W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 07:02 PM GMT

PDB ID	:	4PH0
Title	:	capsid protein from bovine leukemia virus
Authors	:	Trajtenberg, F.; Obal, G.; Pritsch, O.; Buschiazzo, A.
Deposited on	:	2014-05-03
Resolution	:	2.75 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
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-20026982

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 2.75 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		0.221
Clashscore		16
Ramachandran outliers		0.1%
Sidechain outliers		1.6%
RSRZ outliers		8.6%

Worse   *Better*

∎ Percentile relative to all X-ray structures

❏ Percentile relative to X-ray structures of similar resolution
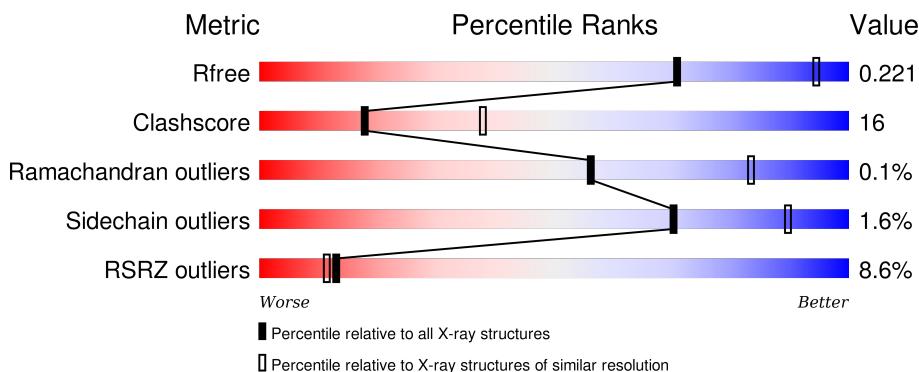
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	3050 (2.78-2.70)
Clashscore	102246	3424 (2.78-2.70)
Ramachandran outliers	100387	3367 (2.78-2.70)
Sidechain outliers	100360	3368 (2.78-2.70)
RSRZ outliers	91569	3055 (2.78-2.70)

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	215	7% 57% / 36% / 7%
1	B	215	11% 58% / 30% / 13%
1	C	215	6% 69% / 22% / • 7%
1	D	215	2% 69% / 22% / • 8%
1	E	215	7% 64% / 26% / 10%
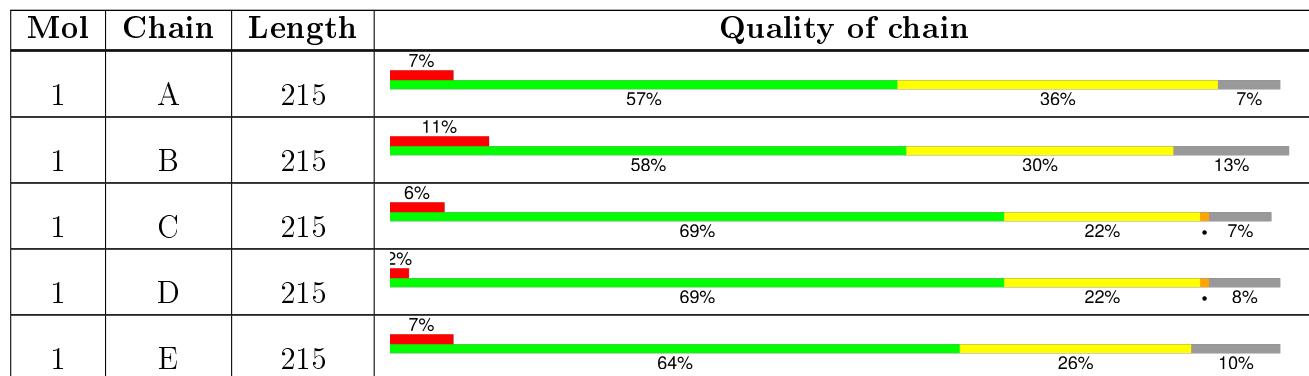
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	215	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 9078 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 BLV capsid.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	201	Total	C	N	O	S	0	0	0
			1549	972	278	295	4			
1	B	188	Total	C	N	O	S	0	0	0
			1450	907	259	280	4			
1	C	199	Total	C	N	O	S	0	0	0
			1532	960	273	295	4			
1	D	198	Total	C	N	O	S	0	0	0
			1535	962	276	293	4			
1	E	193	Total	C	N	O	S	0	0	0
			1493	937	267	285	4			
1	F	199	Total	C	N	O	S	0	0	0
			1519	957	267	291	4			

