A:132:PHE:CZ	2:B:46:LEU:HD21	2.28	0.67
2:F:69:PRO:O	2:F:70:MET:HB2	1.96	0.66
1:A:39:ASP:OD1	1:A:39:ASP:N	2.27	0.66
2:F:87:LYS:HE3	2:F:89:ILE:HD12	1.79	0.64
2:E:55:THR:HA	3:E:167:HOH:O	1.97	0.64
2:F:58:THR:HG23	2:F:111:ASP:OD1	1.98	0.64
1:D:144:PRO:HG2	1:D:147:LEU:HG	1.80	0.63
1:A:148:LYS:CA	3:A:282:HOH:O	2.46	0.62
2:C:69:PRO:O	2:C:70:MET:HB2	1.99	0.62
1:D:222:GLN:HE21	2:F:136:GLY:HA2	1.64	0.62
2:B:129:LYS:CE	1:D:65:PRO:HD3	2.31	0.60
1:D:233:VAL:C	3:D:243:HOH:O	2.40	0.60
1:A:227:ARG:HB3	2:C:78:ASP:O	2.01	0.60
2:B:13:LEU:HD22	2:C:29:ILE:HB	1.85	0.59
2:C:71:TYR:CD2	2:C:126:ILE:CD1	2.85	0.58
2:C:69:PRO:HB3	2:C:105:GLU:HG3	1.84	0.58
2:E:110:ASP:OD2	2:E:110:ASP:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:87:LYS:HE3	2:C:89:ILE:CD1	2.34	0.57
2:B:42:LEU:CD1	2:B:122:PHE:HB3	2.35	0.56
1:D:189:ILE:HD12	1:D:205:PRO:HG3	1.86	0.56
2:F:94:ARG:HG2	3:F:169:HOH:O	2.04	0.56
1:D:94:LEU:HD11	1:D:139:LYS:HG2	1.87	0.55
1:D:178:ASN:HD22	1:D:193:TYR:HB3	1.72	0.55
1:D:127:GLY:O	2:E:137:LYS:HD3	2.08	0.54
2:B:71:TYR:OH	1:D:66:PRO:HG2	2.08	0.54
2:C:99:SER:HB2	2:C:110:ASP:HB2	1.89	0.54
2:B:1:ALA:HB3	2:C:149:GLN:O	2.08	0.53
2:F:39:THR:HG22	2:F:126:ILE:O	2.08	0.53
2:C:39:THR:HG22	2:C:126:ILE:O	2.10	0.52
1:D:9:SER:HA	2:E:23:TYR:O	2.09	0.52
1:D:25:LEU:O	1:D:26:ASP:HB2	2.08	0.52
2:B:81:ASN:ND2	2:B:81:ASN:O	2.43	0.52
2:B:34:ASN:HB2	1:D:28:ALA:HB2	1.92	0.50
1:D:61:PHE:CE1	1:D:82:GLN:HB2	2.47	0.50
2:B:69:PRO:O	2:B:70:MET:HB2	2.11	0.49
1:D:126:VAL:HB	2:E:29:ILE:HB	1.93	0.49
2:B:128:SER:O	2:B:130:GLY:N	2.46	0.48
2:F:71:TYR:CD2	2:F:126:ILE:CD1	2.96	0.48
1:A:183:THR:HG23	3:A:277:HOH:O	2.13	0.48
1:D:65:PRO:HG2	1:D:68:PHE:CD2	2.49	0.48
2:B:83:GLN:O	2:B:128:SER:HB2	2.14	0.48
1:A:222:GLN:HE21	2:C:136:GLY:HA2	1.79	0.48
2:B:129:LYS:HA	1:D:79:ARG:HD3	1.96	0.48
1:D:125:ASP:OD1	2:E:30:THR:HG23	2.14	0.48
1:A:160:TRP:CZ3	1:A:169:ALA:HB2	2.48	0.47
2:C:29:ILE:HG23	2:C:41:LEU:CD1	2.44	0.47
1:A:183:THR:HG22	3:A:285:HOH:O	2.15	0.47
1:A:226:ASP:CG	1:A:227:ARG:H	2.17	0.47
2:B:84:PHE:HB2	2:B:127:GLY:O	2.15	0.47
1:A:18:GLU:HG2	1:A:32:VAL:HG23	1.97	0.46
1:A:167:LEU:HB2	1:A:204:LEU:HD21	1.97	0.46
1:D:160:TRP:CZ3	1:D:169:ALA:HB2	2.50	0.46
