Full wwPDB X-ray Structure Validation Report (i)

Aug 23, 2023 – 07:48 AM EDT

PDB ID	:	3DRY
Title	:	X-ray crystal structure of human KCTD5 protein crystallized in low-salt buffer
Authors	:	Tereshko, V.; Dementieva, I.; Goldstein, S.A.N.
Deposited on	:	2008-07-11
Resolution	:	3.30 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

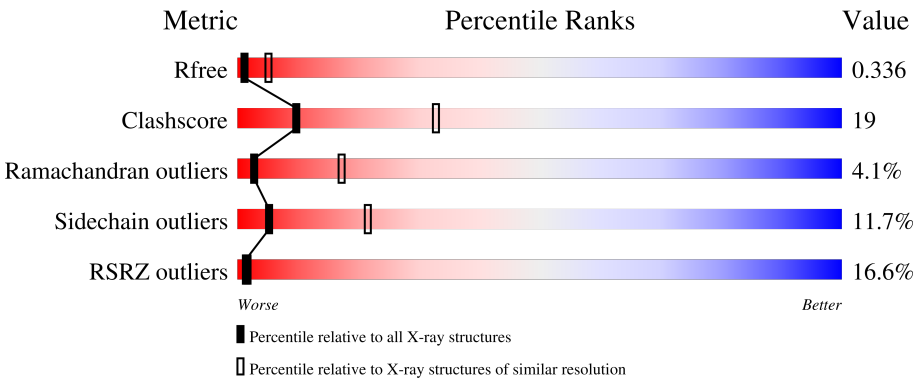
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	202	11% 56% 23% • 18%
1	B	202	12% 50% 28% • 19%
1	C	202	13% 45% 36% 7% 12%
1	D	202	15% 49% 28% 8% 15%
1	E	202	17% 48% 30% • 19%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 6810 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 BTB/POZ domain-containing protein KCTD5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	166	1338	845	225	262	6	0	0	0
			Total	C	N	O	S			
1	B	164	1328	840	223	259	6	0	0	0
			Total	C	N	O	S			
1	C	178	1433	904	243	280	6	0	0	0
			Total	C	N	O	S			
1	D	172	1383	873	235	269	6	0	0	0
			Total	C	N	O	S			
1	E	164	1328	840	223	259	6	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

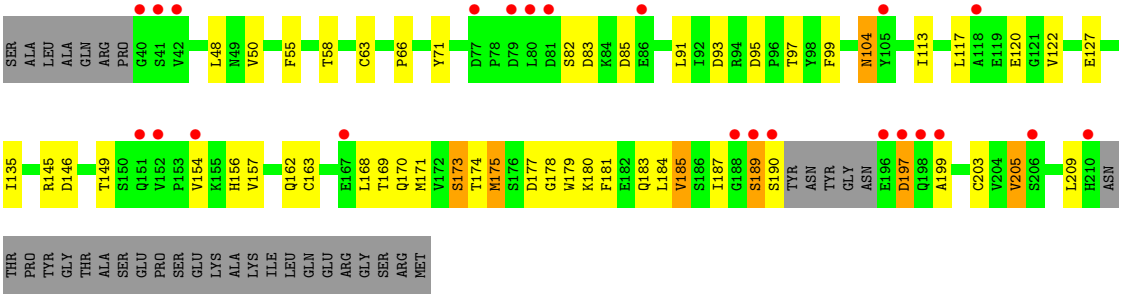
Chain	Residue	Modelled	Actual	Comment	Reference
A	33	SER	-	expression tag	UNP Q9NXV2
B	33	SER	-	expression tag	UNP Q9NXV2
C	33	SER	-	expression tag	UNP Q9NXV2
D	33	SER	-	expression tag	UNP Q9NXV2
E	33	SER	-	expression tag	UNP Q9NXV2

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.

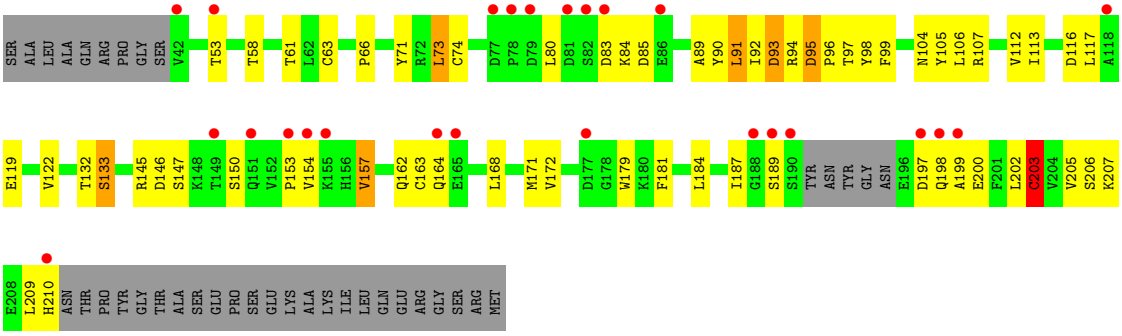
• Molecule 1: BTB/POZ domain-containing protein KCTD5

Chain A:



