



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 03:11 pm 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
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)	:	recalc28949

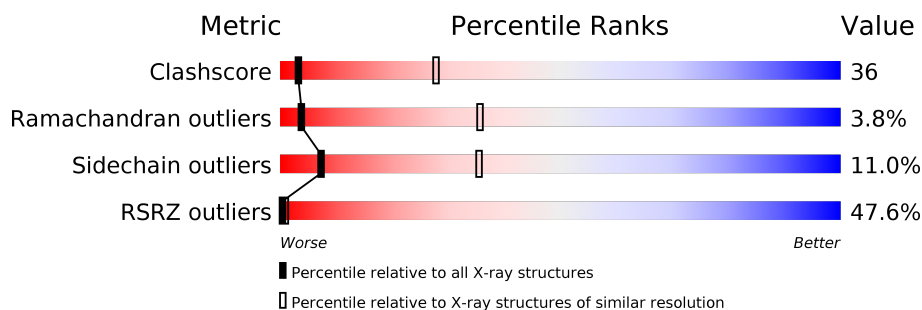
1 Overall quality at a glance

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	112137	1103 (4.20-3.60)
Ramachandran outliers	110173	1062 (4.20-3.60)
Sidechain outliers	110143	1053 (4.20-3.60)
RSRZ outliers	101464	1020 (4.20-3.60)

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 $\leq 5\%$. 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	<div> <div>45%</div> <div>44% 37% 5% 14%</div> </div>
1	B	188	<div> <div>36%</div> <div>47% 44% 7% .</div> </div>
1	C	188	<div> <div>54%</div> <div>44% 41% 13% ..</div> </div>

2 Entry composition

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.

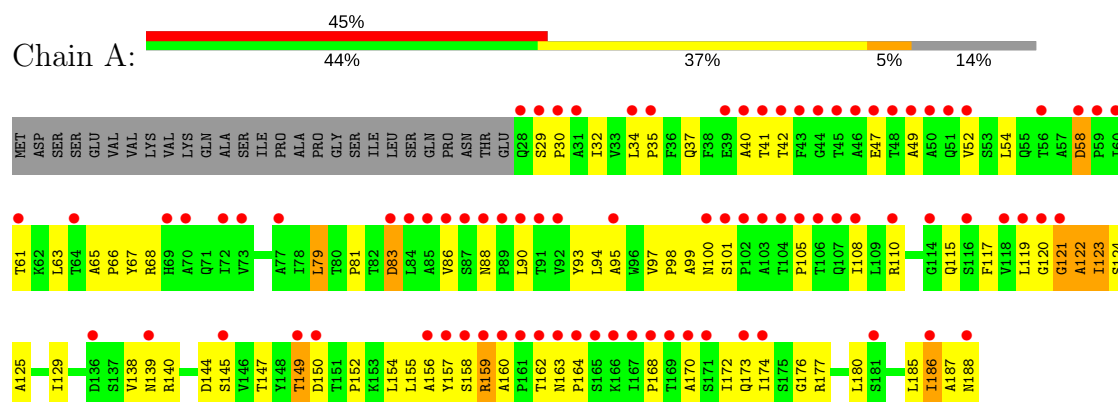
- Molecule 1 is a protein called COAT PROTEIN.