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 errors 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: BLV capsid
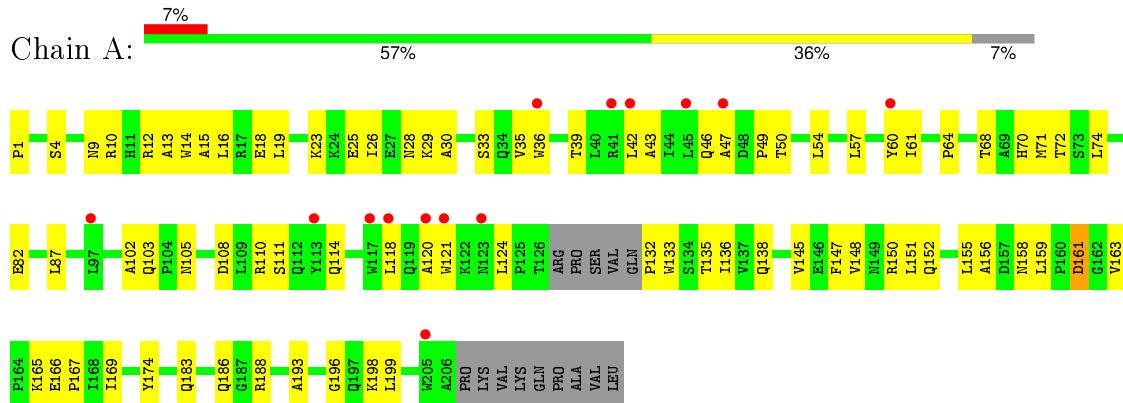
- Molecule 1: BLV capsid
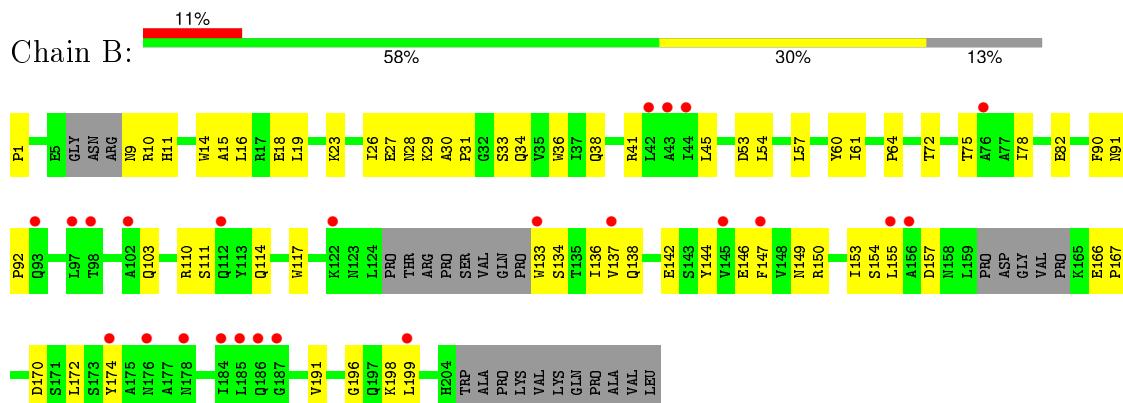
- Molecule 1: BLV capsid
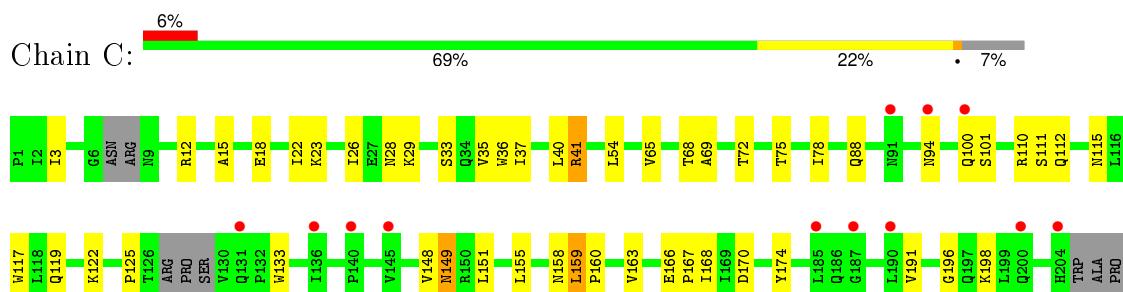
LYS VAL LYS GLN PRO ALA VAL LEU

- Molecule 1: BLV capsid

Chain D:

- Molecule 1: BLV capsid

Chain E:

