Full wwPDB X-ray Structure Validation Report (i)

Feb 4, 2024 – 03:30 PM EST

PDB ID	:	1RKE
Title	:	Human vinculin head (1-258) in complex with human vinculin tail (879-1066)
Authors	:	Izard, T.; Evans, G.; Borgon, R.A.; Rush, C.L.; Bricogne, G.; Bois, P.R.
Deposited on	:	2003-11-21
Resolution	:	2.35 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 (i)) were used in the production of this report:

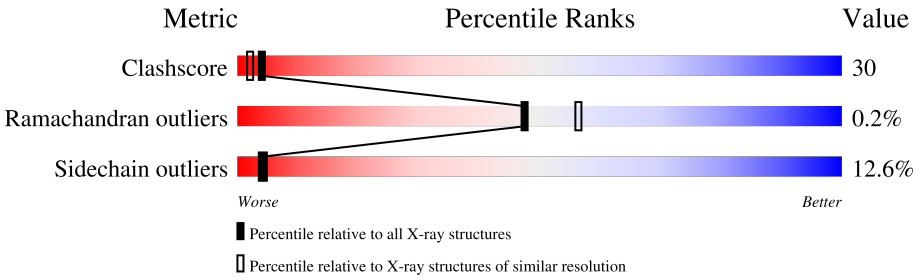
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.35 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	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	262	58% 38% 5%
2	B	185	51% 35% 10% 5%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3660 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 Vinculin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	S	0	1	0
			2070	1302	357	397	14			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	HIS	-	expression tag	UNP P18206
A	-2	HIS	-	expression tag	UNP P18206
A	-1	HIS	-	expression tag	UNP P18206
A	0	HIS	-	expression tag	UNP P18206

- Molecule 2 is a protein called VCL protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	176	Total	C	N	O	S	0	2	0
			1386	852	256	264	14			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	128	Total	O	0	0
			128	128		
3	B	76	Total	O	0	0
			76	76		

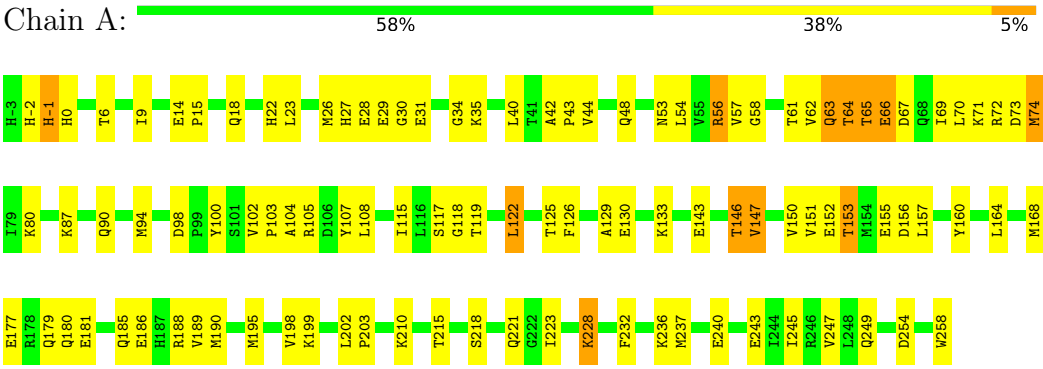
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

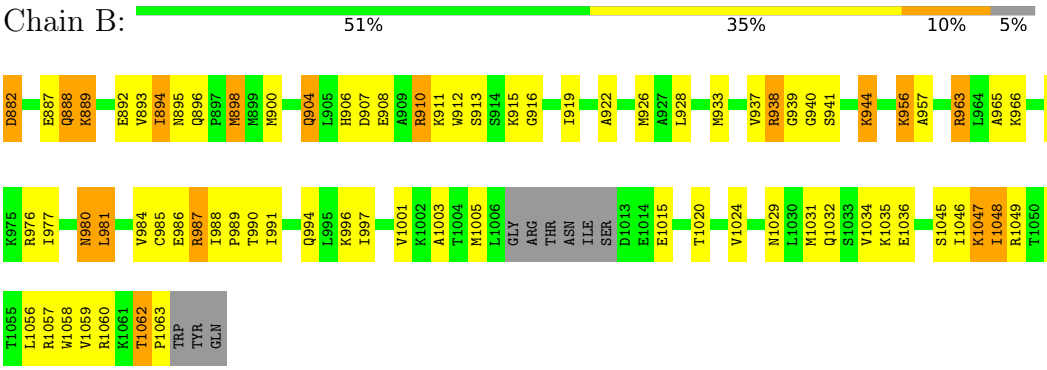
- Molecule 1: Vinculin

Chain A:



