Full wwPDB X-ray Structure Validation Report (i)

Feb 28, 2014 – 03:27 AM GMT

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)

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1 Overall quality at a glance (i)

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	Percentile Ranks	Value
Clashscore		30
Ramachandran outliers		0.2%
Sidechain outliers		12.6%

Worse — *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
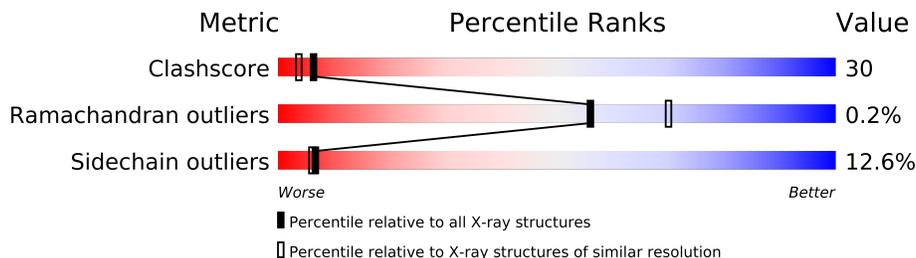
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1064 (2.38-2.34)
Ramachandran outliers	78287	1048 (2.38-2.34)
Sidechain outliers	78261	1049 (2.38-2.34)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	262	
2	B	185	

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 3660 atoms, of which 0 are hydrogen and 0 are deuterium.

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 2070	C 1302	N 357	O 397	S 14	0	1	0

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 1386	C 852	N 256	O 264	S 14	0	2	0

- Molecule 3 is water.

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

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

- Molecule 1: Vinculin

Chain A:
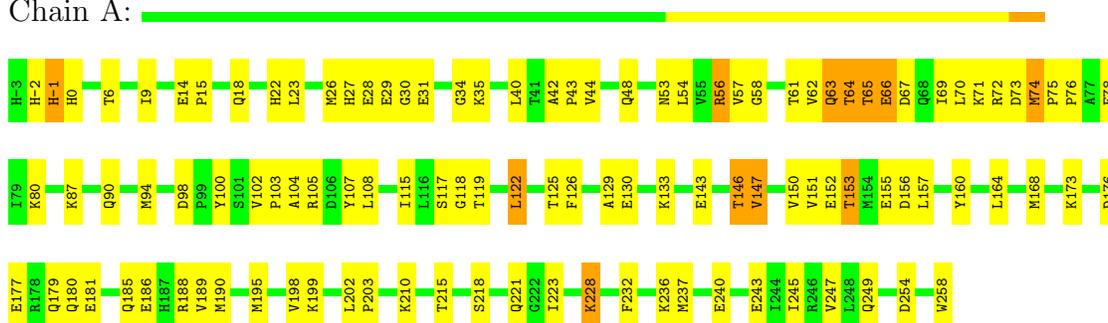
- Molecule 2: VCL protein

Chain B:
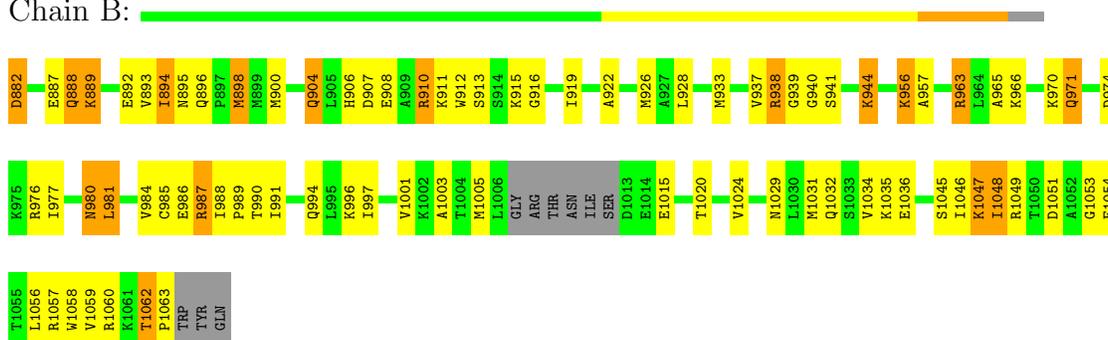
4 Data and refinement statistics ⓘ

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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   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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 30.