2:F:29:ILE:HG23	2:F:41:LEU:CD1	2.46	0.46
2:C:71:TYR:CE2	2:C:126:ILE:CD1	2.99	0.46
1:D:144:PRO:HB2	1:D:146:GLU:CG	2.32	0.45
1:A:128:VAL:HG11	2:B:43:VAL:CG1	2.46	0.45
1:A:25:LEU:HB3	3:A:241:HOH:O	2.17	0.45
2:C:99:SER:CB	2:C:110:ASP:HB2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:LYS:HB2	1:D:75:GLN:HG3	1.98	0.45
1:D:18:GLU:HG2	1:D:32:VAL:HG23	1.97	0.45
2:B:114:LEU:HD22	2:B:119:GLN:HG2	1.99	0.45
1:D:169:ALA:HB3	1:D:194:ILE:HD12	1.99	0.44
2:F:98:ILE:HD13	2:F:112:VAL:HG11	1.98	0.44
1:D:128:VAL:O	1:D:128:VAL:HG23	2.18	0.44
2:F:99:SER:O	2:F:106:ASN:ND2	2.50	0.44
1:A:45:GLN:OE1	1:A:102:ILE:HD11	2.17	0.44
1:A:226:ASP:HB3	3:A:236:HOH:O	2.18	0.44
1:A:146:GLU:H	1:A:146:GLU:HG2	1.32	0.44
2:B:129:LYS:HE3	1:D:65:PRO:CD	2.42	0.44
2:B:39:THR:HB	1:D:62:VAL:HG21	2.00	0.43
2:E:7:PHE:CE2	2:F:23:TYR:HB3	2.54	0.43
2:E:86:THR:HG22	2:E:125:SER:HA	1.99	0.43
2:B:46:LEU:HD13	2:B:62:PHE:CE2	2.54	0.43
1:A:145:ASN:ND2	3:A:246:HOH:O	2.52	0.43
1:A:179:ILE:HD12	1:A:194:ILE:HD11	2.01	0.43
2:C:111:ASP:C	2:C:112:VAL:HG23	2.39	0.43
1:A:178:ASN:HD22	1:A:193:TYR:HB3	1.84	0.42
2:E:114:LEU:HD22	2:E:119:GLN:HG2	2.01	0.42
1:A:45:GLN:HE21	1:A:47:ARG:CZ	2.32	0.42
2:E:41:LEU:O	2:E:124:ARG:HA	2.19	0.42
2:E:87:LYS:HB3	2:E:126:ILE:HD11	2.01	0.42
2:F:92:ASP:HB2	3:F:178:HOH:O	2.19	0.42
1:A:46:SER:HA	1:A:98:CYS:O	2.19	0.41
2:B:86:THR:HG22	2:B:125:SER:HA	2.02	0.41
2:C:128:SER:OG	2:C:131:GLY:O	2.38	0.41
2:E:77:GLN:OE1	2:E:137:LYS:HB2	2.20	0.41
2:F:71:TYR:CE2	2:F:126:ILE:CD1	3.04	0.41
2:E:16:PRO:HG2	2:E:18:ARG:NH2	2.35	0.41
1:A:9:SER:HA	2:B:23:TYR:O	2.20	0.41
1:D:132:PHE:HA	2:E:142:VAL:O	2.21	0.41
2:B:137:LYS:H	2:B:137:LYS:HG2	1.67	0.40
1:D:128:VAL:CG2	1:D:128:VAL:O	2.69	0.40
2:F:74:PHE:HB3	2:F:138:TYR:HB3	2.03	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	197/235 (84%)	191 (97%)	4 (2%)	2 (1%)	18	26
1	D	183/235 (78%)	173 (94%)	9 (5%)	1 (0%)	32	46
2	B	144/149 (97%)	134 (93%)	8 (6%)	2 (1%)	13	18
2	C	133/149 (89%)	128 (96%)	5 (4%)	0	100	100
2	E	147/149 (99%)	145 (99%)	2 (1%)	0	100	100
2	F	128/149 (86%)	123 (96%)	4 (3%)	1 (1%)	22	33
All	All	932/1066 (87%)	894 (96%)	32 (3%)	6 (1%)	28	41

