Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:23 AM GMT

PDB ID	:	2WWS
Title	:	PHYSALIS MOTTLE VIRUS: NATURAL EMPTY CAPSID
Authors	:	Sagurthi, S.R.; Rajaram, V.; Savithri, H.S.; Murthy, M.R.N.
Deposited on	:	2009-10-27
Resolution	:	3.90 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:

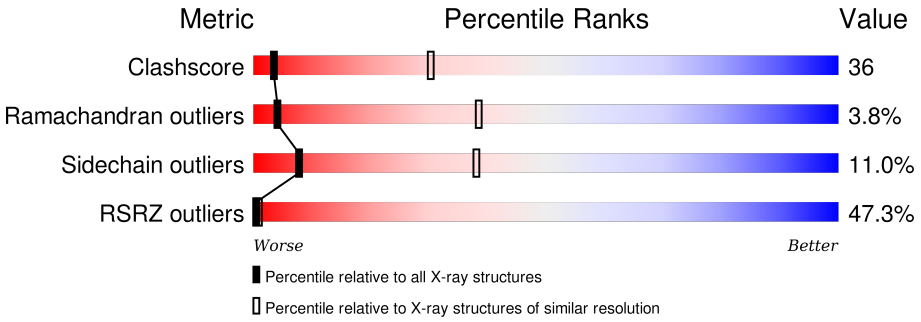
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.90 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))
Clashscore	102246	1031 (4.24-3.56)
Ramachandran outliers	100387	1012 (4.26-3.54)
Sidechain outliers	100360	1004 (4.26-3.54)
RSRZ outliers	91569	1018 (4.28-3.52)

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	188	44% 44% 37% 5% 14%
1	B	188	36% 47% 44% 7% •
1	C	188	54% 44% 41% 13% ••

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3976 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 COAT PROTEIN.

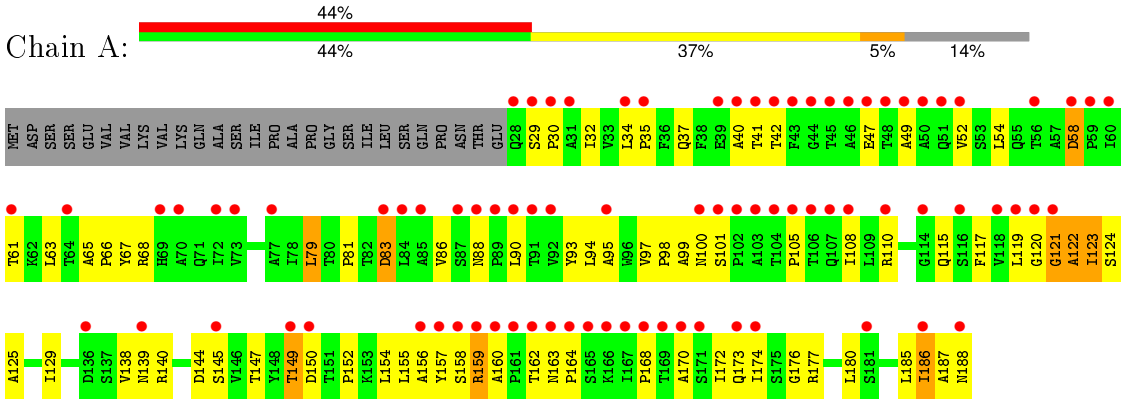
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	161	Total	C	N	O	S	0	0	0
			1210	774	203	230	3			
1	B	185	Total	C	N	O	S	0	0	0
			1383	882	232	266	3			
1	C	185	Total	C	N	O	S	0	0	0
			1383	882	232	266	3			

3 Residue-property plots (i)

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.

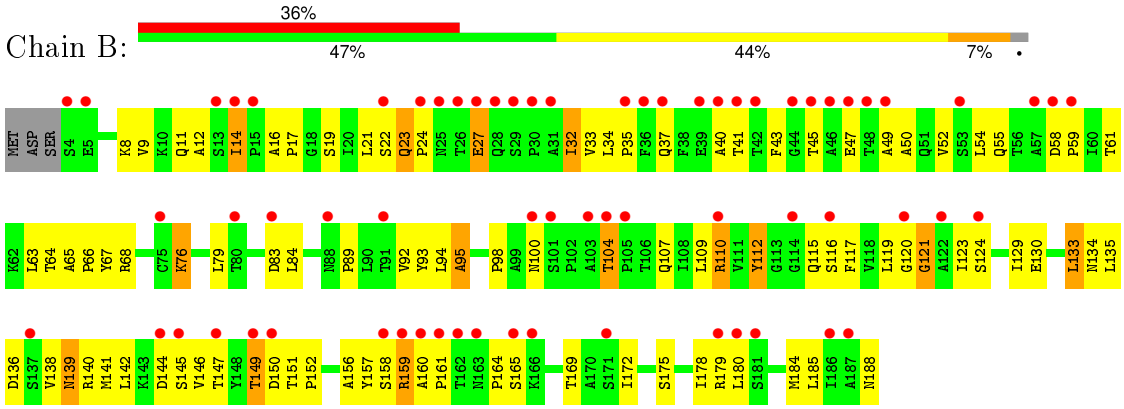
- Molecule 1: COAT PROTEIN

Chain A:



