Full wwPDB X-ray Structure Validation Report (i)

Oct 11, 2021 – 12:41 PM EDT

PDB ID	:	2FQM
Title	:	Crystal structure of the oligomerization domain of the phosphoprotein of vesicular stomatitis virus
Authors	:	Ding, H.; Green, T.J.; Lu, S.; Luo, M.
Deposited on	:	2006-01-18
Resolution	:	2.30 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 (i) symbol.

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

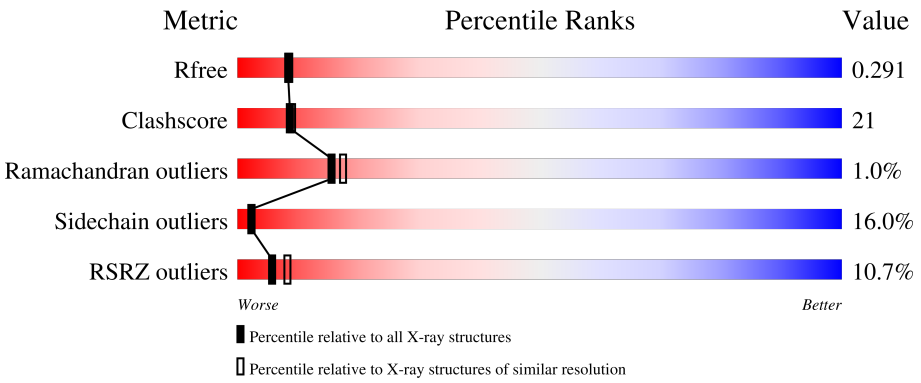
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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% 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	75	15% 48% 28% 11% 13%
1	B	75	5% 59% 19% 7% 16%
1	C	75	3% 56% 23% 11% 11%
1	D	75	7% 60% 31% • • •
1	E	75	15% 51% 41% • •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	75	13% 51% 31% • 15%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3277 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 Phosphoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	65	517	326	90	99	2	0	0	0
1	B	63	495	311	87	95	2	0	0	0
1	C	67	533	337	93	101	2	0	0	0
1	D	72	571	360	98	110	3	0	0	0
1	E	72	571	360	98	110	3	0	0	0
1	F	64	506	320	86	98	2	0	0	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	GLY	-	cloning artifact	UNP P04880
A	104	SER	-	cloning artifact	UNP P04880
A	105	HIS	-	cloning artifact	UNP P04880
A	106	MET	-	cloning artifact	UNP P04880
A	139	MET	LEU	engineered mutation	UNP P04880
B	103	GLY	-	cloning artifact	UNP P04880
B	104	SER	-	cloning artifact	UNP P04880
B	105	HIS	-	cloning artifact	UNP P04880
B	106	MET	-	cloning artifact	UNP P04880
B	139	MET	LEU	engineered mutation	UNP P04880
C	103	GLY	-	cloning artifact	UNP P04880
C	104	SER	-	cloning artifact	UNP P04880
C	105	HIS	-	cloning artifact	UNP P04880
C	106	MET	-	cloning artifact	UNP P04880
C	139	MET	LEU	engineered mutation	UNP P04880
D	-4	GLY	-	cloning artifact	UNP P04880
D	-3	SER	-	cloning artifact	UNP P04880

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	HIS	-	cloning artifact	UNP P04880
D	-1	MET	-	cloning artifact	UNP P04880
D	139	MET	LEU	engineered mutation	UNP P04880
E	-4	GLY	-	cloning artifact	UNP P04880
E	-3	SER	-	cloning artifact	UNP P04880
E	-2	HIS	-	cloning artifact	UNP P04880
E	-1	MET	-	cloning artifact	UNP P04880
E	139	MET	LEU	engineered mutation	UNP P04880
F	103	GLY	-	cloning artifact	UNP P04880
F	104	SER	-	cloning artifact	UNP P04880
F	105	HIS	-	cloning artifact	UNP P04880
F	106	MET	-	cloning artifact	UNP P04880
F	139	MET	LEU	engineered mutation	UNP P04880

- Molecule 2 is water.