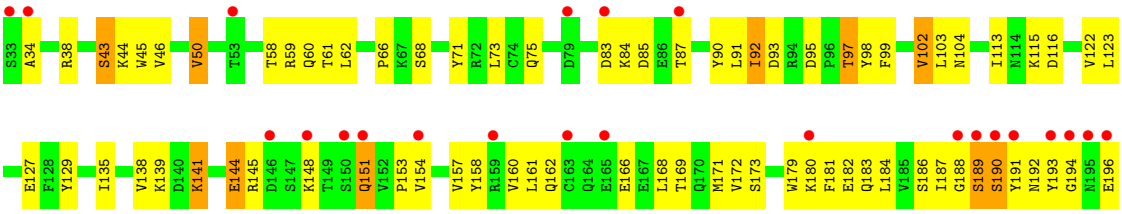
• Molecule 1: BTB/POZ domain-containing protein KCTD5

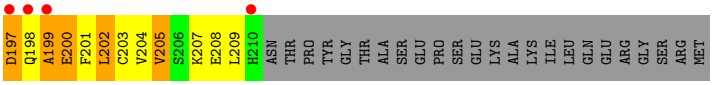
Chain B:



• Molecule 1: BTB/POZ domain-containing protein KCTD5

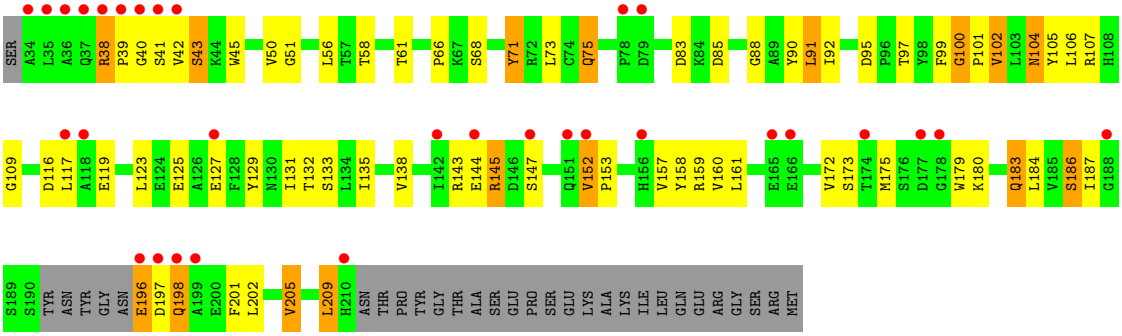
Chain C:





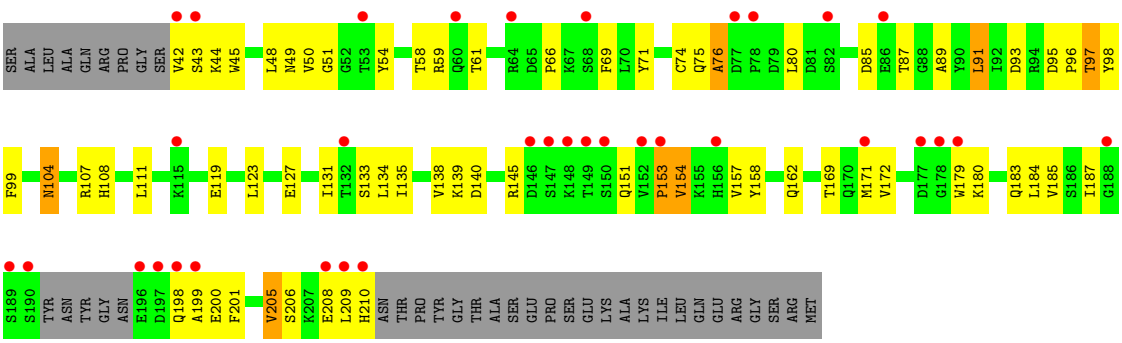
• Molecule 1: BTB/POZ domain-containing protein KCTD5

Chain D:



• Molecule 1: BTB/POZ domain-containing protein KCTD5

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	102.99Å 106.79Å 110.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.30 19.98 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-3.30) 99.7 (19.98-3.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.19 (at 3.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.253 , 0.308 0.266 , 0.336	Depositor DCC
R_{free} test set	1913 reflections (10.24%)	wwPDB-VP
Wilson B-factor (Å^2)	72.5	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 88.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.025 for -h,l,k	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	6810	wwPDB-VP
Average B, all atoms (Å^2)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% 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	0.60	1/1361 (0.1%)	0.60	0/1837
1	B	0.54	0/1351	0.63	0/1824
1	C	0.72	4/1460 (0.3%)	0.70	0/1974
1	D	0.69	1/1407 (0.1%)	0.71	0/1900
1	E	0.54	0/1351	0.61	0/1824
All	All	0.63	6/6930 (0.1%)	0.65	0/9359

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	C	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	190	SER	C-O	11.53	1.45	1.23
1	C	208	GLU	CD-OE2	8.42	1.34	1.25
1	C	192	ASN	CG-OD1	7.15	1.39	1.24
1	C	192	ASN	C-O	7.06	1.36	1.23
1	C	208	GLU	CD-OE1	6.40	1.32	1.25
1	D	147	SER	CB-OG	-5.08	1.35	1.42

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	151	GLN	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	1338	0	1321	46	0
1	B	1328	0	1313	49	0
1	C	1433	0	1409	87	0
1	D	1383	0	1370	61	0
1	E	1328	0	1313	48	0
All	All	6810	0	6726	261	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 19.