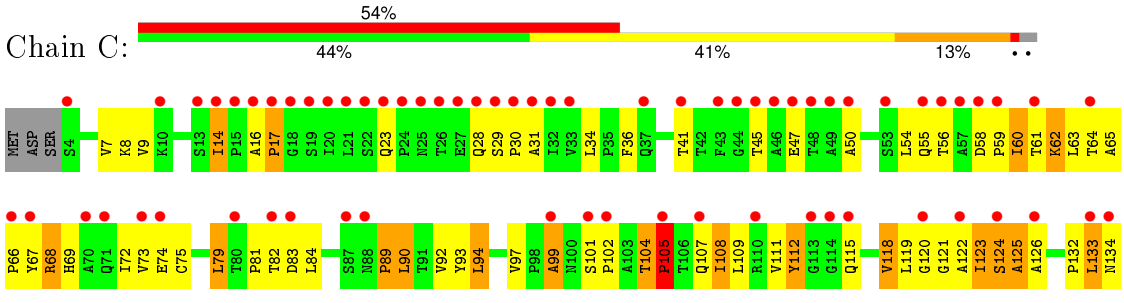
- Molecule 1: COAT PROTEIN

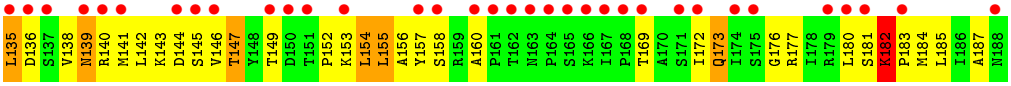
Chain B:



- Molecule 1: COAT PROTEIN

Chain C:




L135
D136
S137
V138
N139
R140
M141
L142
K143
D144
S145
V146
T147
Y148
T149
D150
T151
P152
K153
L154
L155
A156
Y157
S158
R159
A160
P161
T162
N163
P164
S165
K166
I167
P168
T169
A170
S171
I172
Q173
I174
S175
G176
R177
I178
R179
L180
S181
K182
P183
M184
L185
I186
A187
N188

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	325.76Å 325.76Å 738.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.90 19.97 – 3.90	Depositor EDS
% Data completeness (in resolution range)	79.4 (20.00-3.90) 63.9 (19.97-3.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.70 (at 3.94Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.230 , 0.242 (Not available) , (Not available)	Depositor DCC
R_{free} test set	NotAvailable	DCC
Wilson B-factor (Å^2)	59.7	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	1.33 , -11.2	EDS
Estimated twinning fraction	0.408 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 210128 reflections	Xtriage
F_o,F_c correlation	0.10	EDS
Total number of atoms	3976	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% 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

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	0.49	0/1236	0.73	1/1695 (0.1%)
1	B	0.51	0/1412	0.69	0/1936
1	C	0.53	0/1412	0.72	0/1936
All	All	0.51	0/4060	0.72	1/5567 (0.0%)

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	A	121	GLY	N-CA-C	-5.71	98.84	113.10

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	1210	0	1254	78	0
1	B	1383	0	1435	99	0
1	C	1383	0	1435	127	0
All	All	3976	0	4124	294	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 36.