- Molecule 1: BLV capsid

Chain F:
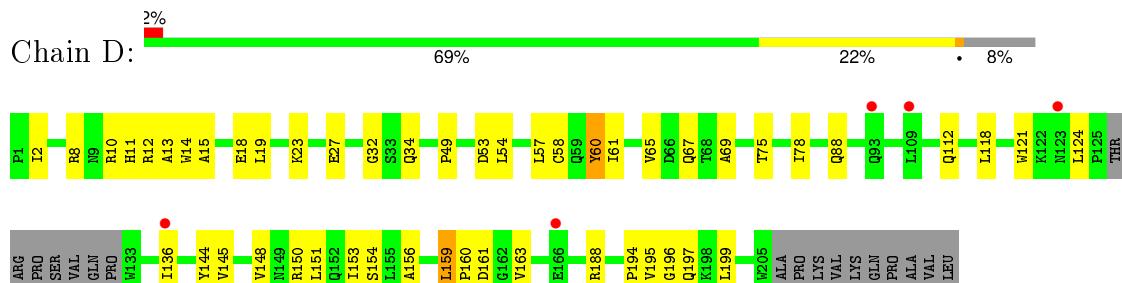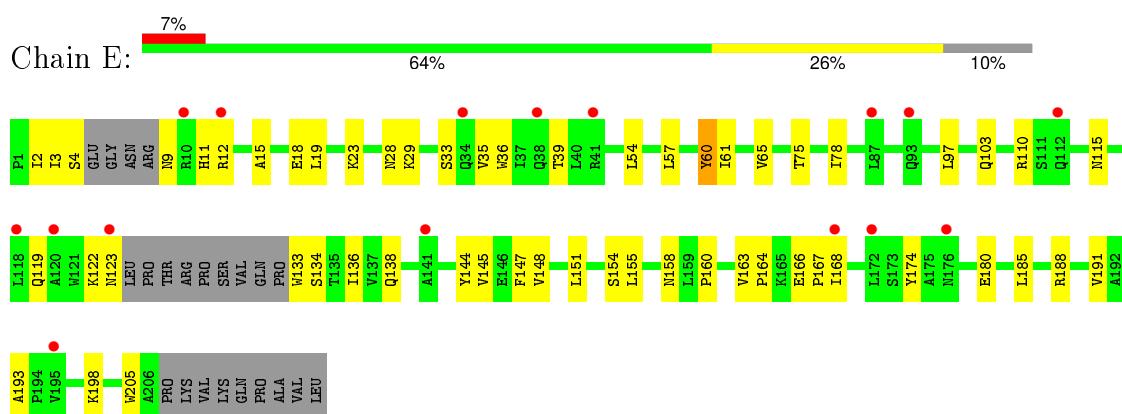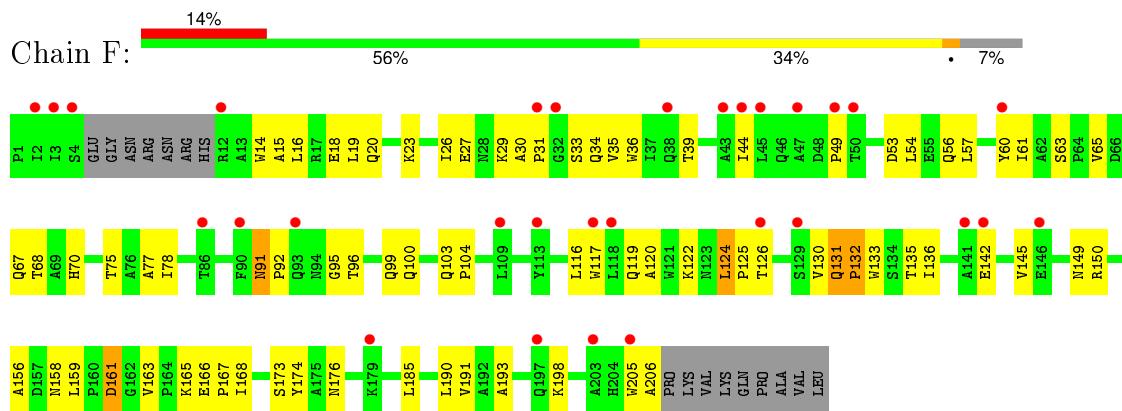
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	94.28Å 94.28Å 257.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.14 – 2.75	Depositor
	47.14 – 2.75	EDS
% Data completeness	99.9 (47.14-2.75)	Depositor
(in resolution range)	99.9 (47.14-2.75)	EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.81 (at 2.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.180 , 0.221	Depositor
	0.180 , 0.221	DCC
R_{free} test set	1674 reflections (5.00%)	DCC
Wilson B-factor (Å^2)	82.2	Xtriage
Anisotropy	0.498	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 76.1	EDS
Estimated twinning fraction	0.420 for k,h,-l	Xtriage
	0.398 for h,-h-k,-l	
Reported twinning fraction	0.420 for k,h,-l	Depositor
L-test for twinning[2]	$< |L| > = 0.39, < L^2 > = 0.22$	Xtriage
Outliers	0 of 33497 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9078	wwPDB-VP
Average B, all atoms (Å^2)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.00% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.43	0/1582	0.65	0/2159
1	B	0.45	0/1474	0.66	0/2005
1	C	0.44	0/1562	0.63	0/2131
1	D	0.44	0/1567	0.67	0/2138
1	E	0.41	0/1523	0.64	0/2077
1	F	0.45	0/1552	0.73	1/2123 (0.0%)
All	All	0.44	0/9260	0.66	1/12633 (0.0%)

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	F	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	131	GLN	N-CA-C	5.32	125.36	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	124	LEU	Peptide

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	1549	0	1527	60	0
1	B	1450	0	1431	60	0
1	C	1532	0	1517	43	1
1	D	1535	0	1516	35	1
1	E	1493	0	1474	45	0
1	F	1519	0	1494	60	0
All	All	9078	0	8959	284	1