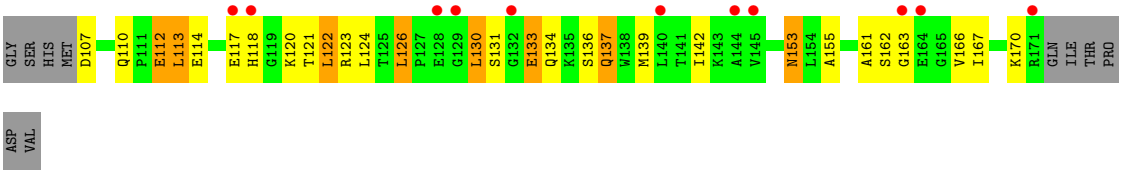
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	22	22	22	0	0
			Total	O		
2	B	13	13	13	0	0
			Total	O		
2	C	11	11	11	0	0
			Total	O		
2	D	13	13	13	0	0
			Total	O		
2	E	16	16	16	0	0
			Total	O		
2	F	9	9	9	0	0

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 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: Phosphoprotein

Chain A:

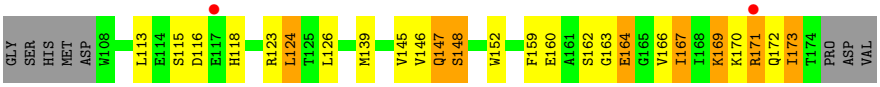


• Molecule 1: Phosphoprotein

Chain B:

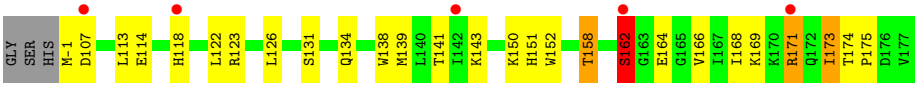
• Molecule 1: Phosphoprotein

Chain C:



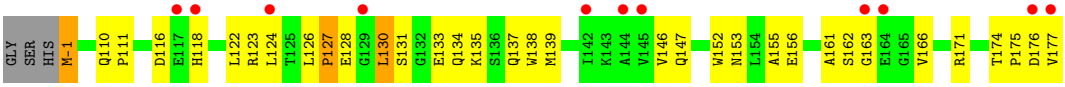
• Molecule 1: Phosphoprotein

Chain D:



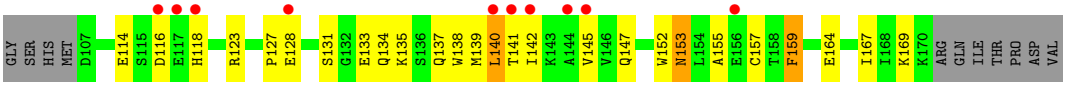
• Molecule 1: Phosphoprotein

Chain E:



• Molecule 1: Phosphoprotein

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	74.38Å 74.38Å 157.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 28.97 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.8 (20.00-2.30) 98.7 (28.97-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	13.11 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.225 , 0.290 0.230 , 0.291	Depositor DCC
R_{free} test set	992 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å^2)	42.0	Xtriage
Anisotropy	0.259	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 71.0	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	0.94	EDS
Total number of atoms	3277	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.74% 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 (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	0.90	0/527	0.90	0/709
1	B	0.88	0/503	0.94	0/675
1	C	0.87	0/543	0.92	0/731
1	D	0.94	1/582 (0.2%)	0.91	1/785 (0.1%)
1	E	0.84	0/582	0.86	0/785
1	F	0.74	0/516	0.88	0/695
All	All	0.87	1/3253 (0.0%)	0.90	1/4380 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	139	MET	SD-CE	-7.19	1.37	1.77

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	139	MET	CG-SD-CE	-6.10	90.44	100.20

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	517	0	516	25	0
1	B	495	0	501	21	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	533	0	538	23	0
1	D	571	0	574	25	0
1	E	571	0	574	41	0
1	F	506	0	503	36	0
2	A	22	0	0	4	0
2	B	13	0	0	2	0
2	C	11	0	0	0	0
2	D	13	0	0	1	0
2	E	16	0	0	0	0
2	F	9	0	0	1	0
All	All	3277	0	3206	132	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 21.