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			

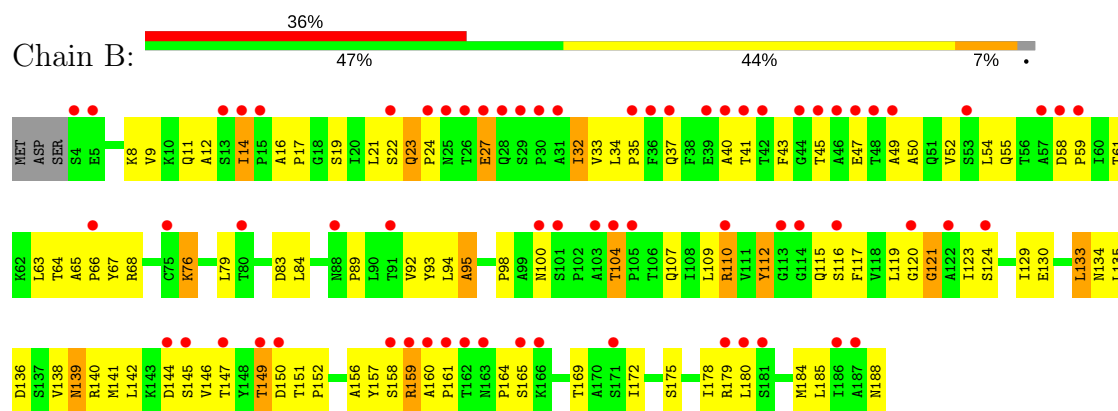
3 Residue-property plots

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.