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 (284) 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:A:133:TRP:HB3	1:A:158:ASN:HD22	1.29	0.94
1:C:133:TRP:HD1	1:C:158:ASN:HB2	1.32	0.94
1:F:124:LEU:O	1:F:126:THR:N	2.06	0.86
1:F:136:ILE:O	1:F:176:ASN:ND2	2.10	0.84
1:D:159:LEU:HD22	1:D:160:PRO:HD2	1.62	0.82
1:A:145:VAL:HG13	1:F:65:VAL:HG11	1.62	0.80
1:F:23:LYS:HB2	1:F:60:TYR:HE2	1.48	0.78
1:C:133:TRP:CD1	1:C:158:ASN:HB2	2.18	0.78
1:E:193:ALA:O	1:E:198:LYS:NZ	2.15	0.78
1:B:138:GLN:NE2	1:B:142:GLU:O	2.17	0.77
1:A:161:ASP:OD1	1:A:161:ASP:N	2.16	0.77
1:A:72:THR:HG23	1:B:196:GLY:HA2	1.67	0.77
1:C:170:ASP:O	1:C:198:LYS:NZ	2.18	0.76
1:B:142:GLU:OE1	1:B:150:ARG:NH1	2.18	0.75
1:F:163:VAL:HG12	1:F:168:ILE:HD11	1.67	0.75
1:A:25:GLU:O	1:A:29:LYS:NZ	2.13	0.74
1:A:12:ARG:NH1	1:A:13:ALA:O	2.20	0.74
1:F:142:GLU:OE1	1:F:150:ARG:NH1	2.22	0.73
1:F:16:LEU:HA	1:F:19:LEU:HD12	1.71	0.72
1:F:119:GLN:O	1:F:122:LYS:HG2	1.88	0.72
1:F:193:ALA:O	1:F:198:LYS:NZ	2.23	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:95:GLY:O	1:F:100:GLN:NE2	2.24	0.71
1:C:75:THR:HA	1:C:78:ILE:HD12	1.73	0.71
1:F:161:ASP:OD1	1:F:161:ASP:N	2.24	0.70
1:A:16:LEU:HA	1:A:19:LEU:HD12	1.73	0.70
1:A:42:LEU:HD11	1:F:14:TRP:HB2	1.74	0.69
1:E:75:THR:HA	1:E:78:ILE:HD12	1.74	0.69
1:B:82:GLU:HG3	1:B:90:PHE:CE2	2.27	0.69
1:B:150:ARG:HA	1:B:153:ILE:HD12	1.74	0.69
1:D:15:ALA:HB3	1:D:18:GLU:HG3	1.75	0.69
1:C:101:SER:HB2	1:C:110:ARG:HA	1.76	0.67
1:B:57:LEU:O	1:B:61:ILE:HG12	1.96	0.66
1:B:170:ASP:O	1:B:198:LYS:NZ	2.29	0.65
1:C:159:LEU:HD22	1:C:160:PRO:HD2	1.79	0.65
1:F:133:TRP:HB3	1:F:158:ASN:HD22	1.62	0.65
1:F:131:GLN:O	1:F:133:TRP:N	2.30	0.64
1:A:70:HIS:NE2	1:A:120:ALA:HB3	2.11	0.64
1:E:166:GLU:HB2	1:E:167:PRO:HD3	1.79	0.64
1:F:159:LEU:HD22	1:F:165:LYS:HG2	1.80	0.64
1:B:75:THR:HA	1:B:78:ILE:HD12	1.78	0.64
1:C:3:ILE:HD11	1:C:12:ARG:HE	1.63	0.64
1:F:34:GLN:HE21	1:F:156:ALA:HB1	1.63	0.63
1:E:160:PRO:HB2	1:E:163:VAL:HG21	1.81	0.63
1:C:88:GLN:O	1:C:112:GLN:NE2	2.30	0.62
1:F:75:THR:HA	1:F:78:ILE:HD12	1.81	0.62
1:F:26:ILE:HD12	1:F:39:THR:HB	1.80	0.62
1:C:41:ARG:HH21	1:C:41:ARG:HB2	1.64	0.62
1:B:166:GLU:H	1:B:166:GLU:CD	2.03	0.61
1:B:138:GLN:HB2	1:B:147:PHE:CD1	2.36	0.61
1:B:133:TRP:HB3	1:B:154:SER:HB3	1.81	0.61
1:A:26:ILE:HA	1:A:29:LYS:HD3	1.82	0.61
1:D:65:VAL:HG11	1:E:145:VAL:HG13	1.83	0.61
1:C:166:GLU:CD	1:C:166:GLU:H	2.04	0.61
1:F:165:LYS:HA	1:F:168:ILE:HD12	1.83	0.61
1:A:71:MET:SD	1:A:74:LEU:HD23	2.41	0.60
1:E:65:VAL:HG11	1:F:145:VAL:HG13	1.81	0.60
1:B:34:GLN:O	1:B:38:GLN:HG2	2.01	0.60
1:E:136:ILE:HD12	1:E:151:LEU:HA	1.84	0.60
1:D:136:ILE:HD12	1:D:151:LEU:HA	1.84	0.60
1:B:54:LEU:HD23	1:B:57:LEU:HD12	1.84	0.60
1:C:65:VAL:HG11	1:D:145:VAL:HG13	1.83	0.59
1:A:166:GLU:CD	1:A:166:GLU:H	2.06	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:ALA:HB1	1:C:125:PRO:HD2	1.83	0.59
1:E:163:VAL:HG12	1:E:168:ILE:HD11	1.85	0.59
1:C:29:LYS:HE2	1:C:35:VAL:HG11	1.84	0.58
1:B:23:LYS:HD2	1:B:60:TYR:CE2	2.39	0.58
1:A:25:GLU:OE1	1:F:60:TYR:OH	2.18	0.58
1:D:57:LEU:O	1:D:61:ILE:HG12	2.03	0.58
1:C:68:THR:HG21	1:D:195:VAL:HG13	1.85	0.58
1:E:160:PRO:HB2	1:E:163:VAL:CG2	2.34	0.57
1:B:9:ASN:C	1:B:10:ARG:HD3	2.25	0.57
1:F:53:ASP:O	1:F:56:GLN:HB2	2.03	0.57
1:E:23:LYS:HD2	1:E:60:TYR:CE1	2.40	0.57
1:B:33:SER:O	1:B:36:TRP:HB3	2.05	0.56
1:F:70:HIS:NE2	1:F:117:TRP:O	2.35	0.56
1:E:57:LEU:O	1:E:61:ILE:HG12	2.04	0.56
1:F:26:ILE:HB	1:F:39:THR:HG21	1.87	0.56
1:B:23:LYS:O	1:B:27:GLU:N	2.39	0.56
1:F:166:GLU:CD	1:F:166:GLU:H	2.10	0.55
1:A:103:GLN:HG2	1:A:105:ASN:H	1.72	0.55
1:E:4:SER:O	1:E:9:ASN:N	2.40	0.55
1:E:166:GLU:H	1:E:166:GLU:CD	2.10	0.55
1:F:57:LEU:O	1:F:61:ILE:HG12	2.07	0.55
1:F:33:SER:O	1:F:36:TRP:HB3	2.07	0.54
1:F:96:THR:O	1:F:100:GLN:HG3	2.07	0.54
1:B:166:GLU:HB2	1:B:167:PRO:HD3	1.89	0.54
1:C:111:SER:O	1:C:115:ASN:ND2	2.40	0.54
1:E:115:ASN:O	1:E:119:GLN:HG2	2.07	0.54
1:A:14:TRP:CG	1:A:19:LEU:HD21	2.43	0.54
1:A:68:THR:OG1	1:B:149:ASN:OD1	2.22	0.54
1:F:124:LEU:HB3	1:F:125:PRO:HD3	1.88	0.54
1:E:138:GLN:HB2	1:E:147:PHE:CG	2.43	0.54
1:C:101:SER:HB2	1:C:110:ARG:CA	2.37	0.53
1:F:70:HIS:NE2	1:F:120:ALA:HB3	2.24	0.53