All (132) 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:138:TRP:HE1	1:F:141:THR:HG21	1.18	1.09
1:F:131:SER:H	1:F:134:GLN:NE2	1.53	1.06
1:D:169:LYS:HE3	1:D:171:ARG:HB3	1.44	0.96
1:F:131:SER:H	1:F:134:GLN:HE21	1.15	0.95
1:C:167:ILE:HD11	1:D:123:ARG:CZ	1.97	0.94
1:F:138:TRP:O	1:F:141:THR:HG22	1.73	0.89
1:D:173:ILE:H	1:D:173:ILE:HD13	1.41	0.85
1:E:128:GLU:H	1:F:137:GLN:HE22	1.24	0.85
1:F:133:GLU:O	1:F:137:GLN:HG3	1.79	0.82
1:F:131:SER:N	1:F:134:GLN:HE21	1.79	0.80
1:E:123:ARG:NH1	1:F:167:ILE:HD11	1.96	0.79
1:F:138:TRP:NE1	2:F:68:HOH:O	2.20	0.74
1:C:167:ILE:HD11	1:D:123:ARG:NH1	2.05	0.72
1:E:174:THR:HG23	1:E:175:PRO:HA	1.71	0.72
1:D:162:SER:HB3	2:D:76:HOH:O	1.92	0.69
1:C:167:ILE:HD11	1:D:123:ARG:NH2	2.09	0.68
1:E:130:LEU:H	1:E:130:LEU:HD23	1.57	0.68
1:E:156:GLU:O	1:E:171:ARG:HG2	1.94	0.67
1:F:131:SER:N	1:F:134:GLN:NE2	2.33	0.67
1:E:131:SER:O	1:E:135:LYS:HG3	1.95	0.67
1:D:162:SER:OG	1:D:164:GLU:HG3	1.95	0.66
1:B:153:ASN:HD22	1:B:153:ASN:C	1.99	0.66
1:E:131:SER:H	1:E:134:GLN:HE21	1.44	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:131:SER:H	1:E:134:GLN:NE2	1.94	0.65
1:E:138:TRP:NE1	1:F:141:THR:HG21	2.01	0.65
1:F:138:TRP:CZ3	1:F:142:ILE:HD11	2.32	0.65
1:C:146:VAL:C	1:C:148:SER:H	2.01	0.63
1:A:137:GLN:HE21	1:B:127:PRO:HG3	1.62	0.63
1:A:153:ASN:HD22	1:A:155:ALA:H	1.45	0.63
1:A:166:VAL:HG11	1:B:142:ILE:CD1	2.30	0.61
1:B:110:GLN:HE22	1:C:147:GLN:HE21	1.49	0.61
1:E:174:THR:HG23	1:E:175:PRO:CA	2.31	0.60
1:A:153:ASN:HD22	1:A:153:ASN:C	2.05	0.60
1:E:128:GLU:N	1:F:137:GLN:HE22	1.96	0.59
1:F:153:ASN:ND2	1:F:155:ALA:HB3	2.18	0.59
1:E:128:GLU:H	1:F:137:GLN:NE2	1.99	0.58
1:B:153:ASN:ND2	1:B:155:ALA:H	2.02	0.58
1:A:133:GLU:OE1	2:A:57:HOH:O	2.18	0.57
1:C:124:LEU:HG	1:D:141:THR:HG23	1.87	0.57
1:A:153:ASN:ND2	1:A:155:ALA:H	2.02	0.57
1:E:137:GLN:NE2	1:F:127:PRO:HG3	2.20	0.57
1:E:131:SER:OG	1:E:133:GLU:HG2	2.05	0.57
1:F:114:GLU:OE2	1:F:123:ARG:HD2	2.05	0.56
1:B:153:ASN:HD22	1:B:155:ALA:H	1.53	0.56
1:D:126:LEU:HD23	1:D:138:TRP:CE3	2.41	0.55
1:A:121:THR:HG23	1:B:167:ILE:HG23	1.88	0.55