All (261) 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:162:GLN:HE21	1:A:199:ALA:CB	1.57	1.16
1:C:196:GLU:CD	1:C:197:ASP:H	1.62	0.99
1:E:157:VAL:HG13	1:E:209:LEU:HD11	1.45	0.99
1:C:190:SER:O	1:C:191:TYR:CD2	2.21	0.94
1:C:196:GLU:O	1:C:197:ASP:HB2	1.65	0.92
1:A:162:GLN:HE21	1:A:199:ALA:HB3	1.31	0.92
1:C:190:SER:O	1:C:191:TYR:CG	2.23	0.91
1:C:196:GLU:OE1	1:C:197:ASP:N	2.03	0.91
1:D:73:LEU:HD23	1:D:90:TYR:CG	2.07	0.90
1:C:50:VAL:HG21	1:C:99:PHE:CD1	2.07	0.90
1:C:160:VAL:HG22	1:C:204:VAL:HG22	1.56	0.86
1:A:162:GLN:NE2	1:A:199:ALA:CB	2.39	0.85
1:C:50:VAL:HG21	1:C:99:PHE:CE1	2.11	0.85
1:D:85:ASP:HB3	1:D:91:LEU:HD11	1.60	0.84
1:C:196:GLU:CG	1:C:197:ASP:H	1.93	0.82
1:A:162:GLN:HE21	1:A:199:ALA:HB2	1.45	0.81
1:B:168:LEU:O	1:B:172:VAL:HG23	1.81	0.81
1:C:196:GLU:O	1:C:197:ASP:CB	2.27	0.81
1:A:185:VAL:HG11	1:E:184:LEU:HD11	1.60	0.81
1:C:199:ALA:O	1:C:200:GLU:HB2	1.80	0.80
1:C:168:LEU:HD23	1:D:160:VAL:HG11	1.63	0.80
1:B:95:ASP:OD2	1:B:97:THR:HG22	1.84	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:189:SER:O	1:C:190:SER:HB2	1.84	0.77
1:B:73:LEU:CD1	1:B:80:LEU:HD13	2.14	0.76
1:B:187:ILE:O	1:B:187:ILE:HG22	1.85	0.76
1:B:168:LEU:HD12	1:B:171:MET:HE2	1.67	0.76
1:E:157:VAL:CG1	1:E:209:LEU:HD11	2.17	0.74
1:B:83:ASP:O	1:B:91:LEU:HD13	1.89	0.73
1:A:83:ASP:O	1:A:91:LEU:HD13	1.88	0.73
1:A:157:VAL:HG13	1:A:209:LEU:HD11	1.70	0.73
1:D:45:TRP:CZ3	1:D:58:THR:HG22	2.23	0.72
1:E:42:VAL:HG22	1:E:76:ALA:CB	2.20	0.72
1:B:73:LEU:HD11	1:B:80:LEU:HD13	1.73	0.71
1:C:104:ASN:HD21	1:D:95:ASP:HB2	1.55	0.70
1:B:61:THR:HG23	1:B:106:LEU:O	1.92	0.69
1:A:187:ILE:HG22	1:A:187:ILE:O	1.93	0.69
1:A:162:GLN:NE2	1:A:199:ALA:HB2	2.04	0.69
1:D:66:PRO:HA	1:D:71:TYR:CD1	2.27	0.69
1:C:91:LEU:N	1:C:91:LEU:HD12	2.08	0.68
1:C:45:TRP:CZ3	1:C:58:THR:HG23	2.29	0.67
1:E:85:ASP:HB3	1:E:91:LEU:HD11	1.75	0.67
1:B:184:LEU:H	1:C:183:GLN:HE22	1.43	0.66
1:B:162:GLN:HE21	1:B:199:ALA:HB2	1.60	0.65
1:C:127:GLU:HA	1:C:135:ILE:HD11	1.78	0.65
1:C:184:LEU:H	1:D:183:GLN:HE22	1.45	0.64
1:C:180:LYS:O	1:C:205:VAL:HG23	1.98	0.64
1:D:58:THR:HG23	1:E:93:ASP:HB2	1.80	0.64
1:E:111:LEU:HD11	1:E:138:VAL:HG22	1.79	0.64
1:E:157:VAL:HG13	1:E:209:LEU:CD1	2.26	0.63
1:C:196:GLU:CD	1:C:197:ASP:N	2.40	0.63
1:A:66:PRO:HA	1:A:71:TYR:CD1	2.34	0.63
1:E:61:THR:HG21	1:E:107:ARG:HG3	1.81	0.62
1:E:66:PRO:HA	1:E:71:TYR:CD1	2.34	0.62
1:B:187:ILE:HG13	1:B:202:LEU:HD21	1.82	0.62
1:D:152:VAL:HG23	1:D:152:VAL:O	2.00	0.62
1:C:157:VAL:HG13	1:C:209:LEU:HD12	1.81	0.61
1:C:196:GLU:CG	1:C:197:ASP:N	2.62	0.61
1:C:197:ASP:OD1	1:C:198:GLN:N	2.31	0.61
1:A:127:GLU:HA	1:A:135:ILE:HD11	1.83	0.61
1:C:172:VAL:HG12	1:D:158:TYR:HB2	1.83	0.59
1:B:168:LEU:HD12	1:B:171:MET:CE	2.31	0.59
1:D:180:LYS:O	1:D:205:VAL:HG23	2.03	0.59
1:C:162:GLN:HE21	1:C:199:ALA:CB	2.16	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:97:THR:HG22	1:E:98:TYR:CD1	2.39	0.58
1:C:95:ASP:OD1	1:C:98:TYR:HD1	1.87	0.58