All (294) 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:B:89:PRO:HA	1:B:120:GLY:HA3	1.17	1.16
1:C:139:ASN:HD22	1:C:140:ARG:N	1.58	1.01
1:C:182:LYS:HE2	1:C:182:LYS:C	1.81	1.01
1:C:68:ARG:HG2	1:C:182:LYS:HZ2	1.28	0.98
1:C:31:ALA:HB2	1:C:181:SER:HB3	1.45	0.96
1:C:146:VAL:HG12	1:C:147:THR:H	1.31	0.94
1:A:138:VAL:HG21	1:A:152:PRO:HG3	1.50	0.93
1:B:11:GLN:HG2	1:B:12:ALA:H	1.33	0.91
1:A:159:ARG:HH11	1:A:159:ARG:HB3	1.34	0.89
1:C:68:ARG:HG2	1:C:182:LYS:NZ	1.90	0.87
1:B:139:ASN:HD22	1:B:140:ARG:N	1.73	0.86
1:B:32:ILE:HD13	1:B:33:VAL:H	1.40	0.83
1:B:139:ASN:HB2	1:B:150:ASP:HB2	1.60	0.82
1:A:94:LEU:HD21	1:A:172:ILE:HD13	1.61	0.80
1:C:139:ASN:ND2	1:C:141:MET:H	1.81	0.79
1:B:12:ALA:HB1	1:B:112:TYR:CE2	2.18	0.79
1:C:59:PRO:C	1:C:61:THR:H	1.85	0.79
1:C:146:VAL:HG12	1:C:147:THR:N	1.97	0.78
1:B:159:ARG:HB2	1:B:159:ARG:HH11	1.47	0.78
1:C:90:LEU:HD21	1:C:119:LEU:HB2	1.65	0.78
1:C:72:ILE:HD11	1:C:75:CYS:HB2	1.67	0.77
1:A:97:VAL:HG12	1:A:99:ALA:H	1.51	0.76
1:A:52:VAL:CG2	1:A:154:LEU:HB3	2.16	0.75
1:A:40:ALA:HB1	1:A:52:VAL:HG11	1.68	0.75
1:B:49:ALA:HB2	1:B:157:TYR:HD2	1.52	0.74
1:B:24:PRO:HA	1:B:27:GLU:CG	2.17	0.74
1:C:68:ARG:CG	1:C:182:LYS:HZ2	2.01	0.73
1:B:43:PHE:CE1	1:B:172:ILE:HD13	2.23	0.73
1:B:32:ILE:HD13	1:B:33:VAL:N	2.04	0.73
1:C:14:ILE:HD13	1:C:14:ILE:H	1.54	0.72
1:B:89:PRO:HA	1:B:120:GLY:CA	2.10	0.72
1:C:108:ILE:O	1:C:111:VAL:HG22	1.89	0.71
1:A:41:THR:HG22	1:A:42:THR:N	2.04	0.71
1:B:180:LEU:H	1:B:180:LEU:HD22	1.56	0.70
1:C:31:ALA:CB	1:C:181:SER:HB3	2.21	0.70
1:A:97:VAL:CG1	1:A:101:SER:HB3	2.21	0.70
1:C:182:LYS:HE2	1:C:182:LYS:O	1.91	0.70
1:C:64:THR:HG22	1:C:180:LEU:HD21	1.73	0.70
1:A:129:ILE:HD12	1:A:129:ILE:N	2.06	0.69
1:A:47:GLU:HB2	1:A:160:ALA:HB2	1.77	0.67
1:C:138:VAL:HG21	1:C:152:PRO:HB3	1.75	0.67
1:B:24:PRO:HA	1:B:27:GLU:HG3	1.76	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:PRO:HB3	1:A:119:LEU:HD13	1.77	0.67
1:C:139:ASN:HD22	1:C:140:ARG:H	1.40	0.67
1:B:159:ARG:HB2	1:B:159:ARG:NH1	2.10	0.66
1:B:37:GLN:HG3	1:B:175:SER:HB3	1.76	0.66
1:A:95:ALA:HB2	1:A:108:ILE:HG23	1.77	0.66
1:A:186:ILE:H	1:A:186:ILE:HD13	1.60	0.66
1:B:8:LYS:HG2	1:B:130:GLU:HB3	1.77	0.66
1:B:43:PHE:HE1	1:B:172:ILE:HD13	1.61	0.66
1:B:180:LEU:N	1:B:180:LEU:HD22	2.10	0.66
1:A:100:ASN:HD21	1:A:149:THR:HB	1.61	0.66
1:C:54:LEU:HD12	1:C:60:ILE:HD13	1.77	0.66
1:C:82:THR:HG22	1:C:84:LEU:H	1.59	0.66
1:A:97:VAL:HG11	1:A:101:SER:HB3	1.77	0.66
1:B:49:ALA:HB2	1:B:157:TYR:CD2	2.31	0.65
1:A:121:GLY:O	1:A:123:ILE:HG13	1.95	0.65
1:A:83:ASP:O	1:A:86:VAL:HG22	1.97	0.65
1:C:9:VAL:HG12	1:C:115:GLN:HE22	1.62	0.64
1:A:105:PRO:O	1:A:108:ILE:HG12	1.97	0.64
1:C:47:GLU:HB2	1:C:160:ALA:HB2	1.80	0.63
1:C:90:LEU:CD2	1:C:119:LEU:HB2	2.28	0.63
1:C:60:ILE:HD12	1:C:142:LEU:HD13	1.80	0.63
1:B:185:LEU:H	1:B:185:LEU:HD12	1.63	0.63
1:C:139:ASN:HD22	1:C:139:ASN:C	1.98	0.63
1:B:139:ASN:HD22	1:B:139:ASN:C	1.99	0.63
1:B:139:ASN:ND2	1:B:141:MET:H	1.96	0.63
1:B:150:ASP:OD2	1:C:145:SER:HB3	1.99	0.63
1:B:185:LEU:N	1:B:185:LEU:HD12	2.14	0.63
1:C:59:PRO:O	1:C:61:THR:N	2.32	0.62
1:C:79:LEU:HD22	1:C:119:LEU:HD11	1.81	0.62
1:A:108:ILE:HD11	1:A:155:LEU:HB3	1.82	0.62
1:A:41:THR:CG2	1:A:42:THR:N	2.63	0.62