- Molecule 2: VCL protein

Chain B:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	86.60Å 161.65Å 36.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.35	Depositor
% Data completeness (in resolution range)	99.8 (15.00-2.35)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	BUSTER-TNT	Depositor
R, R_{free}	0.206 , 0.278	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3660	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

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	0.47	0/2102	0.60	0/2848
2	B	0.45	0/1396	0.62	0/1869
All	All	0.46	0/3498	0.61	0/4717

There are no bond length outliers.

There are no bond angle outliers.

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	2070	0	2108	122	0
2	B	1386	0	1439	93	0
3	A	128	0	0	5	0
3	B	76	0	0	9	0
All	All	3660	0	3547	211	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 30.

All (211) 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:94:MET:HE2	1:A:104:ALA:HB2	1.19	1.13

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:907:ASP:HA	2:B:910:ARG:HD3	1.30	1.11
2:B:937:VAL:HG11	2:B:1020:THR:HG23	1.38	1.05
1:A:65:THR:HG22	1:A:71:LYS:HE3	1.37	1.04
2:B:888:GLN:HG3	2:B:894:ILE:HD13	1.35	1.04
2:B:1049:ARG:NE	2:B:1051:ASP:HB2	1.72	1.04
1:A:69:ILE:HD13	1:A:72:ARG:HH12	1.23	0.99
1:A:153:THR:HG22	1:A:156:ASP:H	1.30	0.97
2:B:1049:ARG:HE	2:B:1051:ASP:HB2	1.29	0.97
1:A:74:MET:HB3	1:A:75:PRO:HD3	1.54	0.90
2:B:926[B]:MET:HE3	2:B:1031:MET:HE1	1.54	0.90
2:B:895:ASN:HD22	2:B:898:MET:H	1.22	0.87
2:B:926[B]:MET:HE3	2:B:1031:MET:CE	2.04	0.87
1:A:185:GLN:HE22	1:A:188:ARG:HH21	1.19	0.87
1:A:94:MET:HE2	1:A:104:ALA:CB	2.06	0.84
2:B:980:ASN:HD22	2:B:980:ASN:N	1.72	0.84
2:B:937:VAL:CG1	2:B:1020:THR:HG23	2.08	0.84
1:A:228:LYS:O	1:A:228:LYS:HD3	1.79	0.83
2:B:907:ASP:HA	2:B:910:ARG:CD	2.11	0.79
1:A:53:ASN:O	1:A:57:VAL:HG23	1.81	0.79
2:B:980:ASN:HD22	2:B:980:ASN:H	1.32	0.78
2:B:900[B]:MET:O	2:B:904:GLN:HG2	1.83	0.77
1:A:65:THR:HG21	1:A:70:LEU:HD23	1.66	0.77
1:A:147:VAL:HG12	1:A:160:TYR:HE1	1.50	0.76
1:A:245:ILE:O	1:A:249:GLN:HG3	1.85	0.76
2:B:888:GLN:CG	2:B:894:ILE:HD13	2.15	0.76
1:A:153:THR:HG23	1:A:155:GLU:H	1.51	0.76
1:A:31:GLU:HG2	1:A:105:ARG:NE	2.00	0.75
2:B:922:ALA:O	2:B:926[A]:MET:HG3	1.86	0.73
1:A:27:HIS:HB2	1:A:108:LEU:HD23	1.69	0.73
1:A:75:PRO:HB2	1:A:76:PRO:HD3	1.70	0.73
1:A:44:VAL:O	1:A:48:GLN:HG3	1.90	0.71
1:A:31:GLU:HG2	1:A:105:ARG:HE	1.55	0.71
2:B:895:ASN:ND2	2:B:898:MET:H	1.89	0.70
2:B:882:ASP:N	3:B:15:HOH:O	2.24	0.70
2:B:1049:ARG:CZ	2:B:1051:ASP:HB2	2.22	0.69
2:B:1032:GLN:O	2:B:1036:GLU:HG3	1.93	0.69