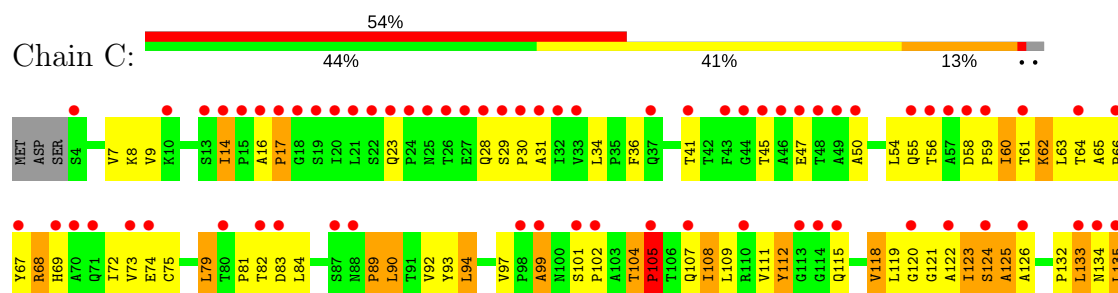
• Molecule 1: COAT PROTEIN



• Molecule 1: COAT PROTEIN



• Molecule 1: COAT PROTEIN



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	T167	P168	T169	A170	S171	I172	Q173	I174	S175	G176	R177	I178	R179	L180	S181	P183	M184	L185	T186	A187	N188
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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 , -10.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.408 for h,-h-k,-l	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.49	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(°)	Ideal(°)
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:B:43:PHE:CE1	1:B:172:ILE:HD13	2.23	0.73
1:C:68:ARG:CG	1:C:182:LYS:HZ2	2.01	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:180:LEU:N	1:B:180:LEU:HD22	2.10	0.66
1:B:43:PHE:HE1	1:B:172:ILE:HD13	1.61	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:A:121:GLY:O	1:A:123:ILE:HG13	1.95	0.65
1:B:49:ALA:HB2	1:B:157:TYR:CD2	2.31	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:B:185:LEU:H	1:B:185:LEU:HD12	1.63	0.63
1:C:60:ILE:HD12	1:C:142:LEU:HD13	1.80	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:C:139:ASN:HD22	1:C:139:ASN:C	1.98	0.63
1:B:185:LEU:N	1:B:185:LEU:HD12	2.14	0.63
1:B:150:ASP:OD2	1:C:145:SER:HB3	1.99	0.63
1:C:59:PRO:O	1:C:61:THR:N	2.32	0.62
1:A:108:ILE:HD11	1:A:155:LEU:HB3	1.82	0.62
1:C:79:LEU:HD22	1:C:119:LEU:HD11	1.81	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:A:93:TYR:O	1:A:156:ALA:HA	2.02	0.60
1:B:23:GLN:N	1:B:24:PRO:CD	2.64	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:GLN:HG2	1:B:12:ALA:N	2.10	0.60
1:C:139:ASN:ND2	1:C:140:ARG:N	2.41	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:16:ALA:N	1:C:17:PRO:HD3	2.18	0.59
1:C:41:THR:HG21	1:C:50:ALA:HB3	1.83	0.59
1:A:54:LEU:HD21	1:A:174:ILE:HG21	1.85	0.59
1:A:159:ARG:NH1	1:A:159:ARG:HB3	2.13	0.58
1:A:97:VAL:HG13	1:A:98:PRO:HD2	1.85	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:B:135:LEU:HD23	1:B:135:LEU:H	1.67	0.57
1:C:58:ASP:HB2	1:C:59:PRO:HA	1.85	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:A:187:ALA:O	1:A:188:ASN:HB2	2.02	0.57
1:B:23:GLN:N	1:B:24:PRO:HD2	2.20	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:42:THR:OG1	1:A:168:PRO:HB3	2.07	0.55
1:A:52:VAL:HG22	1:A:154:LEU:HB3	1.88	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:133:LEU:HD13	1:C:135:LEU:CD1	2.36	0.55
1:C:68:ARG:HG2	1:C:182:LYS:HD3	1.88	0.55
1:B:110:ARG:CB	1:B:110:ARG:HH11	2.19	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:TYR:O	1:B:156:ALA:HA	2.06	0.55
1:C:155:LEU:N	1:C:155:LEU:HD23	2.20	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: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:C:68:ARG:HA	1:C:143:LYS:HE2	1.90	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: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:139:ASN:C	1:C:139:ASN:ND2	2.63	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:A:108:ILE:CD1	1:A:155:LEU:HB3	2.42	0.49
1:B:178:ILE:CG2	1:B:179:ARG:N	2.76	0.49
1:B:19:SER:OG	1:C:23:GLN:NE2	2.44	0.49
1:B:19:SER:HB2	1:C:145:SER:HB2	1.94	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:C:182:LYS:HE2	1:C:183:PRO:N	2.26	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:B:98:PRO:HB3	1:B:138:VAL:HG12	1.95	0.49
1:C:111:VAL:O	1:C:111:VAL:HG23	2.13	0.49
1:A:129:ILE:H	1:A:129:ILE:CD1	2.26	0.49
1:B:16:ALA:HB1	1:C:68:ARG:NH2	2.28	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: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:68:ARG:O	1:C:68:ARG:HG3	2.13	0.48