1:A:98:PRO:HA	1:A:138:VAL:HG12	1.80	0.62
1:C:68:ARG:HG2	1:C:182:LYS:CD	2.30	0.61
1:A:34:LEU:HD23	1:A:34:LEU:H	1.64	0.61
1:B:104:THR:HG23	1:B:107:GLN:OE1	2.01	0.61
1:C:72:ILE:HD11	1:C:75:CYS:CB	2.30	0.61
1:B:79:LEU:HD22	1:B:119:LEU:HD21	1.83	0.61
1:C:123:ILE:HD13	1:C:123:ILE:O	2.01	0.60
1:A:129:ILE:HD12	1:A:129:ILE:H	1.65	0.60
1:B:23:GLN:N	1:B:24:PRO:CD	2.64	0.60
1:A:93:TYR:O	1:A:156:ALA:HA	2.02	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:ASN:ND2	1:C:140:ARG:N	2.41	0.60
1:B:11:GLN:HG2	1:B:12:ALA:N	2.10	0.60
1:B:55:GLN:HB2	1:B:151:THR:HG21	1.84	0.60
1:C:34:LEU:HD12	1:C:180:LEU:HD12	1.84	0.60
1:C:59:PRO:C	1:C:61:THR:N	2.53	0.60
1:B:138:VAL:HG21	1:B:152:PRO:HB3	1.82	0.59
1:C:41:THR:HG21	1:C:50:ALA:HB3	1.83	0.59
1:C:16:ALA:N	1:C:17:PRO:HD3	2.18	0.59
1:A:54:LEU:HD21	1:A:174:ILE:HG21	1.85	0.59
1:A:97:VAL:HG13	1:A:98:PRO:HD2	1.85	0.58
1:A:159:ARG:NH1	1:A:159:ARG:HB3	2.13	0.58
1:B:117:PHE:CD1	1:B:129:ILE:HD13	2.37	0.58
1:C:155:LEU:H	1:C:155:LEU:HD23	1.67	0.58
1:C:9:VAL:CG1	1:C:115:GLN:HE22	2.16	0.58
1:C:81:PRO:HG3	1:C:119:LEU:HD22	1.85	0.58
1:C:58:ASP:HB2	1:C:59:PRO:HA	1.85	0.57
1:B:135:LEU:HD23	1:B:135:LEU:H	1.67	0.57
1:A:98:PRO:O	1:A:99:ALA:HB3	2.05	0.57
1:B:41:THR:HG21	1:B:50:ALA:HB3	1.86	0.57
1:C:93:TYR:CZ	1:C:109:LEU:HD11	2.40	0.57
1:B:23:GLN:N	1:B:24:PRO:HD2	2.20	0.57
1:A:187:ALA:O	1:A:188:ASN:HB2	2.02	0.57
1:A:122:ALA:C	1:A:124:SER:H	2.08	0.57
1:C:93:TYR:CE2	1:C:109:LEU:HD11	2.40	0.57
1:C:82:THR:HB	1:C:169:THR:O	2.04	0.57
1:B:178:ILE:HG22	1:B:179:ARG:N	2.20	0.57
1:C:120:GLY:H	1:C:125:ALA:HB1	1.68	0.56
1:B:24:PRO:HA	1:B:27:GLU:HG2	1.87	0.56
1:C:146:VAL:CG1	1:C:147:THR:H	2.11	0.56
1:C:93:TYR:O	1:C:156:ALA:HA	2.05	0.56
1:B:67:TYR:CG	1:B:180:LEU:HB3	2.41	0.55
1:B:49:ALA:CB	1:B:157:TYR:HD2	2.17	0.55
1:C:36:PHE:CD2	1:C:60:ILE:HG22	2.41	0.55
1:A:52:VAL:HG22	1:A:154:LEU:HB3	1.88	0.55
1:A:42:THR:OG1	1:A:168:PRO:HB3	2.07	0.55
1:C:133:LEU:HD13	1:C:135:LEU:CD1	2.36	0.55
1:A:86:VAL:HA	1:A:121:GLY:H	1.72	0.55
1:B:123:ILE:HG13	1:B:124:SER:N	2.21	0.55
1:C:118:VAL:O	1:C:118:VAL:HG22	2.05	0.55
1:C:68:ARG:HG2	1:C:182:LYS:HD3	1.88	0.55
1:C:155:LEU:N	1:C:155:LEU:HD23	2.20	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:ARG:CB	1:B:110:ARG:HH11	2.19	0.55
1:B:93:TYR:O	1:B:156:ALA:HA	2.06	0.55
1:C:73:VAL:HG13	1:C:74:GLU:N	2.22	0.55
1:C:58:ASP:HB3	1:C:61:THR:OG1	2.06	0.55
1:B:120:GLY:O	1:B:121:GLY:C	2.44	0.55
1:B:16:ALA:HA	1:C:182:LYS:HG2	1.88	0.55
1:C:92:VAL:HG12	1:C:93:TYR:N	2.22	0.55
1:A:52:VAL:HG23	1:A:154:LEU:HB3	1.86	0.54
1:C:65:ALA:N	1:C:66:PRO:HD2	2.23	0.54
1:B:161:PRO:HG2	1:B:164:PRO:HG3	1.89	0.54
1:C:105:PRO:O	1:C:108:ILE:HG12	2.08	0.53
1:A:159:ARG:HH11	1:A:159:ARG:CB	2.13	0.53
1:C:68:ARG:HA	1:C:143:LYS:HE2	1.90	0.53
1:A:186:ILE:N	1:A:186:ILE:HD13	2.23	0.53
1:C:120:GLY:N	1:C:125:ALA:HB1	2.23	0.53
1:A:97:VAL:HG13	1:A:101:SER:HB3	1.91	0.52
1:B:119:LEU:HD12	1:B:119:LEU:H	1.74	0.52
1:A:41:THR:CG2	1:A:42:THR:H	2.22	0.52
1:C:73:VAL:CG1	1:C:177:ARG:HB2	2.39	0.52
1:C:104:THR:HG23	1:C:107:GLN:OE1	2.10	0.52
1:C:154:LEU:HD22	1:C:155:LEU:N	2.24	0.52
1:C:139:ASN:C	1:C:139:ASN:ND2	2.63	0.52
1:A:34:LEU:HD23	1:A:34:LEU:N	2.25	0.52
1:A:58:ASP:O	1:A:61:THR:HB	2.10	0.52