1:C:123:LEU:HD21	1:C:139:LYS:HE2	1.84	0.58
1:A:113:ILE:HD11	1:A:122:VAL:HG21	1.86	0.58
1:C:102:VAL:HG12	1:C:103:LEU:N	2.19	0.57
1:D:38:ARG:O	1:D:40:GLY:N	2.37	0.57
1:C:196:GLU:OE1	1:C:197:ASP:CA	2.52	0.57
1:D:127:GLU:HA	1:D:135:ILE:HD11	1.86	0.57
1:E:42:VAL:HG22	1:E:76:ALA:HB1	1.86	0.57
1:E:75:GLN:O	1:E:76:ALA:CB	2.53	0.57
1:E:127:GLU:HA	1:E:135:ILE:HD11	1.86	0.57
1:D:172:VAL:HG12	1:E:158:TYR:HB2	1.86	0.57
1:A:163:CYS:SG	1:A:171:MET:SD	2.97	0.56
1:A:104:ASN:HD21	1:B:95:ASP:HB2	1.69	0.56
1:E:187:ILE:HG22	1:E:187:ILE:O	2.06	0.56
1:A:180:LYS:NZ	1:B:153:PRO:HG2	2.20	0.56
1:C:115:LYS:NZ	1:D:117:LEU:O	2.38	0.56
1:D:92:ILE:HG21	1:D:129:TYR:OH	2.05	0.56
1:D:184:LEU:N	1:E:183:GLN:HE22	2.04	0.56
1:C:91:LEU:N	1:C:91:LEU:CD1	2.69	0.56
1:A:157:VAL:HG13	1:A:209:LEU:HD21	1.88	0.56
1:B:107:ARG:NE	1:C:93:ASP:OD1	2.39	0.55
1:D:38:ARG:HB3	1:D:41:SER:HB2	1.88	0.55
1:E:123:LEU:HD11	1:E:139:LYS:HE3	1.87	0.55
1:C:190:SER:C	1:C:191:TYR:CD2	2.78	0.55
1:D:104:ASN:HD21	1:E:95:ASP:HB2	1.71	0.55
1:E:75:GLN:O	1:E:76:ALA:HB3	2.06	0.55
1:B:172:VAL:HG12	1:C:158:TYR:HB2	1.87	0.55
1:C:45:TRP:CE3	1:C:58:THR:HG23	2.42	0.55
1:B:61:THR:HG21	1:B:107:ARG:HG3	1.87	0.55
1:A:85:ASP:HB3	1:A:91:LEU:HD11	1.89	0.55
1:B:73:LEU:CD1	1:B:80:LEU:CD1	2.85	0.55
1:A:162:GLN:NE2	1:A:199:ALA:HB3	2.13	0.54
1:B:162:GLN:HE21	1:B:199:ALA:CB	2.20	0.54
1:C:188:GLY:O	1:C:200:GLU:OE1	2.25	0.54
1:C:160:VAL:CG1	1:C:202:LEU:HD13	2.38	0.54
1:C:189:SER:O	1:C:190:SER:CB	2.54	0.54
1:D:38:ARG:HB3	1:D:41:SER:CB	2.38	0.54
1:C:66:PRO:HA	1:C:71:TYR:CD1	2.43	0.54
1:C:97:THR:HG22	1:C:98:TYR:CD1	2.43	0.54
1:C:83:ASP:O	1:C:91:LEU:HD13	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:PHE:CZ	1:C:184:LEU:HD23	2.43	0.53
1:E:42:VAL:HG13	1:E:76:ALA:HB2	1.89	0.53
1:C:193:TYR:CD2	1:C:194:GLY:N	2.77	0.53
1:A:163:CYS:HG	1:A:171:MET:CE	2.21	0.53
1:C:123:LEU:HD21	1:C:139:LYS:CE	2.38	0.53
1:A:95:ASP:HB2	1:E:104:ASN:HD21	1.74	0.52
1:B:113:ILE:HD11	1:B:122:VAL:HG21	1.91	0.52
1:E:153:PRO:O	1:E:154:VAL:C	2.47	0.52
1:C:161:LEU:HD12	1:C:205:VAL:HG11	1.92	0.52
1:C:171:MET:HE2	1:C:172:VAL:HG22	1.91	0.52
1:D:175:MET:HE1	1:D:179:TRP:O	2.10	0.52
1:A:113:ILE:CD1	1:A:122:VAL:HG21	2.38	0.52
1:E:131:ILE:HG22	1:E:134:LEU:H	1.75	0.52
1:B:84:LYS:HA	1:B:89:ALA:O	2.10	0.52
1:D:187:ILE:HG22	1:D:187:ILE:O	2.09	0.51
1:A:157:VAL:CG1	1:A:209:LEU:HD21	2.40	0.51
1:B:162:GLN:NE2	1:B:199:ALA:HB2	2.26	0.51
1:A:180:LYS:HZ3	1:B:153:PRO:HG2	1.76	0.51
1:C:171:MET:HE2	1:C:172:VAL:CG2	2.41	0.51
1:C:179:TRP:CD1	1:C:207:LYS:HD2	2.45	0.51
1:B:179:TRP:CE2	1:B:207:LYS:HD2	2.45	0.51
1:D:99:PHE:O	1:D:100:GLY:C	2.48	0.51
1:D:73:LEU:HD23	1:D:90:TYR:CB	2.40	0.51
1:B:187:ILE:O	1:B:187:ILE:CG2	2.55	0.51
1:D:161:LEU:CD1	1:D:205:VAL:HG11	2.42	0.50
1:C:160:VAL:HG22	1:C:204:VAL:CG2	2.33	0.50
1:A:187:ILE:HD11	1:E:201:PHE:HZ	1.77	0.50
1:B:164:GLN:HA	1:B:200:GLU:HB3	1.94	0.50
1:B:96:PRO:O	1:B:99:PHE:N	2.44	0.50