1:A:82:GLU:HG2	1:A:87:LEU:HD12	1.90	0.53
1:E:144:TYR:O	1:E:148:VAL:HG23	2.09	0.52
1:A:174:TYR:HB2	1:A:198:LYS:HE2	1.91	0.52
1:B:15:ALA:O	1:B:18:GLU:HB2	2.10	0.52
1:B:154:SER:O	1:B:157:ASP:HB2	2.09	0.52
1:B:16:LEU:HA	1:B:19:LEU:HD12	1.91	0.52
1:A:166:GLU:HB2	1:A:167:PRO:HD3	1.91	0.52
1:D:75:THR:HA	1:D:78:ILE:HD12	1.91	0.52
1:E:136:ILE:CD1	1:E:151:LEU:HA	2.40	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:136:ILE:HD12	1:D:151:LEU:HD12	1.92	0.51
1:E:65:VAL:HG21	1:F:145:VAL:O	2.10	0.51
1:E:29:LYS:HE3	1:E:35:VAL:HG11	1.92	0.51
1:F:54:LEU:HD23	1:F:57:LEU:HD12	1.91	0.50
1:A:156:ALA:HA	1:A:165:LYS:NZ	2.26	0.50
1:C:72:THR:OG1	1:D:196:GLY:HA3	2.11	0.50
1:A:155:LEU:HD22	1:A:159:LEU:HB2	1.92	0.50
1:F:185:LEU:O	1:F:190:LEU:N	2.41	0.50
1:E:35:VAL:O	1:E:39:THR:OG1	2.17	0.50
1:C:33:SER:O	1:C:36:TRP:HB3	2.12	0.50
1:A:29:LYS:HG2	1:A:35:VAL:HG22	1.94	0.50
1:B:28:ASN:OD1	1:B:28:ASN:N	2.42	0.50
1:B:111:SER:HA	1:B:114:GLN:OE1	2.12	0.50
1:A:148:VAL:HG12	1:F:65:VAL:HG22	1.93	0.50
1:E:133:TRP:CE3	1:E:134:SER:HB3	2.47	0.50
1:D:23:LYS:O	1:D:27:GLU:N	2.45	0.50
1:C:148:VAL:O	1:C:151:LEU:HB3	2.12	0.50
1:E:19:LEU:HB3	1:E:60:TYR:CE2	2.47	0.49
1:C:15:ALA:HB3	1:C:18:GLU:HG3	1.94	0.49
1:A:49:PRO:O	1:A:110:ARG:HD2	2.12	0.49
1:D:136:ILE:HD11	1:D:154:SER:CB	2.43	0.49
1:C:3:ILE:HD11	1:C:12:ARG:NE	2.26	0.49
1:B:38:GLN:HA	1:B:41:ARG:NH1	2.28	0.49
1:C:163:VAL:HG12	1:C:168:ILE:HD11	1.95	0.49
1:D:136:ILE:CD1	1:D:151:LEU:HA	2.43	0.49
1:A:136:ILE:CD1	1:A:151:LEU:HA	2.43	0.49
1:A:152:GLN:NE2	1:F:68:THR:OG1	2.24	0.48
1:F:77:ALA:HB1	1:F:116:LEU:HD22	1.94	0.48
1:D:32:GLY:HA2	1:D:121:TRP:HB3	1.95	0.48
1:A:136:ILE:HG22	1:A:150:ARG:HH21	1.78	0.48
1:A:30:ALA:HB3	1:A:33:SER:HB3	1.95	0.48
1:C:23:LYS:HA	1:C:26:ILE:HG22	1.96	0.48
1:A:28:ASN:OD1	1:A:28:ASN:N	2.46	0.48
1:A:64:PRO:HB2	1:B:149:ASN:HD21	1.78	0.48
1:D:8:ARG:HB3	1:D:10:ARG:HG2	1.96	0.48
1:E:180:GLU:HG3	1:E:205:TRP:CZ2	2.49	0.48
1:A:183:GLN:HA	1:A:186:GLN:OE1	2.12	0.48
1:F:163:VAL:CG1	1:F:168:ILE:HD11	2.40	0.47
1:C:166:GLU:HB2	1:C:167:PRO:HD3	1.96	0.47
1:E:15:ALA:HB3	1:E:18:GLU:HG3	1.96	0.47
1:C:159:LEU:HD22	1:C:160:PRO:CD	2.43	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:SER:O	1:A:36:TRP:HB3	2.14	0.47
1:C:54:LEU:HB3	1:C:117:TRP:CE2	2.49	0.47
1:E:180:GLU:HG3	1:E:205:TRP:HZ2	1.79	0.47
1:E:174:TYR:HD1	1:E:185:LEU:HD12	1.79	0.47
1:E:2:ILE:HD13	1:E:11:HIS:HA	1.97	0.47
1:C:155:LEU:HD23	1:C:155:LEU:HA	1.73	0.47
1:A:72:THR:HG23	1:B:196:GLY:CA	2.42	0.47
1:D:23:LYS:HD2	1:D:60:TYR:CE1	2.50	0.47
1:C:155:LEU:HD22	1:C:159:LEU:HD23	1.97	0.46
1:F:166:GLU:HB2	1:F:167:PRO:HD3	1.97	0.46
1:A:121:TRP:CE3	1:A:124:LEU:HD11	2.50	0.46
1:B:150:ARG:O	1:B:153:ILE:HB	2.14	0.46
1:E:78:ILE:HG23	1:E:97:LEU:HD23	1.96	0.46
1:C:29:LYS:N	1:C:29:LYS:HD2	2.30	0.46
1:F:132:PRO:HB2	1:F:135:THR:HG21	1.97	0.46
1:C:36:TRP:O	1:C:40:LEU:HG	2.15	0.46
1:E:33:SER:O	1:E:36:TRP:HB3	2.15	0.46
1:D:69:ALA:HB1	1:D:124:LEU:HD22	1.97	0.46
1:B:34:GLN:HE21	1:B:38:GLN:NE2	2.14	0.46
1:A:4:SER:HA	1:A:9:ASN:OD1	2.16	0.46
1:F:91:ASN:HA	1:F:92:PRO:HD2	1.81	0.46
1:D:88:GLN:HB3	1:D:112:GLN:HE22	1.81	0.46
1:A:121:TRP:HE3	1:A:124:LEU:HD11	1.81	0.46
1:A:50:THR:HB	1:A:102:ALA:HA	1.98	0.46
1:E:19:LEU:HB3	1:E:60:TYR:CD2	2.51	0.45
1:B:133:TRP:HB3	1:B:154:SER:CB	2.46	0.45
1:B:34:GLN:HG2	1:B:38:GLN:HE21	1.80	0.45
1:A:193:ALA:O	1:A:198:LYS:NZ	2.37	0.45
1:F:161:ASP:C	1:F:163:VAL:H	2.20	0.45
1:A:57:LEU:O	1:A:61:ILE:HG12	2.17	0.45
1:E:180:GLU:HG2	1:E:180:GLU:H	1.60	0.45
1:F:23:LYS:HB2	1:F:60:TYR:CE2	2.39	0.45
1:E:174:TYR:CD2	1:E:191:VAL:HG13	2.51	0.45
1:B:155:LEU:HA	1:B:155:LEU:HD23	1.78	0.45
1:B:138:GLN:HB2	1:B:147:PHE:CG	2.51	0.45
1:A:110:ARG:HG2	1:A:114:GLN:NE2	2.32	0.45
1:D:14:TRP:HE1	1:D:53:ASP:HB3	1.80	0.45
1:F:174:TYR:CG	1:F:191:VAL:HG13	2.52	0.45
1:F:34:GLN:NE2	1:F:156:ALA:HB1	2.29	0.45
1:E:60:TYR:HD1	1:E:60:TYR:O	2.00	0.45
1:E:103:GLN:O	1:E:110:ARG:NH1	2.44	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:196:GLY:HA2	1:D:199:LEU:HD12	1.99	0.44
1:D:14:TRP:HB3	1:D:19:LEU:HD11	2.00	0.44
1:B:144:TYR:CD2	1:B:199:LEU:HD23	2.52	0.44
1:F:20:GLN:NE2	1:F:60:TYR:OH	2.50	0.44