2:B:971:GLN:OE1	2:B:1054:PHE:HB3	1.94	0.68
2:B:895:ASN:HD22	2:B:898:MET:HB2	1.59	0.68
2:B:900[A]:MET:O	2:B:904:GLN:HG2	1.93	0.67
2:B:926[B]:MET:HE1	2:B:1034:VAL:HG21	1.76	0.67
2:B:976:ARG:O	2:B:980:ASN:ND2	2.28	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:938:ARG:CG	2:B:938:ARG:HH11	2.08	0.67
1:A:232:PHE:CE2	1:A:236:LYS:HD2	2.30	0.66
2:B:919:ILE:HD12	2:B:1056:LEU:HD11	1.76	0.66
2:B:926[B]:MET:CE	2:B:1034:VAL:HG21	2.26	0.66
2:B:906:HIS:ND1	3:B:21:HOH:O	2.28	0.65
1:A:228:LYS:HD3	1:A:228:LYS:C	2.14	0.65
2:B:938:ARG:O	2:B:940:GLY:N	2.30	0.65
2:B:944:LYS:HD3	2:B:1003:ALA:O	1.96	0.65
2:B:980:ASN:N	2:B:980:ASN:ND2	2.45	0.65
2:B:895:ASN:ND2	2:B:898:MET:HB2	2.12	0.65
2:B:1045:SER:O	2:B:1048:ILE:HD11	1.96	0.64
1:A:69:ILE:HD13	1:A:72:ARG:NH1	2.06	0.64
1:A:153:THR:HB	1:A:156:ASP:OD2	1.97	0.64
2:B:887:GLU:H	2:B:887:GLU:CD	2.00	0.63
2:B:926[B]:MET:CE	2:B:1031:MET:HE1	2.27	0.63
1:A:185:GLN:HE22	1:A:188:ARG:NH2	1.94	0.63
2:B:938:ARG:HH11	2:B:938:ARG:HB3	1.64	0.63
1:A:58:GLY:HA3	1:A:126:PHE:HZ	1.64	0.63
2:B:987:ARG:HH22	2:B:1032:GLN:NE2	1.97	0.63
1:A:65:THR:CG2	1:A:71:LYS:HE3	2.22	0.63
1:A:58:GLY:CA	1:A:126:PHE:HZ	2.13	0.62
2:B:910:ARG:HH11	2:B:910:ARG:CB	2.13	0.62
1:A:195:MET:O	1:A:199:LYS:HG3	1.98	0.62
2:B:938:ARG:HH11	2:B:938:ARG:HG3	1.65	0.62
1:A:56:ARG:HD2	3:A:351:HOH:O	1.99	0.61
1:A:164:LEU:HD12	1:A:164:LEU:O	1.99	0.61
2:B:926[B]:MET:HE3	2:B:1031:MET:HE2	1.83	0.61
2:B:981:LEU:O	2:B:984:VAL:HG22	2.01	0.60
2:B:963:ARG:NH1	2:B:963:ARG:HG2	2.15	0.60
2:B:926[B]:MET:HG2	2:B:1031:MET:HE1	1.82	0.60
2:B:938:ARG:N	2:B:938:ARG:HD2	2.16	0.60
1:A:90:GLN:NE2	1:A:107:TYR:HE2	1.99	0.60
1:A:0:HIS:HB2	2:B:1029:ASN:HD21	1.65	0.59
2:B:974:ASP:OD2	2:B:977:ILE:HD12	2.02	0.59
2:B:1053:GLY:O	2:B:1054:PHE:HB2	2.02	0.59
2:B:926[B]:MET:HE1	2:B:1034:VAL:CG2	2.32	0.59
1:A:202:LEU:HB3	1:A:203:PRO:CD	2.32	0.58
2:B:910:ARG:HH11	2:B:910:ARG:HB2	1.66	0.58
1:A:90:GLN:NE2	1:A:107:TYR:CE2	2.72	0.58
2:B:963:ARG:HG2	2:B:963:ARG:HH11	1.69	0.58
1:A:14:GLU:HG2	1:A:15:PRO:HD3	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:GLU:O	1:A:190:MET:HG3	2.04	0.57
1:A:74:MET:HG3	1:A:78:PHE:CZ	2.39	0.57
2:B:898:MET:CE	2:B:933:MET:HB3	2.34	0.57
1:A:56:ARG:HH11	1:A:56:ARG:HG3	1.70	0.56
2:B:892:GLU:HB3	2:B:894:ILE:HD12	1.88	0.56
2:B:926[B]:MET:HG2	2:B:1031:MET:CE	2.35	0.56
1:A:6:THR:HB	1:A:181:GLU:HG3	1.88	0.56
2:B:912:TRP:CZ3	2:B:1060:ARG:HD3	2.40	0.56
1:A:22[B]:HIS:HD2	1:A:23:LEU:HD23	1.70	0.56
1:A:57:VAL:HG22	3:A:351:HOH:O	2.06	0.55
1:A:65:THR:HG22	1:A:71:LYS:CE	2.25	0.55
1:A:65:THR:HG23	1:A:66:GLU:N	2.20	0.55