1:D:184:LEU:HD13	1:D:201:PHE:CD2	2.47	0.50
1:C:162:GLN:NE2	1:C:199:ALA:HB2	2.27	0.50
1:C:196:GLU:OE1	1:C:197:ASP:HA	2.11	0.50
1:A:120:GLU:N	1:A:120:GLU:OE1	2.44	0.50
1:B:112:VAL:HG23	1:B:112:VAL:O	2.12	0.50
1:D:73:LEU:HD23	1:D:90:TYR:CD2	2.46	0.50
1:D:99:PHE:O	1:D:102:VAL:HB	2.11	0.49
1:B:96:PRO:O	1:B:98:TYR:N	2.46	0.49
1:A:169:THR:O	1:A:173:SER:OG	2.31	0.49
1:C:160:VAL:HG11	1:C:202:LEU:HD13	1.92	0.49
1:D:104:ASN:O	1:D:107:ARG:N	2.45	0.49
1:A:50:VAL:HG21	1:A:99:PHE:CD1	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:GLN:HE21	1:C:199:ALA:HB2	1.77	0.49
1:B:184:LEU:HA	1:B:203:CYS:HA	1.94	0.49
1:B:154:VAL:HG11	1:B:210:HIS:HB2	1.95	0.49
1:C:199:ALA:O	1:C:200:GLU:CB	2.55	0.49
1:B:91:LEU:CD1	1:B:91:LEU:N	2.76	0.48
1:D:196:GLU:OE2	1:D:198:GLN:NE2	2.47	0.48
1:C:186:SER:O	1:C:187:ILE:HD13	2.14	0.48
1:D:106:LEU:HD21	1:D:131:ILE:HD13	1.95	0.48
1:D:186:SER:O	1:D:187:ILE:HD13	2.14	0.48
1:B:84:LYS:HA	1:B:91:LEU:HD13	1.96	0.48
1:C:92:ILE:HD13	1:C:129:TYR:HE2	1.78	0.48
1:E:69:PHE:CE1	1:E:80:LEU:HD11	2.49	0.48
1:B:58:THR:N	1:C:93:ASP:OD2	2.34	0.48
1:B:168:LEU:HD23	1:C:202:LEU:HD11	1.95	0.48
1:C:102:VAL:CG1	1:C:103:LEU:N	2.77	0.48
1:C:85:ASP:HB3	1:C:91:LEU:HD11	1.96	0.47
1:E:45:TRP:CZ3	1:E:58:THR:HG22	2.49	0.47
1:C:168:LEU:O	1:C:172:VAL:HG23	2.14	0.47
1:E:180:LYS:O	1:E:205:VAL:HG23	2.14	0.47
1:D:104:ASN:O	1:D:105:TYR:C	2.52	0.47
1:D:157:VAL:HG13	1:D:209:LEU:CD1	2.44	0.47
1:A:181:PHE:CE1	1:A:184:LEU:HD23	2.50	0.47
1:A:183:GLN:HE22	1:E:184:LEU:H	1.62	0.47
1:E:66:PRO:HA	1:E:71:TYR:CG	2.50	0.47
1:E:171:MET:HE3	1:E:172:VAL:HG23	1.95	0.47
1:C:103:LEU:HD12	1:C:103:LEU:O	2.15	0.47
1:D:157:VAL:HG13	1:D:209:LEU:HD11	1.96	0.47
1:D:175:MET:HE2	1:D:175:MET:HB3	1.84	0.46
1:A:177:ASP:OD2	1:A:178:GLY:N	2.49	0.46
1:E:91:LEU:N	1:E:91:LEU:CD1	2.78	0.46
1:A:179:TRP:HE3	1:A:205:VAL:HG23	1.80	0.46
1:D:50:VAL:HG21	1:D:99:PHE:CE1	2.51	0.46
1:A:97:THR:O	1:A:117:LEU:HD21	2.15	0.46
1:E:58:THR:O	1:E:59:ARG:C	2.53	0.46
1:D:91:LEU:N	1:D:91:LEU:HD13	2.31	0.45
1:D:91:LEU:N	1:D:91:LEU:CD1	2.79	0.45
1:B:181:PHE:HB3	1:C:158:TYR:CE1	2.51	0.45
1:C:46:VAL:CG1	1:C:90:TYR:CE2	2.99	0.45
1:E:50:VAL:HG21	1:E:99:PHE:CD1	2.51	0.45
1:E:45:TRP:CE3	1:E:58:THR:HG22	2.52	0.45
1:A:58:THR:HG23	1:B:93:ASP:HB2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:ASP:O	1:D:91:LEU:N	2.48	0.45
1:E:179:TRP:HE3	1:E:205:VAL:HG22	1.81	0.45
1:E:69:PHE:HE1	1:E:80:LEU:HD11	1.82	0.45
1:A:93:ASP:OD2	1:E:58:THR:HG23	2.17	0.45
1:A:179:TRP:CE3	1:A:205:VAL:HG23	2.51	0.45
1:A:50:VAL:HG21	1:A:99:PHE:CE1	2.52	0.45
1:C:97:THR:HG22	1:C:98:TYR:N	2.32	0.45
1:E:54:TYR:OH	1:E:87:THR:HG21	2.15	0.45
1:E:48:LEU:O	1:E:89:ALA:HB1	2.18	0.44
1:C:62:LEU:HD13	1:C:73:LEU:HD22	1.98	0.44
1:C:184:LEU:HA	1:C:203:CYS:HA	1.99	0.44
1:C:151:GLN:NE2	1:C:153:PRO:HB3	2.32	0.44
1:A:91:LEU:CD1	1:A:91:LEU:N	2.79	0.44
1:A:99:PHE:O	1:A:99:PHE:CG	2.70	0.44
1:D:99:PHE:O	1:D:102:VAL:N	2.51	0.44