1:C:107:GLN:O	1:C:108:ILE:C	2.50	0.48
1:C:181:SER:O	1:C:182:LYS:O	2.31	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:133:LEU:HD11	1:C:152:PRO:HB3	1.96	0.48
1:B:100:ASN:HD22	1:B:149:THR:HB	1.79	0.48
1:C:82:THR:HG22	1:C:83:ASP:N	2.28	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:A:110:ARG:HD2	1:B:188:ASN:OXT	2.16	0.46
1:C:68:ARG:NE	1:C:182:LYS:HZ2	2.13	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:A:41:THR:HG22	1:A:42:THR:H	1.79	0.46
1:B:14:ILE:HG23	1:B:14:ILE:O	2.16	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:C:182:LYS:CE	1:C:182:LYS:O	2.62	0.46
1:C:72:ILE:HG23	1:C:72:ILE:O	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:B:135:LEU:CD2	1:B:135:LEU:H	2.30	0.45
1:C:72:ILE:HG22	1:C:140:ARG:O	2.17	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:B:94:LEU:O	1:B:95:ALA:HB2	2.17	0.44
1:C:97:VAL:HG22	1:C:155:LEU:CD2	2.47	0.44
1:A:81:PRO:HA	1:A:170:ALA:CB	2.47	0.44
1:B:139:ASN:ND2	1:B:139:ASN:C	2.69	0.44
1:C:185:LEU:HD12	1:C:185:LEU:N	2.32	0.44
1:B:61:THR:O	1:B:63:LEU:N	2.51	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:A:79:LEU:CD2	1:A:119:LEU:HD11	2.47	0.44
1:B:22:SER:C	1:B:24:PRO:HD2	2.38	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:A:187:ALA:O	1:A:188:ASN:CB	2.66	0.43
1:C:92:VAL:CG1	1:C:93:TYR:N	2.81	0.43
1:B:14:ILE:HD13	1:B:14:ILE:O	2.18	0.43
1:B:16:ALA:N	1:B:17:PRO:CD	2.80	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: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: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: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:A:98:PRO:O	1:A:150:ASP:HA	2.18	0.43
1:B:120:GLY:O	1:B:121:GLY:O	2.37	0.43
1:C:89:PRO:HB3	1:C:121:GLY:HA3	2.00	0.43
1:B:47:GLU:HB2	1:B:160:ALA:HB2	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:VAL:O	1:B:93:TYR:HD2	2.02	0.43
1:B:185:LEU:CD1	1:B:185:LEU:H	2.30	0.43
1:C:61:THR:C	1:C:63:LEU:H	2.21	0.43
1:A:49:ALA:HB2	1:A:157:TYR:HD1	1.83	0.42
1:B:110:ARG:HB2	1:B:110:ARG:HH11	1.84	0.42
1:C:59:PRO:HA	1:C:62:LYS:HG3	2.00	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:B:45:THR:HA	1:B:165:SER:O	2.19	0.42
1:C:99:ALA:HB3	1:C:149:THR:O	2.18	0.42
1:A:144:ASP:CG	1:A:145:SER:H	2.22	0.42
1:B:92:VAL:HG12	1:B:93:TYR:N	2.34	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:A:29:SER:OG	1:A:30:PRO:CD	2.68	0.42
1:C:101:SER:HA	1:C:102:PRO:HD3	1.71	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:B:61:THR:C	1:B:63:LEU:N	2.73	0.42
1:C:97:VAL:O	1:C:153:LYS:HB3	2.20	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:A:65:ALA:N	1:A:66:PRO:CD	2.83	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:C:144:ASP:CG	1:C:145:SER:H	2.23	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:A:120:GLY:C	1:A:122:ALA:H	2.21	0.41
1:B:76:LYS:HD3	1:B:130:GLU:HG2	2.03	0.41
1:C:157:TYR:CD2	1:C:158:SER:N	2.89	0.41
1:C:74:GLU:HG2	1:C:177:ARG:HG3	2.03	0.41
1:A:67:TYR:CD2	1:A:67:TYR:N	2.89	0.41
1:B:150:ASP:OD2	1:C:145:SER:CB	2.68	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:A:176:GLY:C	1:A:177:ARG:HG3	2.42	0.40
1:B:133:LEU:HD22	1:B:134:ASN:N	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:GLU:HB2	1:A:160:ALA:CA	2.52	0.40
1:A:94:LEU:HD21	1:A:172:ILE:CD1	2.42	0.40
1:C:146:VAL:CG1	1:C:147:THR:N	2.69	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%)	6	44
1	B	183/188 (97%)	154 (84%)	26 (14%)	3 (2%)	11	53
1	C	183/188 (97%)	146 (80%)	24 (13%)	13 (7%)	1	21
All	All	525/564 (93%)	438 (83%)	67 (13%)	20 (4%)	4	35