2:B:980:ASN:H	2:B:980:ASN:ND2	2.00	0.55
2:B:898:MET:HE3	2:B:933:MET:HB3	1.89	0.55
1:A:56:ARG:HH11	1:A:56:ARG:CG	2.19	0.55
1:A:56:ARG:HB2	1:A:56:ARG:NH1	2.22	0.55
2:B:944:LYS:NZ	3:B:139:HOH:O	2.40	0.55
2:B:1001:VAL:HG21	3:B:182:HOH:O	2.06	0.54
1:A:74:MET:HE3	1:A:126:PHE:CE2	2.42	0.54
1:A:74:MET:SD	1:A:122:LEU:HD12	2.47	0.54
1:A:74:MET:HB3	1:A:75:PRO:CD	2.32	0.54
1:A:185:GLN:NE2	1:A:188:ARG:HH21	1.99	0.54
1:A:29:GLU:HB3	1:A:35:LYS:HD3	1.89	0.53
1:A:62:VAL:HG13	1:A:71:LYS:HG3	1.89	0.53
2:B:938:ARG:HH11	2:B:938:ARG:CB	2.20	0.53
1:A:27:HIS:HB2	1:A:108:LEU:CD2	2.36	0.53
1:A:62:VAL:HG12	1:A:62:VAL:O	2.09	0.53
2:B:893:VAL:HB	3:B:65:HOH:O	2.08	0.53
1:A:151:VAL:HG13	1:A:156:ASP:HB2	1.90	0.53
1:A:243:GLU:O	1:A:247:VAL:HG23	2.08	0.53
2:B:1032:GLN:NE2	3:B:120:HOH:O	2.42	0.53
2:B:919:ILE:HD12	2:B:1056:LEU:CD1	2.38	0.53
1:A:90:GLN:O	1:A:94:MET:HG3	2.09	0.53
1:A:6:THR:OG1	1:A:9:ILE:HG13	2.09	0.52
1:A:147:VAL:CG1	1:A:160:TYR:HE1	2.20	0.52
1:A:173:LYS:NZ	1:A:177:GLU:OE2	2.43	0.52
1:A:22[B]:HIS:CD2	1:A:23:LEU:HD23	2.45	0.52
2:B:963:ARG:HH11	2:B:963:ARG:CG	2.22	0.52
1:A:218:SER:HB3	1:A:221:GLN:CG	2.40	0.52
2:B:938:ARG:HG3	2:B:938:ARG:NH1	2.25	0.50
1:A:42:ALA:HB3	1:A:43:PRO:CD	2.42	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:VAL:HG12	1:A:57:VAL:O	2.11	0.50
1:A:70:LEU:HD13	1:A:129:ALA:HB2	1.92	0.50
1:A:102:VAL:N	1:A:103:PRO:HD2	2.27	0.50
1:A:75:PRO:HB2	1:A:76:PRO:CD	2.39	0.50
2:B:889:LYS:O	2:B:892:GLU:HB2	2.11	0.50
2:B:1049:ARG:HG2	2:B:1051:ASP:H	1.77	0.49
1:A:215:THR:HG22	1:A:223:ILE:HG22	1.94	0.49
2:B:895:ASN:HD22	2:B:898:MET:N	2.01	0.49
1:A:72:ARG:HG2	1:A:73:ASP:OD1	2.13	0.48
2:B:990:THR:O	2:B:994:GLN:HG3	2.12	0.48
2:B:908:GLU:HA	2:B:911:LYS:HE3	1.96	0.48
2:B:988:ILE:N	2:B:989:PRO:CD	2.76	0.48
2:B:888:GLN:HG3	2:B:894:ILE:CD1	2.26	0.48
2:B:894:ILE:HG22	2:B:896:GLN:OE1	2.13	0.48
2:B:956:LYS:HB3	2:B:956:LYS:HE2	1.55	0.48
1:A:22[B]:HIS:O	1:A:26:MET:HE2	2.14	0.48
1:A:130:GLU:HA	1:A:130:GLU:OE1	2.14	0.47
1:A:74:MET:HE1	1:A:126:PHE:CD2	2.49	0.47
1:A:151:VAL:HG11	1:A:157:LEU:HA	1.96	0.47
2:B:1045:SER:HA	2:B:1048:ILE:HD13	1.96	0.47
1:A:189:VAL:HA	3:A:367:HOH:O	2.14	0.47
1:A:30:GLY:O	1:A:34:GLY:HA2	2.14	0.47
1:A:40:LEU:HA	1:A:43:PRO:HG2	1.97	0.46
1:A:42:ALA:HB3	1:A:43:PRO:HD3	1.96	0.46
1:A:153:THR:HG23	1:A:155:GLU:N	2.25	0.46
1:A:54:LEU:CD2	1:A:119:THR:HG23	2.45	0.46
2:B:1047:LYS:HE2	2:B:1047:LYS:HB3	1.42	0.46
1:A:168:MET:CE	1:A:237:MET:CE	2.93	0.46
1:A:22[B]:HIS:CD2	1:A:23:LEU:N	2.84	0.46
1:A:74:MET:CE	1:A:126:PHE:CE2	2.99	0.46
1:A:74:MET:CE	1:A:126:PHE:CD2	2.99	0.45
2:B:915:LYS:O	2:B:1057:ARG:HD3	2.17	0.45