1:C:60:ILE:O	1:C:60:ILE:HG13	2.08	0.52
1:B:144:ASP:OD1	1:B:145:SER:N	2.38	0.51
1:C:67:TYR:CD2	1:C:180:LEU:HB3	2.44	0.51
1:B:159:ARG:CB	1:B:159:ARG:HH11	2.20	0.51
1:C:58:ASP:HA	1:C:61:THR:OG1	2.11	0.51
1:B:110:ARG:HH12	1:C:187:ALA:HB1	1.75	0.51
1:B:146:VAL:HG12	1:B:147:THR:N	2.26	0.50
1:A:157:TYR:CG	1:A:158:SER:N	2.79	0.50
1:B:55:GLN:CB	1:B:151:THR:HG21	2.41	0.50
1:A:122:ALA:O	1:A:124:SER:N	2.45	0.50
1:B:40:ALA:HB1	1:B:52:VAL:HG21	1.94	0.50
1:B:123:ILE:HG13	1:B:124:SER:H	1.77	0.49
1:B:19:SER:HB2	1:C:145:SER:HB2	1.94	0.49
1:B:19:SER:OG	1:C:23:GLN:NE2	2.44	0.49
1:C:182:LYS:HE2	1:C:183:PRO:N	2.26	0.49
1:A:108:ILE:CD1	1:A:155:LEU:HB3	2.42	0.49
1:C:14:ILE:N	1:C:14:ILE:HD13	2.23	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:ILE:CG2	1:B:179:ARG:N	2.76	0.49
1:A:120:GLY:C	1:A:122:ALA:N	2.61	0.49
1:B:150:ASP:OD1	1:C:68:ARG:HD2	2.13	0.49
1:B:32:ILE:CD1	1:B:33:VAL:N	2.74	0.49
1:C:111:VAL:HG23	1:C:111:VAL:O	2.13	0.49
1:B:98:PRO:HB3	1:B:138:VAL:HG12	1.95	0.49
1:B:16:ALA:HB1	1:C:68:ARG:NH2	2.28	0.49
1:A:129:ILE:H	1:A:129:ILE:CD1	2.26	0.49
1:C:94:LEU:HD11	1:C:172:ILE:HD13	1.95	0.49
1:C:157:TYR:CG	1:C:158:SER:N	2.81	0.48
1:C:29:SER:HB2	1:C:30:PRO:HD2	1.94	0.48
1:C:68:ARG:O	1:C:68:ARG:HG3	2.13	0.48
1:B:66:PRO:HG2	1:B:67:TYR:CE2	2.48	0.48
1:B:110:ARG:NH1	1:C:187:ALA:HB1	2.28	0.48
1:C:181:SER:O	1:C:182:LYS:O	2.31	0.48
1:C:107:GLN:O	1:C:108:ILE:C	2.50	0.48
1:C:133:LEU:HD11	1:C:152:PRO:HB3	1.96	0.48
1:B:34:LEU:HD13	1:B:35:PRO:HD2	1.95	0.48
1:B:9:VAL:HG23	1:B:9:VAL:O	2.13	0.48
1:C:82:THR:HG22	1:C:83:ASP:N	2.28	0.48
1:B:100:ASN:HD22	1:B:149:THR:HB	1.79	0.48
1:C:82:THR:CG2	1:C:83:ASP:N	2.76	0.47
1:C:134:ASN:OD1	1:C:136:ASP:HB2	2.13	0.47
1:A:100:ASN:ND2	1:A:149:THR:HB	2.28	0.47
1:A:185:LEU:HD12	1:A:185:LEU:N	2.29	0.47
1:B:12:ALA:HB1	1:B:112:TYR:CD2	2.49	0.47
1:B:79:LEU:HD22	1:B:119:LEU:CD2	2.45	0.47
1:B:93:TYR:CE2	1:B:116:SER:HB2	2.50	0.47
1:C:154:LEU:C	1:C:154:LEU:HD22	2.34	0.47
1:C:61:THR:C	1:C:63:LEU:N	2.68	0.46
1:B:119:LEU:HD12	1:B:119:LEU:N	2.31	0.46
1:C:68:ARG:NE	1:C:182:LYS:HZ2	2.13	0.46
1:A:110:ARG:HD2	1:B:188:ASN:OXT	2.16	0.46
1:C:185:LEU:H	1:C:185:LEU:HD12	1.80	0.46
1:A:97:VAL:HG13	1:A:98:PRO:CD	2.45	0.46
1:C:111:VAL:O	1:C:112:TYR:C	2.53	0.46
1:C:176:GLY:C	1:C:177:ARG:HG2	2.36	0.46
1:A:61:THR:C	1:A:63:LEU:N	2.69	0.46
1:C:182:LYS:CE	1:C:182:LYS:O	2.62	0.46
1:A:41:THR:HG22	1:A:42:THR:H	1.79	0.46
1:B:58:ASP:N	1:B:59:PRO:HD2	2.31	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:ILE:HG23	1:B:14:ILE:O	2.16	0.46
1:C:72:ILE:O	1:C:72:ILE:HG23	2.16	0.45
1:C:69:HIS:HA	1:C:143:LYS:O	2.16	0.45
1:B:94:LEU:N	1:B:94:LEU:HD12	2.31	0.45
1:A:90:LEU:N	1:A:90:LEU:HD23	2.31	0.45
1:A:68:ARG:O	1:A:68:ARG:HG2	2.17	0.45
1:A:67:TYR:CD2	1:A:180:LEU:HD13	2.51	0.45
1:C:72:ILE:HG22	1:C:140:ARG:O	2.17	0.45
1:B:135:LEU:CD2	1:B:135:LEU:H	2.30	0.45
1:C:8:LYS:HE2	1:C:132:PRO:HG3	1.99	0.45
1:B:65:ALA:HB3	1:B:66:PRO:HD3	1.99	0.44
1:C:97:VAL:HG22	1:C:155:LEU:CD2	2.47	0.44
1:B:94:LEU:O	1:B:95:ALA:HB2	2.17	0.44
1:B:139:ASN:ND2	1:B:139:ASN:C	2.69	0.44
1:A:81:PRO:HA	1:A:170:ALA:CB	2.47	0.44
1:C:185:LEU:N	1:C:185:LEU:HD12	2.32	0.44
1:C:123:ILE:CG2	1:C:124:SER:N	2.80	0.44
1:C:16:ALA:N	1:C:17:PRO:CD	2.79	0.44