1:C:37:ILE:HG22	1:C:41:ARG:HH22	1.81	0.44
1:C:155:LEU:O	1:C:159:LEU:N	2.50	0.44
1:E:23:LYS:HD2	1:E:60:TYR:HE1	1.81	0.44
1:A:54:LEU:O	1:A:57:LEU:HB2	2.18	0.44
1:D:12:ARG:NH1	1:D:13:ALA:O	2.51	0.44
1:F:142:GLU:OE2	1:F:150:ARG:HD3	2.18	0.44
1:F:15:ALA:HB3	1:F:18:GLU:HG3	1.98	0.44
1:C:119:GLN:O	1:C:122:LYS:HB2	2.17	0.44
1:B:54:LEU:HB3	1:B:117:TRP:NE1	2.32	0.44
1:B:26:ILE:HD11	1:B:36:TRP:CD2	2.52	0.44
1:A:196:GLY:HA2	1:A:199:LEU:HD12	2.00	0.44
1:E:3:ILE:HD13	1:E:12:ARG:NE	2.33	0.44
1:B:103:GLN:O	1:B:110:ARG:NH1	2.51	0.44
1:E:65:VAL:HG23	1:F:149:ASN:OD1	2.18	0.44
1:A:136:ILE:HG22	1:A:150:ARG:NH2	2.32	0.44
1:D:150:ARG:HA	1:D:153:ILE:HD12	1.99	0.44
1:A:23:LYS:HD2	1:A:60:TYR:CE2	2.52	0.44
1:F:15:ALA:HB3	1:F:18:GLU:CG	2.48	0.44
1:D:118:LEU:HA	1:D:118:LEU:HD23	1.85	0.43
1:C:41:ARG:HB2	1:C:41:ARG:NH2	2.31	0.43
1:F:103:GLN:HA	1:F:104:PRO:HD3	1.84	0.43
1:D:194:PRO:HD2	1:D:197:GLN:OE1	2.18	0.43
1:A:138:GLN:HB2	1:A:147:PHE:CG	2.53	0.43
1:D:54:LEU:HD23	1:D:57:LEU:HD12	1.99	0.43
1:D:144:TYR:O	1:D:148:VAL:HG23	2.18	0.43
1:E:54:LEU:O	1:E:57:LEU:HB2	2.18	0.43
1:A:118:LEU:O	1:A:121:TRP:HD1	2.02	0.43
1:D:49:PRO:HB2	1:D:53:ASP:HB2	2.00	0.43
1:B:57:LEU:HA	1:B:57:LEU:HD23	1.78	0.43
1:C:155:LEU:O	1:C:159:LEU:HB2	2.18	0.43
1:E:164:PRO:HB2	1:E:167:PRO:HD2	2.01	0.43
1:A:108:ASP:O	1:A:111:SER:HB2	2.19	0.43
1:B:54:LEU:O	1:B:57:LEU:HB2	2.19	0.43
1:B:41:ARG:O	1:B:45:LEU:HG	2.19	0.43
1:F:63:SER:O	1:F:67:GLN:HG3	2.18	0.43
1:B:72:THR:HG23	1:C:196:GLY:O	2.18	0.43
1:A:15:ALA:HB3	1:A:18:GLU:HG3	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:TRP:HB3	1:A:158:ASN:ND2	2.12	0.43
1:E:122:LYS:HG3	1:E:123:ASN:N	2.34	0.43
1:E:154:SER:O	1:E:158:ASN:ND2	2.42	0.43
1:D:34:GLN:HG2	1:D:156:ALA:HB1	2.00	0.43
1:F:16:LEU:O	1:F:20:GLN:N	2.49	0.43
1:F:23:LYS:O	1:F:27:GLU:N	2.43	0.43
1:B:174:TYR:CG	1:B:191:VAL:HG13	2.54	0.42
1:B:137:VAL:HG12	1:B:138:GLN:N	2.33	0.42
1:D:136:ILE:HD11	1:D:154:SER:HB2	2.00	0.42
1:A:64:PRO:CB	1:B:149:ASN:HD21	2.31	0.42
1:E:164:PRO:HB2	1:E:167:PRO:CD	2.49	0.42
1:C:23:LYS:O	1:C:26:ILE:HG22	2.19	0.42
1:B:26:ILE:HA	1:B:29:LYS:HD3	2.02	0.42
1:C:174:TYR:CG	1:C:191:VAL:HG13	2.55	0.42
1:C:94:ASN:HB2	1:C:100:GLN:NE2	2.33	0.42
1:B:9:ASN:O	1:B:10:ARG:HD3	2.20	0.42
1:B:142:GLU:CD	1:B:150:ARG:HH11	2.22	0.42
1:E:29:LYS:HA	1:E:29:LYS:HD3	1.91	0.42
1:F:44:ILE:HG23	1:F:49:PRO:HD2	2.01	0.42
1:A:161:ASP:C	1:A:163:VAL:H	2.22	0.42
1:B:133:TRP:CZ3	1:B:172:LEU:HD11	2.55	0.42
1:F:30:ALA:HA	1:F:31:PRO:HD3	1.90	0.42
1:F:96:THR:HG23	1:F:99:GLN:OE1	2.20	0.41
1:B:34:GLN:CG	1:B:38:GLN:HE21	2.33	0.41
1:A:155:LEU:HD12	1:A:169:ILE:HD11	2.03	0.41
1:C:18:GLU:O	1:C:22:ILE:HG13	2.19	0.41
1:D:2:ILE:HD13	1:D:11:HIS:HA	2.02	0.41
1:D:161:ASP:O	1:D:163:VAL:HG23	2.21	0.41
1:F:29:LYS:HE2	1:F:35:VAL:HG21	2.02	0.41
1:B:146:GLU:HA	1:B:149:ASN:HB2	2.03	0.41
1:B:144:TYR:HD2	1:B:199:LEU:HD23	1.84	0.41
1:B:30:ALA:HA	1:B:31:PRO:HD3	1.90	0.41
1:B:136:ILE:HG23	1:B:136:ILE:HD12	1.93	0.41
1:A:43:ALA:O	1:A:46:GLN:HB2	2.20	0.41
1:F:205:TRP:CG	1:F:206:ALA:N	2.89	0.41
1:A:138:GLN:HB2	1:A:147:PHE:CD1	2.55	0.41
1:A:35:VAL:O	1:A:39:THR:OG1	2.23	0.41
1:D:15:ALA:HB3	1:D:18:GLU:CG	2.48	0.41
1:B:133:TRP:CZ3	1:B:134:SER:HB3	2.56	0.41
1:E:133:TRP:CZ3	1:E:155:LEU:HD21	2.56	0.41
1:A:136:ILE:HD12	1:A:151:LEU:HA	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:174:TYR:CG	1:E:191:VAL:HG13	2.56	0.41
1:F:130:VAL:C	1:F:132:PRO:HD2	2.40	0.41
1:A:1:PRO:HG3	1:A:47:ALA:HB1	2.02	0.41
1:B:64:PRO:HB2	1:C:149:ASN:OD1	2.21	0.41
1:D:58:CYS:HB3	1:D:67:GLN:HG2	2.02	0.41
1:A:156:ALA:HA	1:A:165:LYS:HZ1	1.86	0.41
1:D:161:ASP:C	1:D:163:VAL:H	2.24	0.41
1:B:144:TYR:CE2	1:B:199:LEU:HA	2.56	0.40
1:B:91:ASN:HA	1:B:92:PRO:HD2	1.83	0.40
1:B:14:TRP:HE1	1:B:53:ASP:HB3	1.87	0.40
1:F:174:TYR:CD1	1:F:191:VAL:HG13	2.57	0.40
1:B:1:PRO:O	1:B:11:HIS:HA	2.22	0.40
1:B:54:LEU:HD23	1:B:54:LEU:HA	1.89	0.40
1:C:15:ALA:O	1:C:18:GLU:HB2	2.22	0.40
1:A:87:LEU:HA	1:A:87:LEU:HD23	1.77	0.40
1:C:54:LEU:HB3	1:C:117:TRP:NE1	2.36	0.40
1:A:132:PRO:HB2	1:A:135:THR:HG23	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:ASN:O	1:D:10:ARG:NH2[6_654]	2.11	0.09