1:D:159:ARG:HG3	1:D:179:TRP:CZ3	2.52	0.44
1:B:157:VAL:CG2	1:B:209:LEU:HD11	2.47	0.44
1:C:190:SER:O	1:C:191:TYR:CE2	2.68	0.44
1:C:190:SER:C	1:C:191:TYR:CG	2.86	0.44
1:C:90:TYR:C	1:C:91:LEU:HD12	2.38	0.44
1:A:175:MET:CE	1:A:179:TRP:O	2.66	0.44
1:B:105:TYR:HD2	1:B:106:LEU:HD23	1.82	0.44
1:E:42:VAL:HG22	1:E:76:ALA:HB2	1.97	0.44
1:A:175:MET:HE3	1:A:179:TRP:O	2.18	0.43
1:B:66:PRO:HA	1:B:71:TYR:CD1	2.53	0.43
1:D:125:GLU:O	1:D:129:TYR:HD1	2.01	0.43
1:B:105:TYR:OH	1:B:133:SER:HB2	2.17	0.43
1:A:91:LEU:N	1:A:91:LEU:HD12	2.33	0.43
1:C:182:GLU:HB2	1:C:204:VAL:HG12	2.00	0.43
1:D:143:ARG:O	1:D:145:ARG:N	2.51	0.43
1:C:44:LYS:O	1:C:59:ARG:N	2.49	0.43
1:C:84:LYS:HE3	1:C:90:TYR:CE2	2.53	0.43
1:C:162:GLN:HE21	1:C:199:ALA:HB3	1.82	0.43
1:D:161:LEU:HD12	1:D:205:VAL:HG11	2.00	0.43
1:A:183:GLN:HG2	1:A:184:LEU:N	2.33	0.43
1:D:73:LEU:HD12	1:D:73:LEU:H	1.84	0.43
1:D:184:LEU:H	1:E:183:GLN:HE22	1.65	0.43
1:D:105:TYR:O	1:D:109:GLY:N	2.49	0.43
1:A:170:GLN:O	1:A:174:THR:HG23	2.19	0.42
1:C:95:ASP:OD1	1:C:98:TYR:CD1	2.70	0.42
1:D:172:VAL:HG12	1:E:158:TYR:CB	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:51:GLY:HA3	1:E:96:PRO:HD3	2.01	0.42
1:B:84:LYS:HE3	1:B:90:TYR:CZ	2.54	0.42
1:B:99:PHE:O	1:B:99:PHE:CG	2.72	0.42
1:C:122:VAL:HG12	1:C:138:VAL:HG11	2.02	0.42
1:B:92:ILE:O	1:B:94:ARG:N	2.51	0.42
1:B:104:ASN:OD1	1:B:112:VAL:HG21	2.19	0.42
1:D:104:ASN:ND2	1:E:95:ASP:OD1	2.53	0.42
1:C:193:TYR:HD2	1:C:194:GLY:N	2.18	0.42
1:B:85:ASP:N	1:B:91:LEU:HD11	2.35	0.41
1:C:141:LYS:HD3	1:C:144:GLU:OE2	2.20	0.41
1:D:123:LEU:HA	1:D:138:VAL:HG11	2.02	0.41
1:B:172:VAL:HG12	1:C:158:TYR:CB	2.50	0.41
1:C:66:PRO:HA	1:C:71:TYR:CG	2.55	0.41
1:D:66:PRO:HA	1:D:71:TYR:CG	2.54	0.41
1:C:181:PHE:HZ	1:C:184:LEU:HD23	1.84	0.41
1:D:41:SER:O	1:D:43:SER:N	2.53	0.41
1:D:45:TRP:CZ3	1:D:58:THR:CG2	3.00	0.41
1:D:100:GLY:O	1:D:101:PRO:C	2.57	0.41
1:B:96:PRO:O	1:B:97:THR:C	2.59	0.41
1:A:48:LEU:HB2	1:A:55:PHE:HB2	2.03	0.41
1:A:154:VAL:HG23	1:A:156:HIS:CE1	2.55	0.41
1:D:75:GLN:HE21	1:D:75:GLN:HB3	1.63	0.41
1:E:91:LEU:N	1:E:91:LEU:HD13	2.36	0.41
1:B:163:CYS:HG	1:B:171:MET:CE	2.34	0.41
1:C:97:THR:CG2	1:C:98:TYR:N	2.84	0.41
1:A:181:PHE:CZ	1:A:184:LEU:HD23	2.56	0.41
1:D:61:THR:HG21	1:D:107:ARG:HG3	2.03	0.40
1:D:184:LEU:HD13	1:D:201:PHE:HD2	1.84	0.40
1:C:184:LEU:H	1:D:183:GLN:NE2	2.13	0.40
1:C:193:TYR:CB	1:C:197:ASP:OD2	2.70	0.40
1:D:56:LEU:HD12	1:D:56:LEU:HA	1.85	0.40
1:E:134:LEU:O	1:E:138:VAL:HG23	2.20	0.40
1:E:162:GLN:NE2	1:E:199:ALA:HB2	2.37	0.40
1:C:201:PHE:HZ	1:D:202:LEU:HD11	1.87	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	162/202 (80%)	138 (85%)	21 (13%)	3 (2%)	8 34
1	B	160/202 (79%)	134 (84%)	22 (14%)	4 (2%)	5 27
1	C	176/202 (87%)	135 (77%)	31 (18%)	10 (6%)	1 11
1	D	168/202 (83%)	125 (74%)	32 (19%)	11 (6%)	1 9
1	E	160/202 (79%)	133 (83%)	21 (13%)	6 (4%)	3 19
All	All	826/1010 (82%)	665 (80%)	127 (15%)	34 (4%)	3 17