1:B:61:THR:O	1:B:63:LEU:N	2.51	0.44
1:B:22:SER:C	1:B:24:PRO:HD2	2.38	0.44
1:A:79:LEU:CD2	1:A:119:LEU:HD11	2.47	0.44
1:A:47:GLU:HB2	1:A:160:ALA:CB	2.45	0.44
1:A:117:PHE:CE2	1:A:129:ILE:HG23	2.53	0.43
1:C:92:VAL:CG1	1:C:93:TYR:N	2.81	0.43
1:A:187:ALA:O	1:A:188:ASN:CB	2.66	0.43
1:B:16:ALA:N	1:B:17:PRO:CD	2.80	0.43
1:B:14:ILE:HD13	1:B:14:ILE:O	2.18	0.43
1:A:97:VAL:HA	1:A:98:PRO:HD3	1.87	0.43
1:C:65:ALA:N	1:C:66:PRO:CD	2.82	0.43
1:B:157:TYR:CG	1:B:158:SER:N	2.86	0.43
1:C:31:ALA:HB1	1:C:180:LEU:O	2.18	0.43
1:C:68:ARG:HG2	1:C:182:LYS:CE	2.49	0.43
1:A:37:GLN:HA	1:A:174:ILE:O	2.19	0.43
1:C:14:ILE:CD1	1:C:14:ILE:N	2.82	0.43
1:C:184:MET:HG3	1:C:185:LEU:N	2.33	0.43
1:A:138:VAL:HB	1:A:139:ASN:H	1.61	0.43
1:B:84:LEU:HB3	1:B:169:THR:HG22	2.01	0.43
1:B:120:GLY:O	1:B:121:GLY:O	2.37	0.43
1:A:98:PRO:O	1:A:150:ASP:HA	2.18	0.43
1:C:89:PRO:HB3	1:C:121:GLY:HA3	2.00	0.43
1:B:92:VAL:O	1:B:93:TYR:HD2	2.02	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:GLU:HB2	1:B:160:ALA:HB2	2.01	0.43
1:C:61:THR:C	1:C:63:LEU:H	2.21	0.43
1:B:185:LEU:CD1	1:B:185:LEU:H	2.30	0.43
1:A:49:ALA:HB2	1:A:157:TYR:HD1	1.83	0.42
1:C:59:PRO:HA	1:C:62:LYS:HG3	2.00	0.42
1:B:110:ARG:HB2	1:B:110:ARG:HH11	1.84	0.42
1:C:7:VAL:HG13	1:C:7:VAL:O	2.17	0.42
1:C:125:ALA:O	1:C:126:ALA:HB3	2.18	0.42
1:A:163:ASN:CG	1:A:163:ASN:O	2.58	0.42
1:C:99:ALA:HB3	1:C:149:THR:O	2.18	0.42
1:B:45:THR:HA	1:B:165:SER:O	2.19	0.42
1:B:92:VAL:HG12	1:B:93:TYR:N	2.34	0.42
1:A:144:ASP:CG	1:A:145:SER:H	2.22	0.42
1:B:129:ILE:HG22	1:B:130:GLU:N	2.35	0.42
1:C:73:VAL:CG1	1:C:74:GLU:N	2.82	0.42
1:A:154:LEU:HD12	1:A:155:LEU:N	2.35	0.42
1:C:133:LEU:HD13	1:C:135:LEU:HD12	2.01	0.42
1:C:54:LEU:O	1:C:56:THR:N	2.52	0.42
1:C:101:SER:HA	1:C:102:PRO:HD3	1.71	0.42
1:A:29:SER:OG	1:A:30:PRO:CD	2.68	0.42
1:C:97:VAL:O	1:C:153:LYS:HB3	2.20	0.42
1:B:61:THR:C	1:B:63:LEU:N	2.73	0.42
1:C:173:GLN:HB3	1:C:173:GLN:HE21	1.65	0.42
1:A:140:ARG:H	1:A:140:ARG:HG3	1.65	0.41
1:C:144:ASP:CG	1:C:145:SER:H	2.23	0.41
1:B:64:THR:HG22	1:B:180:LEU:HD11	2.03	0.41
1:B:66:PRO:HG2	1:B:67:TYR:CD2	2.55	0.41
1:A:65:ALA:N	1:A:66:PRO:CD	2.83	0.41
1:C:14:ILE:CD1	1:C:14:ILE:H	2.30	0.41
1:C:58:ASP:CB	1:C:61:THR:OG1	2.69	0.41
1:B:76:LYS:HD3	1:B:130:GLU:HG2	2.03	0.41
1:A:120:GLY:C	1:A:122:ALA:H	2.21	0.41
1:C:74:GLU:HG2	1:C:177:ARG:HG3	2.03	0.41
1:C:157:TYR:CD2	1:C:158:SER:N	2.89	0.41
1:B:150:ASP:OD2	1:C:145:SER:CB	2.68	0.41
1:A:67:TYR:CD2	1:A:67:TYR:N	2.89	0.41
1:B:68:ARG:HG2	1:B:184:MET:HB2	2.02	0.40
1:A:95:ALA:CB	1:A:108:ILE:HG23	2.47	0.40
1:A:154:LEU:CD2	1:A:174:ILE:HD11	2.51	0.40
1:B:133:LEU:HD22	1:B:134:ASN:N	2.36	0.40
1:A:176:GLY:C	1:A:177:ARG:HG3	2.42	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:146:VAL:CG1	1:C:147:THR:N	2.69	0.40
1:A:94:LEU:HD21	1:A:172:ILE:CD1	2.42	0.40
1:A:47:GLU:HB2	1:A:160:ALA:CA	2.52	0.40
1:B:83:ASP:OD1	1:B:84:LEU:HD12	2.20	0.40
1:A:97:VAL:CG1	1:A:98:PRO:N	2.81	0.40
1:C:84:LEU:HB3	1:C:169:THR:HG22	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	159/188 (85%)	138 (87%)	17 (11%)	4 (2%)	7 48
1	B	183/188 (97%)	154 (84%)	26 (14%)	3 (2%)	12 56
1	C	183/188 (97%)	146 (80%)	24 (13%)	13 (7%)	1 23
All	All	525/564 (93%)	438 (83%)	67 (13%)	20 (4%)	4 38