1:A:153:THR:CG2	1:A:155:GLU:H	2.27	0.45
1:A:-1:HIS:CD2	2:B:987:ARG:CZ	2.99	0.45
2:B:898:MET:HE1	2:B:933:MET:C	2.36	0.45
1:A:179:GLN:O	1:A:188:ARG:HD2	2.16	0.45
1:A:218:SER:HB3	1:A:221:GLN:HG2	1.97	0.45
1:A:94:MET:HE1	1:A:103:PRO:HB2	1.98	0.45
1:A:75:PRO:HA	1:A:78:PHE:CD1	2.52	0.45
1:A:147:VAL:HG12	1:A:160:TYR:CE1	2.40	0.45
2:B:1057:ARG:HG2	2:B:1059:VAL:HG23	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:LYS:HB3	1:A:133:LYS:HE3	1.75	0.44
1:A:143:GLU:O	1:A:146:THR:HG22	2.17	0.44
1:A:74:MET:HE2	1:A:125:THR:HG22	1.99	0.44
1:A:80:LYS:HD2	1:A:118:GLY:HA2	1.98	0.44
1:A:168:MET:CE	1:A:237:MET:HE1	2.48	0.44
1:A:176:ASP:O	1:A:179:GLN:HG3	2.18	0.44
1:A:64:THR:HG23	1:A:64:THR:O	2.18	0.44
2:B:987:ARG:O	2:B:991:ILE:HG13	2.18	0.44
2:B:984:VAL:C	2:B:986:GLU:H	2.21	0.43
2:B:997:ILE:O	2:B:1001:VAL:HG13	2.18	0.43
1:A:53:ASN:HB2	3:A:372:HOH:O	2.18	0.43
1:A:56:ARG:CG	1:A:56:ARG:NH1	2.80	0.43
1:A:143:GLU:O	1:A:146:THR:HB	2.19	0.43
2:B:895:ASN:OD1	2:B:1024:VAL:HG21	2.17	0.43
1:A:58:GLY:HA2	1:A:126:PHE:HZ	1.83	0.43
1:A:70:LEU:O	1:A:74:MET:HB2	2.18	0.43
1:A:102:VAL:N	1:A:103:PRO:CD	2.81	0.43
1:A:58:GLY:HA2	1:A:126:PHE:CZ	2.53	0.43
1:A:65:THR:HG21	1:A:70:LEU:CD2	2.43	0.43
1:A:65:THR:O	1:A:71:LYS:NZ	2.46	0.43
1:A:90:GLN:HE21	1:A:107:TYR:HE2	1.65	0.42
1:A:98:ASP:C	1:A:100:TYR:H	2.22	0.42
1:A:198:VAL:HG23	1:A:240:GLU:HB3	2.01	0.42
1:A:61:THR:C	1:A:63:GLN:H	2.21	0.42
1:A:179:GLN:NE2	1:A:180:GLN:HG3	2.34	0.42
1:A:258:TRP:HZ2	2:B:1029:ASN:HD22	1.67	0.42
2:B:912:TRP:HH2	3:B:83:HOH:O	2.02	0.42
1:A:202:LEU:HB3	1:A:203:PRO:HD3	2.00	0.42
2:B:898:MET:HE1	2:B:933:MET:O	2.19	0.42
2:B:966:LYS:HE3	2:B:985:CYS:HB3	2.01	0.42
1:A:179:GLN:O	1:A:188:ARG:CD	2.67	0.42
1:A:65:THR:HG23	1:A:67:ASP:H	1.84	0.42
1:A:153:THR:CG2	1:A:155:GLU:HB3	2.50	0.42
1:A:168:MET:HE1	1:A:237:MET:CE	2.50	0.42
1:A:153:THR:CG2	1:A:155:GLU:N	2.84	0.41
1:A:232:PHE:CD2	1:A:236:LYS:HD2	2.55	0.41
2:B:965:ALA:HB3	2:B:985:CYS:SG	2.60	0.41
1:A:65:THR:HG23	1:A:67:ASP:N	2.36	0.41
2:B:1062:THR:HA	2:B:1063:PRO:HD2	1.92	0.41
1:A:243:GLU:OE1	1:A:243:GLU:HA	2.21	0.41
2:B:916:GLY:HA2	3:B:160:HOH:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:GLU:HA	3:A:328:HOH:O	2.21	0.41
2:B:1058:TRP:NE1	3:B:123:HOH:O	2.32	0.41
2:B:926[A]:MET:HG2	2:B:957:ALA:HB3	2.03	0.40
1:A:258:TRP:HE1	2:B:1029:ASN:ND2	2.19	0.40
1:A:147:VAL:CG1	1:A:160:TYR:CE1	3.03	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	261/262 (100%)	252 (97%)	9 (3%)	0	100	100
2	B	174/185 (94%)	166 (95%)	7 (4%)	1 (1%)	25	27
All	All	435/447 (97%)	418 (96%)	16 (4%)	1 (0%)	47	56