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	34	ALA
1	C	43	SER
1	C	190	SER
1	C	197	ASP
1	C	199	ALA
1	C	200	GLU
1	D	71	TYR
1	D	198	GLN
1	E	76	ALA
1	E	154	VAL
1	B	198	GLN
1	C	154	VAL
1	D	42	VAL
1	D	51	GLY
1	D	100	GLY
1	D	144	GLU
1	E	44	LYS
1	A	175	MET
1	B	74	CYS
1	B	203	CYS
1	E	49	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	197	ASP
1	C	166	GLU
1	D	153	PRO
1	A	189	SER
1	B	93	ASP
1	D	152	VAL
1	E	43	SER
1	E	153	PRO
1	D	39	PRO
1	C	50	VAL
1	D	88	GLY
1	C	92	ILE
1	D	102	VAL

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	152/181 (84%)	139 (91%)	13 (9%)	10 35
1	B	151/181 (83%)	131 (87%)	20 (13%)	4 17
1	C	161/181 (89%)	141 (88%)	20 (12%)	4 19
1	D	156/181 (86%)	137 (88%)	19 (12%)	5 20
1	E	151/181 (83%)	133 (88%)	18 (12%)	5 21
All	All	771/905 (85%)	681 (88%)	90 (12%)	5 21

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	CYS
1	A	82	SER
1	A	104	ASN
1	A	145	ARG
1	A	146	ASP
1	A	149	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	168	LEU
1	A	173	SER
1	A	185	VAL
1	A	189	SER
1	A	197	ASP
1	A	203	CYS
1	A	205	VAL
1	B	53	THR
1	B	63	CYS
1	B	73	LEU
1	B	91	LEU
1	B	95	ASP
1	B	116	ASP
1	B	117	LEU
1	B	119	GLU
1	B	132	THR
1	B	133	SER
1	B	145	ARG
1	B	146	ASP
1	B	147	SER
1	B	150	SER
1	B	157	VAL
1	B	189	SER
1	B	197	ASP
1	B	203	CYS
1	B	205	VAL
1	B	206	SER
1	C	38	ARG
1	C	43	SER
1	C	60	GLN
1	C	61	THR
1	C	68	SER
1	C	75	GLN
1	C	87	THR
1	C	97	THR
1	C	102	VAL
1	C	113	ILE
1	C	116	ASP
1	C	141	LYS
1	C	144	GLU
1	C	145	ARG
1	C	148	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	169	THR
1	C	173	SER
1	C	189	SER
1	C	202	LEU
1	C	205	VAL
1	D	38	ARG
1	D	43	SER
1	D	68	SER
1	D	75	GLN
1	D	91	LEU
1	D	97	THR
1	D	104	ASN
1	D	116	ASP
1	D	119	GLU
1	D	132	THR
1	D	133	SER
1	D	145	ARG
1	D	173	SER
1	D	183	GLN
1	D	186	SER
1	D	196	GLU
1	D	197	ASP
1	D	205	VAL
1	D	209	LEU
1	E	74	CYS
1	E	91	LEU
1	E	97	THR
1	E	104	ASN
1	E	108	HIS
1	E	119	GLU
1	E	133	SER
1	E	140	ASP
1	E	145	ARG
1	E	151	GLN
1	E	169	THR
1	E	185	VAL
1	E	198	GLN
1	E	200	GLU
1	E	205	VAL
1	E	206	SER
1	E	208	GLU
1	E	210	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	HIS
1	A	156	HIS
1	A	162	GLN
1	A	183	GLN
1	A	198	GLN
1	B	75	GLN
1	B	162	GLN
1	B	183	GLN
1	C	104	ASN
1	C	108	HIS
1	C	162	GLN
1	C	183	GLN
1	C	198	GLN
1	D	37	GLN
1	D	60	GLN
1	D	75	GLN
1	D	104	ASN
1	D	108	HIS
1	D	183	GLN
1	D	198	GLN
1	E	130	ASN
1	E	162	GLN
1	E	183	GLN
1	E	198	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 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	166/202 (82%)	1.05	23 (13%)	2	2	80, 86, 91, 92	0
1	B	164/202 (81%)	1.15	25 (15%)	2	2	80, 86, 92, 96	0
1	C	178/202 (88%)	1.11	27 (15%)	2	2	76, 85, 91, 92	13 (7%)
1	D	172/202 (85%)	1.18	31 (18%)	1	1	80, 86, 92, 110	0
1	E	164/202 (81%)	1.18	34 (20%)	1	1	80, 86, 91, 92	0
All	All	844/1010 (83%)	1.14	140 (16%)	1	2	76, 86, 91, 110	13 (1%)