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	ILE
1	A	164	PRO
1	C	55	GLN
1	C	122	ALA
1	C	125	ALA
1	A	122	ALA
1	A	125	ALA
1	B	95	ALA
1	B	121	GLY
1	C	60	ILE
1	C	99	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	135	LEU
1	B	112	TYR
1	C	45	THR
1	C	17	PRO
1	C	108	ILE
1	C	112	TYR
1	C	182	LYS
1	C	105	PRO
1	C	89	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	135/159 (85%)	122 (90%)	13 (10%)	10 44
1	B	156/159 (98%)	139 (89%)	17 (11%)	8 39
1	C	156/159 (98%)	137 (88%)	19 (12%)	6 33
All	All	447/477 (94%)	398 (89%)	49 (11%)	8 38

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ILE
1	A	35	PRO
1	A	58	ASP
1	A	79	LEU
1	A	83	ASP
1	A	88	ASN
1	A	115	GLN
1	A	147	THR
1	A	149	THR
1	A	159	ARG
1	A	162	THR
1	A	173	GLN
1	A	186	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	14	ILE
1	B	21	LEU
1	B	23	GLN
1	B	27	GLU
1	B	32	ILE
1	B	54	LEU
1	B	76	LYS
1	B	104	THR
1	B	109	LEU
1	B	110	ARG
1	B	115	GLN
1	B	133	LEU
1	B	136	ASP
1	B	139	ASN
1	B	142	LEU
1	B	149	THR
1	B	159	ARG
1	C	14	ILE
1	C	28	GLN
1	C	62	LYS
1	C	68	ARG
1	C	79	LEU
1	C	90	LEU
1	C	94	LEU
1	C	104	THR
1	C	105	PRO
1	C	118	VAL
1	C	123	ILE
1	C	124	SER
1	C	133	LEU
1	C	139	ASN
1	C	147	THR
1	C	154	LEU
1	C	155	LEU
1	C	173	GLN
1	C	182	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	69	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	100	ASN
1	B	69	HIS
1	B	71	GLN
1	B	88	ASN
1	B	115	GLN
1	B	139	ASN
1	B	173	GLN
1	C	23	GLN
1	C	37	GLN
1	C	69	HIS
1	C	115	GLN
1	C	139	ASN
1	C	173	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 carbohydrates 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