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	209	ALA
2	B	33	ASP
2	B	129	LYS
1	D	85	GLY
2	F	17	ALA
1	A	59	ASP

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	166/204 (81%)	157 (95%)	9 (5%)	26	41
1	D	161/204 (79%)	151 (94%)	10 (6%)	21	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	120/122 (98%)	115 (96%)	5 (4%)	34	53
2	C	110/122 (90%)	103 (94%)	7 (6%)	20	32
2	E	121/122 (99%)	113 (93%)	8 (7%)	19	30
2	F	107/122 (88%)	100 (94%)	7 (6%)	20	31
All	All	785/896 (88%)	739 (94%)	46 (6%)	23	36

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ARG
1	A	39	ASP
1	A	47	ARG
1	A	146	GLU
1	A	163	ASP
1	A	170	GLU
1	A	183	THR
1	A	188	SER
1	A	235	LEU
2	B	15	GLU
2	B	32	MET
2	B	34	ASN
2	B	38	ASP
2	B	129	LYS
2	C	18	ARG
2	C	53	THR
2	C	93	SER
2	C	94	ARG
2	C	95	ASP
2	C	106	ASN
2	C	111	ASP
1	D	20	ARG
1	D	39	ASP
1	D	47	ARG
1	D	125	ASP
1	D	131	GLN
1	D	146	GLU
1	D	170	GLU
1	D	183	THR
1	D	188	SER
1	D	214	VAL
2	E	15	GLU

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Mol	Chain	Res	Type
2	E	30	THR
2	E	32	MET
2	E	77	GLN
2	E	94	ARG
2	E	110	ASP
2	E	129	LYS
2	E	132	LYS
2	F	38	ASP
2	F	93	SER
2	F	94	ARG
2	F	95	ASP
2	F	112	VAL
2	F	116	THR
2	F	129	LYS

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	145	ASN
1	A	178	ASN
1	A	222	GLN
1	D	145	ASN
1	D	178	ASN
1	D	213	ASN
1	D	222	GLN
2	F	106	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	203/235 (86%)	-0.07	8 (3%)	40	39	7, 20, 38, 49	6 (2%)
1	D	191/235 (81%)	0.15	13 (6%)	18	16	9, 24, 41, 50	5 (2%)
2	B	148/149 (99%)	0.38	17 (11%)	5	5	8, 28, 51, 57	1 (0%)
2	C	135/149 (90%)	-0.32	3 (2%)	62	59	6, 19, 39, 47	0
2	E	149/149 (100%)	-0.00	5 (3%)	46	44	8, 27, 46, 53	1 (0%)
2	F	132/149 (88%)	-0.36	3 (2%)	61	58	6, 19, 38, 48	0
All	All	958/1066 (89%)	-0.02	49 (5%)	29	27	6, 23, 45, 57	13 (1%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	34	VAL	9.0
1	D	33	SER	8.8
1	D	34	VAL	8.0
1	A	33	SER	6.8
1	D	63	VAL	6.8
2	B	130	GLY	5.5
1	A	63	VAL	5.1
2	B	93	SER	4.4
2	B	131	GLY	4.3
2	B	27	ALA	4.3
2	E	59	SER	4.0
1	A	235	LEU	3.8
2	E	93	SER	3.6
1	D	163	ASP	3.5
1	D	84	GLY	3.3
1	D	26	ASP	3.3
2	B	80	ASN	3.2
1	D	77	SER	3.2
2	B	81	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	59	SER	3.0
2	B	95	ASP	3.0
2	E	95	ASP	2.9
2	B	94	ARG	2.9
2	C	17	ALA	2.8
2	B	82	HIS	2.8
2	F	110	ASP	2.7
2	C	110	ASP	2.7
2	B	92	ASP	2.6
2	E	94	ARG	2.6
1	D	85	GLY	2.6
2	E	81	ASN	2.6
1	A	50	ASP	2.6
2	F	111	ASP	2.5
2	F	16	PRO	2.5
1	A	8	ALA	2.5
2	B	96	PHE	2.4
2	B	34	ASN	2.3
1	A	39	ASP	2.3
1	D	205	PRO	2.3
2	B	133	LEU	2.2
2	B	137	LYS	2.2
2	B	28	PRO	2.2
1	D	69	ARG	2.2
2	C	16	PRO	2.2
1	A	77	SER	2.2
1	D	104	PRO	2.1
1	D	71	ASP	2.1
1	D	39	ASP	2.1
2	B	78	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.