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	189	SER	18.0
1	C	190	SER	17.0
1	D	36	ALA	15.3
1	A	40	GLY	15.1
1	D	196	GLU	11.9
1	A	190	SER	11.6
1	D	197	ASP	11.2
1	B	190	SER	11.0
1	E	149	THR	10.6
1	C	195	ASN	10.5
1	E	198	GLN	9.9
1	B	81	ASP	9.5
1	A	197	ASP	9.3
1	E	197	ASP	9.1
1	E	190	SER	9.1
1	D	39	PRO	7.9
1	C	194	GLY	7.5
1	C	33	SER	7.4
1	D	166	GLU	7.3
1	A	41	SER	7.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	189	SER	7.0
1	C	191	TYR	6.2
1	D	35	LEU	6.2
1	C	34	ALA	5.9
1	D	34	ALA	5.6
1	C	197	ASP	5.6
1	D	177	ASP	5.5
1	D	38	ARG	5.4
1	B	197	ASP	5.4
1	A	188	GLY	5.2
1	C	198	GLN	5.2
1	B	177	ASP	5.1
1	C	154	VAL	5.1
1	A	42	VAL	5.0
1	A	79	ASP	4.9
1	E	210	HIS	4.9
1	D	188	GLY	4.8
1	E	179	TRP	4.7
1	C	146	ASP	4.7
1	D	198	GLN	4.6
1	D	42	VAL	4.6
1	C	210	HIS	4.5
1	D	151	GLN	4.5
1	B	79	ASP	4.4
1	A	189	SER	4.4
1	C	83	ASP	4.3
1	A	77	ASP	4.3
1	A	210	HIS	4.3
1	A	198	GLN	4.2
1	B	42	VAL	4.2
1	E	150	SER	4.1
1	D	40	GLY	4.1
1	D	41	SER	4.1
1	B	199	ALA	4.1
1	E	132	THR	4.0
1	C	199	ALA	4.0
1	B	210	HIS	3.9
1	A	196	GLU	3.9
1	B	78	PRO	3.9
1	C	163	CYS	3.8
1	E	77	ASP	3.8
1	E	178	GLY	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	188	GLY	3.7
1	A	199	ALA	3.6
1	E	196	GLU	3.5
1	E	146	ASP	3.5
1	C	189	SER	3.5
1	E	209	LEU	3.5
1	B	151	GLN	3.4
1	B	149	THR	3.3
1	B	198	GLN	3.3
1	D	37	GLN	3.3
1	D	165	GLU	3.3
1	D	147	SER	3.2
1	C	193	TYR	3.2
1	D	78	PRO	3.2
1	B	82	SER	3.2
1	C	159	ARG	3.1
1	E	147	SER	3.1
1	E	199	ALA	3.0
1	B	53	THR	3.0
1	A	81	ASP	3.0
1	A	167	GLU	3.0
1	E	208	GLU	2.9
1	D	210	HIS	2.9
1	E	152	VAL	2.9
1	A	105	TYR	2.9
1	D	118	ALA	2.8
1	E	82	SER	2.8
1	B	155	LYS	2.8
1	C	165	GLU	2.8
1	D	156	HIS	2.8
1	A	151	GLN	2.8
1	C	150	SER	2.7
1	D	174	THR	2.7
1	E	43	SER	2.7
1	C	79	ASP	2.7
1	D	199	ALA	2.7
1	B	118	ALA	2.7
1	A	206	SER	2.6
1	B	77	ASP	2.6
1	E	42	VAL	2.6
1	D	79	ASP	2.6
1	E	78	PRO	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	148	LYS	2.5
1	B	154	VAL	2.5
1	B	188	GLY	2.5
1	E	115	LYS	2.4
1	B	86	GLU	2.4
1	E	86	GLU	2.4
1	E	156	HIS	2.4
1	E	177	ASP	2.3
1	B	83	ASP	2.3
1	A	80	LEU	2.3
1	C	180	LYS	2.3
1	E	60	GLN	2.3
1	D	152	VAL	2.3
1	B	164	GLN	2.3
1	A	152	VAL	2.2
1	C	196	GLU	2.2
1	C	53	THR	2.2
1	A	86	GLU	2.2
1	A	154	VAL	2.2
1	B	165	GLU	2.2
1	E	64	ARG	2.2
1	E	53	THR	2.2
1	C	188	GLY	2.2
1	C	87	THR	2.2
1	D	117	LEU	2.1
1	D	142	ILE	2.1
1	E	68	SER	2.1
1	A	118	ALA	2.1
1	D	178	GLY	2.1
1	E	148	LYS	2.1
1	E	153	PRO	2.1
1	E	171	MET	2.0
1	D	127	GLU	2.0
1	D	144	GLU	2.0
1	B	153	PRO	2.0
1	C	151	GLN	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.