1:D:173:ILE:H	1:D:173:ILE:CD1	2.18	0.55
1:A:113:LEU:HD12	1:A:122:LEU:HD23	1.87	0.55
1:E:126:LEU:CD2	1:E:130:LEU:HD11	2.37	0.55
1:A:124:LEU:HD12	1:B:166:VAL:CG2	2.37	0.55
1:B:135:LYS:O	1:B:139:MET:HG2	2.07	0.54
1:D:174:THR:HB	1:D:175:PRO:HD2	1.89	0.54
1:E:127:PRO:HA	1:F:137:GLN:NE2	2.22	0.54
1:A:166:VAL:HG11	1:B:142:ILE:HD13	1.89	0.54
1:C:145:VAL:O	1:C:148:SER:HB3	2.08	0.54
1:B:133:GLU:O	1:B:137:GLN:HG3	2.08	0.53
1:C:160:GLU:OE2	1:C:169:LYS:HE2	2.09	0.53
1:C:173:ILE:N	1:C:173:ILE:HD13	2.23	0.52
1:E:130:LEU:H	1:E:130:LEU:CD2	2.22	0.52
1:A:139:MET:CE	1:B:166:VAL:HG12	2.39	0.52
1:A:110:GLN:O	1:A:112:GLU:HG2	2.10	0.52
1:A:114:GLU:CD	1:A:123:ARG:HD2	2.31	0.51
1:A:162:SER:OG	1:B:123:ARG:NH2	2.43	0.51
1:E:124:LEU:HD11	1:F:145:VAL:CG2	2.41	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:123:ARG:HH12	1:F:167:ILE:HD11	1.72	0.51
1:E:126:LEU:HD22	1:E:130:LEU:HD11	1.92	0.51
1:D:173:ILE:HD13	1:D:173:ILE:N	2.21	0.50
1:E:139:MET:HG2	1:F:159:PHE:HZ	1.76	0.50
1:C:146:VAL:C	1:C:148:SER:N	2.64	0.50
1:E:131:SER:N	1:E:134:GLN:HE21	2.08	0.50
1:C:167:ILE:CG2	1:C:169:LYS:HG2	2.42	0.50
1:C:160:GLU:OE2	1:C:169:LYS:CE	2.60	0.50
1:A:166:VAL:HG11	1:B:142:ILE:HD11	1.93	0.50
1:D:131:SER:H	1:D:134:GLN:NE2	2.11	0.49
1:E:127:PRO:HA	1:F:137:GLN:HE21	1.78	0.49
1:C:166:VAL:CG1	1:C:167:ILE:N	2.76	0.49
1:B:127:PRO:CD	1:B:138:TRP:CH2	2.96	0.49
1:C:159:PHE:CE1	1:C:166:VAL:HG11	2.47	0.49
1:B:123:ARG:HD2	2:B:32:HOH:O	2.13	0.48
1:A:126:LEU:HD23	1:A:130:LEU:HD22	1.94	0.48
1:C:139:MET:SD	1:D:166:VAL:HG23	2.54	0.48
1:B:112:GLU:HG3	1:D:113:LEU:HD12	1.95	0.48
1:D:118:HIS:CD2	1:D:118:HIS:N	2.82	0.48
1:D:174:THR:HB	1:D:175:PRO:CD	2.43	0.48
1:A:126:LEU:HD23	1:A:130:LEU:CD2	2.44	0.48
1:D:158:THR:O	1:D:168:ILE:HA	2.14	0.47
1:F:131:SER:H	1:F:134:GLN:HE22	1.52	0.47
1:E:130:LEU:CD2	1:E:130:LEU:N	2.77	0.47
1:A:131:SER:N	1:A:134:GLN:OE1	2.31	0.47
1:C:164:GLU:HA	1:D:126:LEU:HD12	1.97	0.47
1:E:123:ARG:CZ	1:F:167:ILE:HD11	2.45	0.46
1:A:117:GLU:O	1:A:118:HIS:ND1	2.47	0.46
1:C:146:VAL:O	1:C:148:SER:N	2.49	0.46