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	197/215 (92%)	195 (99%)	2 (1%)	0	100	100
1	B	180/215 (84%)	176 (98%)	4 (2%)	0	100	100
1	C	193/215 (90%)	192 (100%)	1 (0%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	194/215 (90%)	192 (99%)	2 (1%)	0	100	100
1	E	187/215 (87%)	184 (98%)	3 (2%)	0	100	100
1	F	195/215 (91%)	190 (97%)	4 (2%)	1 (0%)	34	62
All	All	1146/1290 (89%)	1129 (98%)	16 (1%)	1 (0%)	56	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	132	PRO

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	162/177 (92%)	159 (98%)	3 (2%)	65	87
1	B	152/177 (86%)	152 (100%)	0	100	100
1	C	163/177 (92%)	160 (98%)	3 (2%)	66	88
1	D	162/177 (92%)	159 (98%)	3 (2%)	65	87
1	E	157/177 (89%)	154 (98%)	3 (2%)	65	87
1	F	159/177 (90%)	156 (98%)	3 (2%)	65	87
All	All	955/1062 (90%)	940 (98%)	15 (2%)	70	89

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	161	ASP
1	A	188	ARG
1	C	41	ARG
1	C	149	ASN
1	C	159	LEU
1	D	60	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	159	LEU
1	D	188	ARG
1	E	28	ASN
1	E	60	TYR
1	E	188	ARG
1	F	91	ASN
1	F	161	ASP
1	F	173	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	158	ASN
1	B	38	GLN
1	B	200	GLN
1	C	59	GLN
1	D	38	GLN
1	E	103	GLN
1	E	105	ASN
1	F	20	GLN
1	F	34	GLN
1	F	38	GLN