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, 95^{th} 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	161/188 (85%)	2.44	83 (51%) 0 1	1, 13, 45, 59	0
1	B	185/188 (98%)	1.83	67 (36%) 0 1	1, 13, 46, 74	0
1	C	185/188 (98%)	2.47	101 (54%) 0 1	11, 23, 39, 52	0
All	All	531/564 (94%)	2.24	251 (47%) 0 1	1, 18, 45, 74	0

All (251) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	162	THR	10.7
1	C	29	SER	10.2
1	C	165	SER	9.8
1	B	26	THR	9.6
1	A	51	GLN	9.1
1	A	31	ALA	8.8
1	C	163	ASN	8.8
1	A	29	SER	8.6
1	A	30	PRO	8.2
1	A	161	PRO	8.1
1	B	28	GLN	7.7
1	A	164	PRO	6.8
1	A	158	SER	6.7
1	A	28	GLN	6.7
1	A	162	THR	6.6
1	C	27	GLU	6.5
1	C	28	GLN	6.5
1	C	87	SER	6.5
1	A	106	THR	6.4
1	A	159	ARG	6.2
1	C	150	ASP	6.0
1	C	45	THR	5.9
1	B	187	ALA	5.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	89	PRO	5.8
1	C	166	LYS	5.6
1	B	58	ASP	5.6
1	B	46	ALA	5.5
1	A	45	THR	5.4
1	B	162	THR	5.4
1	C	49	ALA	5.4
1	C	25	ASN	5.4
1	C	26	THR	5.4
1	B	171	SER	5.3
1	C	48	THR	5.3
1	A	107	GLN	5.2
1	C	44	GLY	5.2
1	A	56	THR	5.2
1	B	124	SER	5.2
1	C	30	PRO	5.1
1	A	181	SER	5.1
1	C	161	PRO	5.1
1	C	71	GLN	5.0
1	C	160	ALA	5.0
1	A	150	ASP	5.0
1	C	83	ASP	4.9
1	C	24	PRO	4.8
1	C	46	ALA	4.8
1	B	163	ASN	4.7
1	C	164	PRO	4.7
1	B	37	GLN	4.7
1	A	171	SER	4.6
1	C	136	ASP	4.6
1	B	40	ALA	4.5
1	A	40	ALA	4.5
1	C	82	THR	4.5
1	A	110	ARG	4.5
1	A	42	THR	4.4
1	C	145	SER	4.4
1	A	88	ASN	4.3
1	B	165	SER	4.3
1	B	48	THR	4.3
1	B	31	ALA	4.3
1	A	48	THR	4.3
1	A	47	GLU	4.3
1	B	149	THR	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	44	GLY	4.1
1	C	126	ALA	4.1
1	B	161	PRO	4.1
1	A	160	ALA	4.1
1	C	20	ILE	4.0
1	B	27	GLU	4.0
1	A	87	SER	4.0
1	C	13	SER	4.0
1	B	25	ASN	3.9
1	C	169	THR	3.9
1	C	17	PRO	3.9
1	A	163	ASN	3.9
1	B	42	THR	3.9
1	B	45	THR	3.9
1	A	41	THR	3.8
1	C	16	ALA	3.8
1	B	57	ALA	3.8
1	B	35	PRO	3.8
1	A	58	ASP	3.8
1	B	15	PRO	3.7
1	A	157	TYR	3.7
1	B	13	SER	3.7
1	A	91	THR	3.7
1	B	181	SER	3.6
1	C	15	PRO	3.6
1	C	99	ALA	3.6
1	C	23	GLN	3.6
1	C	57	ALA	3.5
1	C	56	THR	3.5
1	A	156	ALA	3.5
1	C	64	THR	3.5
1	A	120	GLY	3.5
1	A	173	GLN	3.5
1	C	70	ALA	3.5
1	C	113	GLY	3.4
1	A	166	LYS	3.4
1	C	168	PRO	3.4
1	A	145	SER	3.4
1	C	188	ASN	3.4
1	C	31	ALA	3.4
1	A	46	ALA	3.4
1	C	171	SER	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	88	ASN	3.4
1	A	149	THR	3.4
1	B	145	SER	3.4
1	C	22	SER	3.4
1	C	167	ILE	3.4
1	A	114	GLY	3.4
1	C	43	PHE	3.4
1	A	101	SER	3.3
1	A	61	THR	3.3
1	B	47	GLU	3.3
1	B	30	PRO	3.3
1	A	39	GLU	3.3
1	C	114	GLY	3.3
1	B	160	ALA	3.3
1	B	144	ASP	3.2
1	A	119	LEU	3.2
1	A	100	ASN	3.2
1	C	101	SER	3.2
1	A	104	THR	3.2
1	A	35	PRO	3.2
1	A	83	ASP	3.1
1	A	70	ALA	3.1
1	C	179	ARG	3.1
1	B	53	SER	3.1
1	B	59	PRO	3.1
1	A	69	HIS	3.1
1	A	43	PHE	3.1
1	A	102	PRO	3.1
1	B	41	THR	3.1
1	A	59	PRO	3.1
1	B	29	SER	3.1
1	C	80	THR	3.1
1	C	137	SER	3.0
1	C	139	ASN	3.0
1	B	24	PRO	3.0
1	C	151	THR	3.0
1	A	167	ILE	3.0
1	A	186	ILE	3.0
1	C	172	ILE	3.0
1	B	39	GLU	3.0
1	C	134	ASN	3.0
1	B	104	THR	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	4	SER	2.9
1	A	95	ALA	2.9
1	C	74	GLU	2.9
1	A	116	SER	2.9
1	C	115	GLN	2.9
1	A	139	ASN	2.9
1	C	181	SER	2.9
1	A	50	ALA	2.8
1	B	158	SER	2.8
1	C	50	ALA	2.8
1	A	121	GLY	2.8
1	C	55	GLN	2.8
1	C	59	PRO	2.8
1	B	179	ARG	2.8
1	C	124	SER	2.8
1	A	108	ILE	2.8
1	B	75	CYS	2.8
1	C	141	MET	2.7
1	C	19	SER	2.7
1	C	73	VAL	2.7
1	B	186	ILE	2.7
1	B	105	PRO	2.7
1	C	32	ILE	2.7
1	C	122	ALA	2.6
1	A	174	ILE	2.6
1	B	159	ARG	2.6
1	C	61	THR	2.6
1	A	105	PRO	2.6
1	C	144	ASP	2.6
1	B	44	GLY	2.6
1	C	14	ILE	2.5
1	C	67	TYR	2.5
1	A	85	ALA	2.5
1	C	41	THR	2.5
1	C	175	SER	2.5
1	B	49	ALA	2.5
1	C	110	ARG	2.4
1	B	101	SER	2.4
1	B	22	SER	2.4
1	A	60	ILE	2.4
1	B	80	THR	2.4
1	C	146	VAL	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	122	ALA	2.4
1	A	103	ALA	2.4
1	C	133	LEU	2.4
1	A	170	ALA	2.4
1	B	150	ASP	2.4
1	B	100	ASN	2.4
1	C	149	THR	2.4
1	B	103	ALA	2.4
1	A	92	VAL	2.4
1	A	90	LEU	2.4
1	B	116	SER	2.4
1	A	49	ALA	2.4
1	C	120	GLY	2.3
1	C	21	LEU	2.3
1	A	64	THR	2.3
1	A	72	ILE	2.3
1	C	107	GLN	2.3
1	B	4	SER	2.3
1	C	33	VAL	2.3
1	B	88	ASN	2.3
1	C	66	PRO	2.3
1	C	180	LEU	2.3
1	A	52	VAL	2.3
1	B	110	ARG	2.3
1	A	73	VAL	2.3
1	C	153	LYS	2.3
1	A	168	PRO	2.3
1	A	165	SER	2.2
1	C	158	SER	2.2
1	C	102	PRO	2.2
1	A	77	ALA	2.2
1	B	36	PHE	2.2
1	C	10	LYS	2.2
1	A	84	LEU	2.2
1	B	147	THR	2.2
1	C	47	GLU	2.2
1	C	140	ARG	2.1
1	A	34	LEU	2.1
1	B	180	LEU	2.1
1	A	188	ASN	2.1
1	A	136	ASP	2.1
1	B	91	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	114	GLY	2.1
1	C	174	ILE	2.1
1	C	105	PRO	2.1
1	A	169	THR	2.1
1	A	118	VAL	2.1
1	C	135	LEU	2.1
1	B	166	LYS	2.1
1	C	157	TYR	2.1
1	B	137	SER	2.1
1	C	37	GLN	2.1
1	B	14	ILE	2.0
1	C	18	GLY	2.0
1	B	5	GLU	2.0
1	C	183	PRO	2.0
1	B	120	GLY	2.0
1	B	83	ASP	2.0
1	C	58	ASP	2.0
1	C	53	SER	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.