1:D:150:LYS:C	1:D:151:HIS:HD1	2.20	0.45
1:A:170:LYS:NZ	2:A:15:HOH:O	2.49	0.45
1:E:166:VAL:HG23	1:F:139:MET:SD	2.55	0.45
1:F:153:ASN:HD21	1:F:155:ALA:HB3	1.80	0.45
1:B:129:GLY:HA2	2:B:71:HOH:O	2.16	0.45
1:D:126:LEU:CD2	1:D:138:TRP:CE3	3.00	0.45
1:A:139:MET:HE1	1:B:166:VAL:HG12	1.98	0.45
1:E:153:ASN:OD1	1:E:155:ALA:N	2.49	0.44
1:A:167:ILE:HG23	1:A:167:ILE:HD12	1.60	0.44
1:F:116:ASP:HB3	1:F:118:HIS:O	2.17	0.44
1:D:143:LYS:HD3	1:E:110:GLN:OE1	2.18	0.44
1:A:161:ALA:HB1	2:A:59:HOH:O	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:126:LEU:HB2	1:F:164:GLU:O	2.18	0.43
1:D:114:GLU:CD	1:D:123:ARG:HD2	2.39	0.43
1:C:162:SER:OG	1:C:163:GLY:N	2.48	0.43
1:F:116:ASP:C	1:F:118:HIS:N	2.72	0.43
1:B:131:SER:O	1:B:135:LYS:HD2	2.19	0.43
1:C:160:GLU:OE2	1:C:169:LYS:NZ	2.50	0.43
1:F:159:PHE:CD1	1:F:159:PHE:C	2.93	0.43
1:A:126:LEU:CD2	1:A:130:LEU:HD23	2.48	0.42
1:C:171:ARG:O	1:C:172:GLN:HG3	2.20	0.42
1:E:130:LEU:HG	1:E:135:LYS:HG2	2.01	0.42
1:E:133:GLU:CD	1:E:133:GLU:H	2.22	0.42
1:C:118:HIS:CD2	1:C:118:HIS:N	2.87	0.42
1:E:146:VAL:HG23	1:E:147:GLN:N	2.35	0.42
1:D:143:LYS:HE2	1:E:-1:MET:O	2.20	0.42
1:A:133:GLU:HB2	2:A:57:HOH:O	2.19	0.42
1:E:153:ASN:OD1	1:E:153:ASN:C	2.58	0.41
1:C:166:VAL:HG12	1:C:167:ILE:N	2.35	0.41
1:E:111:PRO:CD	1:F:140:LEU:HD13	2.49	0.41
1:E:162:SER:OG	1:E:163:GLY:N	2.54	0.41
1:F:131:SER:O	1:F:135:LYS:HG3	2.20	0.41
1:E:137:GLN:HE21	1:F:127:PRO:HG3	1.84	0.41
1:E:161:ALA:HB1	1:F:139:MET:CE	2.51	0.41
1:C:139:MET:CE	1:D:162:SER:O	2.69	0.41
1:E:146:VAL:CG2	1:E:147:GLN:N	2.83	0.41
1:E:138:TRP:HE1	1:F:141:THR:CG2	2.08	0.40
1:B:127:PRO:HG2	1:B:138:TRP:CH2	2.56	0.40
1:F:157:CYS:HB3	1:F:169:LYS:O	2.22	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	63/75 (84%)	59 (94%)	3 (5%)	1 (2%)	9	9
1	B	61/75 (81%)	59 (97%)	2 (3%)	0	100	100
1	C	65/75 (87%)	59 (91%)	5 (8%)	1 (2%)	10	10
1	D	70/75 (93%)	67 (96%)	2 (3%)	1 (1%)	11	11
1	E	70/75 (93%)	65 (93%)	4 (6%)	1 (1%)	11	11
1	F	62/75 (83%)	57 (92%)	5 (8%)	0	100	100
All	All	391/450 (87%)	366 (94%)	21 (5%)	4 (1%)	15	17