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 ⓘ

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	40
1	B	156/159 (98%)	139 (89%)	17 (11%)	7	36
1	C	156/159 (98%)	137 (88%)	19 (12%)	6	31
All	All	447/477 (94%)	398 (89%)	49 (11%)	7	35

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 [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

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, 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	161/188 (85%)	2.44	84 (52%) 0 1	1, 13, 45, 59	0
1	B	185/188 (98%)	1.82	67 (36%) 0 1	1, 13, 46, 74	0
1	C	185/188 (98%)	2.46	102 (55%) 0 1	11, 23, 39, 52	0
All	All	531/564 (94%)	2.23	253 (47%) 0 1	1, 18, 45, 74	0

All (253) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	162	THR	10.7
1	C	29	SER	10.1
1	C	165	SER	9.7
1	B	26	THR	9.6
1	A	51	GLN	9.2
1	A	31	ALA	8.8
1	C	163	ASN	8.8
1	A	29	SER	8.4
1	A	30	PRO	8.3
1	A	161	PRO	8.2
1	B	28	GLN	7.7
1	A	164	PRO	6.8
1	A	158	SER	6.6
1	A	162	THR	6.6
1	A	28	GLN	6.6
1	A	159	ARG	6.5
1	A	106	THR	6.4
1	C	28	GLN	6.4
1	C	27	GLU	6.4
1	C	87	SER	6.3
1	B	187	ALA	5.9
1	C	45	THR	5.8
1	A	89	PRO	5.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	150	ASP	5.8
1	C	166	LYS	5.8
1	B	46	ALA	5.5
1	B	58	ASP	5.4
1	A	45	THR	5.4
1	C	49	ALA	5.4
1	B	162	THR	5.4
1	C	44	GLY	5.3
1	C	26	THR	5.3
1	C	25	ASN	5.3
1	B	171	SER	5.2
1	C	48	THR	5.2
1	C	30	PRO	5.2
1	A	56	THR	5.2
1	A	107	GLN	5.1
1	C	161	PRO	5.1
1	B	124	SER	5.1
1	C	71	GLN	5.0
1	A	150	ASP	5.0
1	C	160	ALA	5.0
1	A	181	SER	4.9
1	C	24	PRO	4.9
1	C	164	PRO	4.8
1	C	46	ALA	4.7
1	C	83	ASP	4.7
1	B	163	ASN	4.6
1	B	37	GLN	4.6
1	A	110	ARG	4.6
1	B	40	ALA	4.5
1	A	40	ALA	4.5
1	C	136	ASP	4.4
1	C	82	THR	4.4
1	A	171	SER	4.4
1	A	42	THR	4.4
1	B	48	THR	4.4
1	C	145	SER	4.3
1	A	48	THR	4.3
1	A	88	ASN	4.3
1	B	165	SER	4.2
1	B	31	ALA	4.2
1	A	44	GLY	4.2
1	A	47	GLU	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	126	ALA	4.2
1	B	149	THR	4.1
1	B	161	PRO	4.1
1	C	20	ILE	4.1
1	A	160	ALA	4.0
1	C	17	PRO	3.9
1	B	27	GLU	3.9
1	B	45	THR	3.9
1	A	163	ASN	3.9
1	B	42	THR	3.9
1	C	169	THR	3.9
1	B	25	ASN	3.8
1	A	87	SER	3.8
1	B	35	PRO	3.8
1	A	41	THR	3.8
1	C	13	SER	3.8
1	C	16	ALA	3.8
1	B	15	PRO	3.8
1	B	57	ALA	3.8
1	A	157	TYR	3.7
1	A	58	ASP	3.7
1	C	15	PRO	3.6
1	C	99	ALA	3.6
1	B	13	SER	3.6
1	C	23	GLN	3.6
1	C	56	THR	3.6
1	A	156	ALA	3.6
1	B	181	SER	3.5
1	A	91	THR	3.5
1	C	57	ALA	3.5
1	C	64	THR	3.5
1	A	120	GLY	3.5
1	C	70	ALA	3.5
1	C	113	GLY	3.5
1	A	166	LYS	3.5
1	A	114	GLY	3.5
1	C	168	PRO	3.5
1	C	43	PHE	3.4
1	C	167	ILE	3.4
1	A	173	GLN	3.4
1	C	22	SER	3.4