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(Å²)	Q<0.9
1	A	201/215 (93%)	0.52	14 (6%)	19	18	66, 99, 131, 157	0
1	B	188/215 (87%)	0.79	24 (12%)	5	4	79, 118, 167, 212	0
1	C	199/215 (92%)	0.43	12 (6%)	25	25	52, 85, 117, 150	0
1	D	198/215 (92%)	0.26	5 (2%)	61	63	55, 82, 121, 150	0
1	E	193/215 (89%)	0.57	16 (8%)	14	12	75, 102, 146, 188	0
1	F	199/215 (92%)	0.81	30 (15%)	3	2	64, 110, 158, 183	0
All	All	1178/1290 (91%)	0.56	101 (8%)	13	11	52, 99, 151, 212	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	3	ILE	7.4
1	B	185	LEU	6.0
1	F	4	SER	5.3
1	E	112	GLN	5.0
1	F	129	SER	4.5
1	E	87	LEU	4.5
1	B	42	LEU	4.5
1	E	141	ALA	4.4
1	B	93	GLN	4.4
1	B	112	GLN	4.4
1	F	90	PHE	4.4
1	B	178	ASN	4.2
1	F	49	PRO	4.1
1	B	137	VAL	4.1
1	F	118	LEU	4.1
1	B	102	ALA	3.9
1	F	117	TRP	3.9
1	E	93	GLN	3.9
1	B	155	LEU	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	38	GLN	3.6
1	F	113	TYR	3.6
1	B	176	ASN	3.6
1	E	120	ALA	3.5
1	C	190	LEU	3.5
1	F	93	GLN	3.5
1	F	44	ILE	3.3
1	B	199	LEU	3.3
1	A	42	LEU	3.3
1	C	185	LEU	3.3
1	E	10	ARG	3.3
1	F	60	TYR	3.2
1	A	117	TRP	3.2
1	C	136	ILE	3.2
1	F	197	GLN	3.2
1	A	123	ASN	3.1
1	B	147	PHE	3.0
1	F	2	ILE	3.0
1	A	97	LEU	3.0
1	F	86	THR	2.9
1	E	118	LEU	2.9
1	B	43	ALA	2.9
1	A	41	ARG	2.9
1	F	205	TRP	2.9
1	D	93	GLN	2.9
1	D	109	LEU	2.9
1	C	204	HIS	2.8
1	F	43	ALA	2.8
1	A	113	TYR	2.8
1	C	187	GLY	2.8
1	B	44	ILE	2.8
1	D	136	ILE	2.8
1	A	60	TYR	2.8
1	B	187	GLY	2.8
1	E	172	LEU	2.7
1	B	98	THR	2.7
1	B	97	LEU	2.7
1	F	141	ALA	2.7
1	C	145	VAL	2.6
1	F	126	THR	2.6
1	B	186	GLN	2.6
1	C	140	PRO	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	109	LEU	2.5
1	B	133	TRP	2.5
1	A	47	ALA	2.5
1	A	205	TRP	2.4
1	C	131	GLN	2.4
1	F	142	GLU	2.4
1	B	174	TYR	2.3
1	D	166	GLU	2.3
1	B	156	ALA	2.3
1	F	31	PRO	2.3
1	F	47	ALA	2.3
1	B	145	VAL	2.3
1	F	12	ARG	2.3
1	E	12	ARG	2.3
1	F	179	LYS	2.3
1	A	121	TRP	2.3
1	E	34	GLN	2.2
1	C	91	ASN	2.2
1	C	94	ASN	2.2
1	F	203	ALA	2.2
1	F	50	THR	2.2
1	A	118	LEU	2.2
1	C	200	GLN	2.2
1	A	36	TRP	2.2
1	F	32	GLY	2.1
1	E	176	ASN	2.1
1	C	100	GLN	2.1
1	F	146	GLU	2.1
1	B	76	ALA	2.1
1	E	41	ARG	2.1
1	E	168	ILE	2.1
1	F	38	GLN	2.1
1	E	195	VAL	2.1
1	F	45	LEU	2.1
1	A	45	LEU	2.1
1	B	184	ILE	2.1
1	E	123	ASN	2.1
1	B	122	LYS	2.0
1	D	123	ASN	2.0
1	A	120	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 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.