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	162	SER
1	C	147	GLN
1	A	163	GLY
1	E	176	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	56/65 (86%)	44 (79%)	12 (21%)	1	1
1	B	54/65 (83%)	46 (85%)	8 (15%)	3	3
1	C	58/65 (89%)	44 (76%)	14 (24%)	0	0
1	D	63/65 (97%)	55 (87%)	8 (13%)	4	4
1	E	63/65 (97%)	55 (87%)	8 (13%)	4	4
1	F	55/65 (85%)	49 (89%)	6 (11%)	6	7
All	All	349/390 (90%)	293 (84%)	56 (16%)	2	2

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	112	GLU
1	A	113	LEU
1	A	120	LYS
1	A	122	LEU
1	A	126	LEU
1	A	130	LEU
1	A	133	GLU
1	A	136	SER
1	A	137	GLN
1	A	142	ILE
1	A	153	ASN
1	B	110	GLN
1	B	123	ARG
1	B	131	SER
1	B	140	LEU
1	B	142	ILE
1	B	153	ASN
1	B	160	GLU
1	B	171	ARG
1	C	113	LEU
1	C	115	SER
1	C	116	ASP
1	C	123	ARG
1	C	124	LEU
1	C	126	LEU
1	C	148	SER
1	C	152	TRP
1	C	164	GLU
1	C	167	ILE
1	C	169	LYS
1	C	170	LYS
1	C	171	ARG
1	C	173	ILE
1	D	-1	MET
1	D	107	ASP
1	D	122	LEU
1	D	152	TRP
1	D	158	THR
1	D	162	SER
1	D	171	ARG
1	D	173	ILE
1	E	-1	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	116	ASP
1	E	118	HIS
1	E	122	LEU
1	E	127	PRO
1	E	130	LEU
1	E	152	TRP
1	E	177	VAL
1	F	128	GLU
1	F	140	LEU
1	F	147	GLN
1	F	152	TRP
1	F	153	ASN
1	F	159	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	GLN
1	A	147	GLN
1	A	153	ASN
1	B	110	GLN
1	B	147	GLN
1	B	153	ASN
1	C	118	HIS
1	C	151	HIS
1	D	118	HIS
1	D	134	GLN
1	D	137	GLN
1	E	118	HIS
1	E	134	GLN
1	E	137	GLN
1	E	147	GLN
1	F	134	GLN
1	F	137	GLN
1	F	147	GLN
1	F	151	HIS
1	F	153	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 monosaccharides 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	65/75 (86%)	0.71	11 (16%)	1	2	26, 45, 91, 107	0
1	B	63/75 (84%)	0.51	4 (6%)	20	25	23, 47, 77, 91	0
1	C	67/75 (89%)	0.41	2 (2%)	50	57	27, 51, 77, 95	0
1	D	72/75 (96%)	0.52	5 (6%)	16	22	21, 44, 78, 93	0
1	E	72/75 (96%)	0.85	11 (15%)	2	3	24, 53, 92, 105	0
1	F	64/75 (85%)	0.92	10 (15%)	2	2	29, 57, 91, 111	0
All	All	403/450 (89%)	0.65	43 (10%)	6	8	21, 50, 88, 111	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	171	ARG	7.1
1	A	164	GLU	6.7
1	E	118	HIS	4.2
1	D	171	ARG	4.1
1	F	117	GLU	4.1
1	E	142	ILE	3.7
1	F	128	GLU	3.6
1	A	118	HIS	3.4
1	F	141	THR	3.4
1	F	140	LEU	3.3
1	F	118	HIS	3.3
1	B	118	HIS	3.2
1	E	163	GLY	3.1
1	F	156	GLU	3.0
1	F	116	ASP	3.0
1	E	117	GLU	2.9
1	E	176	ASP	2.9
1	A	117	GLU	2.8
1	F	144	ALA	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	142	ILE	2.8
1	D	118	HIS	2.7
1	B	131	SER	2.7
1	A	128	GLU	2.7
1	A	171	ARG	2.6
1	E	129	GLY	2.6
1	E	124	LEU	2.5
1	C	171	ARG	2.5
1	F	142	ILE	2.5
1	D	107	ASP	2.5
1	E	145	VAL	2.4
1	A	140	LEU	2.3
1	D	162	SER	2.3
1	C	117	GLU	2.3
1	F	145	VAL	2.3
1	E	144	ALA	2.2
1	A	132	GLY	2.2
1	B	117	GLU	2.2
1	A	129	GLY	2.2
1	A	145	VAL	2.2
1	E	164	GLU	2.1
1	A	163	GLY	2.1
1	E	177	VAL	2.1
1	A	144	ALA	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 monosaccharides 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.