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	939	GLY

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.

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	234/233 (100%)	213 (91%)	21 (9%)	9 8
2	B	150/156 (96%)	123 (82%)	27 (18%)	1 1
All	All	384/389 (99%)	336 (88%)	48 (12%)	4 4

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-2	HIS
1	A	-1	HIS
1	A	18	GLN
1	A	56	ARG
1	A	63	GLN
1	A	64	THR
1	A	65	THR
1	A	66	GLU
1	A	74	MET
1	A	87	LYS
1	A	115	ILE
1	A	117	SER
1	A	122	LEU
1	A	146	THR
1	A	147	VAL
1	A	150	VAL
1	A	152	GLU
1	A	153	THR
1	A	210	LYS
1	A	228	LYS
1	A	254	ASP
2	B	882	ASP
2	B	888	GLN
2	B	889	LYS
2	B	894	ILE
2	B	898	MET
2	B	904	GLN
2	B	910	ARG
2	B	913	SER
2	B	928	LEU
2	B	938	ARG
2	B	941	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	944	LYS
2	B	956	LYS
2	B	963	ARG
2	B	970	LYS
2	B	971	GLN
2	B	980	ASN
2	B	981	LEU
2	B	987	ARG
2	B	996	LYS
2	B	1005	MET
2	B	1015	GLU
2	B	1035	LYS
2	B	1046	ILE
2	B	1047	LYS
2	B	1048	ILE
2	B	1062	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-1	HIS
1	A	63	GLN
1	A	184	HIS
1	A	185	GLN
1	A	187	HIS
2	B	888	GLN
2	B	895	ASN
2	B	980	ASN
2	B	1018	GLN
2	B	1028	GLN
2	B	1029	ASN
2	B	1032	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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.