1	C	188	ASN	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	3.3
1	C	114	GLY	3.3
1	C	171	SER	3.3
1	A	46	ALA	3.3
1	C	31	ALA	3.3
1	A	145	SER	3.3
1	A	101	SER	3.3
1	B	145	SER	3.3
1	B	30	PRO	3.3
1	A	39	GLU	3.2
1	B	47	GLU	3.2
1	A	69	HIS	3.2
1	A	119	LEU	3.2
1	C	179	ARG	3.2
1	A	61	THR	3.2
1	A	100	ASN	3.2
1	B	144	ASP	3.2
1	A	104	THR	3.2
1	A	35	PRO	3.2
1	B	160	ALA	3.2
1	C	101	SER	3.1
1	A	70	ALA	3.1
1	A	59	PRO	3.1
1	B	59	PRO	3.1
1	B	53	SER	3.1
1	A	83	ASP	3.1
1	A	102	PRO	3.1
1	B	41	THR	3.1
1	C	80	THR	3.1
1	B	29	SER	3.1
1	A	43	PHE	3.1
1	A	186	ILE	3.0
1	C	172	ILE	3.0
1	A	167	ILE	3.0
1	C	139	ASN	3.0
1	C	115	GLN	3.0
1	C	137	SER	2.9
1	B	104	THR	2.9
1	B	24	PRO	2.9
1	C	151	THR	2.9
1	A	95	ALA	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	116	SER	2.9
1	A	121	GLY	2.9
1	C	134	ASN	2.9
1	A	139	ASN	2.9
1	B	179	ARG	2.9
1	C	4	SER	2.9
1	A	50	ALA	2.9
1	B	39	GLU	2.8
1	C	181	SER	2.8
1	C	74	GLU	2.8
1	C	59	PRO	2.8
1	B	158	SER	2.8
1	C	50	ALA	2.8
1	C	55	GLN	2.8
1	A	108	ILE	2.8
1	B	186	ILE	2.7
1	C	141	MET	2.7
1	C	73	VAL	2.7
1	C	124	SER	2.7
1	C	122	ALA	2.7
1	B	105	PRO	2.7
1	B	159	ARG	2.7
1	C	32	ILE	2.7
1	A	174	ILE	2.6
1	B	44	GLY	2.6
1	A	105	PRO	2.6
1	C	19	SER	2.6
1	B	75	CYS	2.6
1	C	61	THR	2.6
1	C	14	ILE	2.6
1	C	144	ASP	2.5
1	C	110	ARG	2.5
1	C	67	TYR	2.5
1	C	41	THR	2.5
1	A	60	ILE	2.5
1	A	85	ALA	2.5
1	B	49	ALA	2.5
1	B	122	ALA	2.5
1	C	146	VAL	2.4
1	A	49	ALA	2.4
1	B	80	THR	2.4
1	A	103	ALA	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	103	ALA	2.4
1	C	133	LEU	2.4
1	C	149	THR	2.4
1	A	90	LEU	2.4
1	A	92	VAL	2.4
1	C	175	SER	2.4
1	A	170	ALA	2.4
1	B	22	SER	2.4
1	C	153	LYS	2.3
1	B	110	ARG	2.3
1	C	21	LEU	2.3
1	C	66	PRO	2.3
1	C	120	GLY	2.3
1	B	101	SER	2.3
1	A	73	VAL	2.3
1	C	33	VAL	2.3
1	A	72	ILE	2.3
1	A	52	VAL	2.3
1	C	180	LEU	2.3
1	B	100	ASN	2.3
1	A	64	THR	2.3
1	B	150	ASP	2.3
1	C	107	GLN	2.3
1	B	4	SER	2.3
1	A	168	PRO	2.3
1	B	116	SER	2.3
1	C	10	LYS	2.3
1	B	88	ASN	2.2
1	C	102	PRO	2.2
1	A	165	SER	2.2
1	C	140	ARG	2.2
1	A	84	LEU	2.2
1	B	36	PHE	2.2
1	C	158	SER	2.2
1	C	47	GLU	2.1
1	A	77	ALA	2.1
1	B	147	THR	2.1
1	B	114	GLY	2.1
1	B	180	LEU	2.1
1	C	174	ILE	2.1
1	A	34	LEU	2.1
1	A	136	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	169	THR	2.1
1	C	135	LEU	2.1
1	A	118	VAL	2.1
1	B	166	LYS	2.1
1	B	120	GLY	2.1
1	B	91	THR	2.1
1	C	37	GLN	2.1
1	C	69	HIS	2.1
1	C	105	PRO	2.1
1	C	98	PRO	2.1
1	A	188	ASN	2.1
1	A	86	VAL	2.0
1	C	157	TYR	2.0
1	C	18	GLY	2.0
1	C	183	PRO	2.0
1	C	58	ASP	2.0
1	B	66	PRO	2.0
1	B	5	GLU	2.0
1	B	113	GLY	2.0
1	B	14	ILE	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.