All (211) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:94:MET:HE2	1:A:104:ALA:HB2	1.19	1.13

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Atom-1	Atom-2	Distance(Å)	Clash(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
2:B:1049:ARG:HE	2:B:1051:ASP:HB2	1.29	0.97
1:A:153:THR:HG22	1:A:156:ASP:H	1.30	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:926[B]:MET:HE3	2:B:1031:MET:CE	2.04	0.87
2:B:895:ASN:HD22	2:B:898:MET:H	1.22	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:N	2:B:980:ASN:HD22	1.72	0.84
2:B:937:VAL:CG1	2:B:1020:THR:HG23	2.08	0.84
1:A:228:LYS:HD3	1:A:228:LYS:O	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:H	2:B:980:ASN:HD22	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
2:B:888:GLN:CG	2:B:894:ILE:HD13	2.15	0.76
1:A:245:ILE:O	1:A:249:GLN:HG3	1.85	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:926[B]:MET:HE1	2:B:1034:VAL:HG21	1.76	0.67
2:B:900[A]:MET:O	2:B:904:GLN:HG2	1.93	0.67
2:B:976:ARG:O	2:B:980:ASN:ND2	2.28	0.67
2:B:938:ARG:HH11	2:B:938:ARG:CG	2.08	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:232:PHE:CE2	1:A:236:LYS:HD2	2.30	0.66
2:B:926[B]:MET:CE	2:B:1034:VAL:HG21	2.26	0.66
2:B:919:ILE:HD12	2:B:1056:LEU:HD11	1.76	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:980:ASN:N	2:B:980:ASN:ND2	2.45	0.65
2:B:944:LYS:HD3	2:B:1003:ALA:O	1.96	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:HB3	2:B:938:ARG:HH11	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
2:B:910:ARG:CB	2:B:910:ARG:HH11	2.13	0.62
1:A:58:GLY:CA	1:A:126:PHE:HZ	2.13	0.62
2:B:938:ARG:HH11	2:B:938:ARG:HG3	1.65	0.62
1:A:195:MET:O	1:A:199:LYS:HG3	1.98	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:HG2	2:B:963:ARG:NH1	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:HB2	2:B:910:ARG:HH11	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:898:MET:CE	2:B:933:MET:HB3	2.34	0.57
1:A:56:ARG:HG3	1:A:56:ARG:HH11	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:ND2	2:B:980:ASN:H	2.00	0.55
2:B:898:MET:HE3	2:B:933:MET:HB3	1.89	0.55
1:A:56:ARG:CG	1:A:56:ARG:HH11	2.19	0.55
1:A:56:ARG:NH1	1:A:56:ARG:HB2	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:62:VAL:HG12	1:A:62:VAL:O	2.09	0.53
1:A:27:HIS:HB2	1:A:108:LEU:CD2	2.36	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
2:B:1032:GLN:NE2	3:B:120:HOH:O	2.42	0.53
1:A:243:GLU:O	1:A:247:VAL:HG23	2.08	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:147:VAL:CG1	1:A:160:TYR:HE1	2.20	0.52
1:A:6:THR:OG1	1:A:9:ILE:HG13	2.09	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:70:LEU:HD13	1:A:129:ALA:HB2	1.92	0.50
1:A:57:VAL:HG12	1:A:57:VAL:O	2.11	0.50
1:A:42:ALA:HB3	1:A:43:PRO:CD	2.42	0.50
1:A:102:VAL:N	1:A:103:PRO:HD2	2.27	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:153:THR:HG23	1:A:155:GLU:N	2.25	0.46
1:A:42:ALA:HB3	1:A:43:PRO:HD3	1.96	0.46
1:A:54:LEU:CD2	1:A:119:THR:HG23	2.45	0.46
2:B:1047:LYS:HB3	2:B:1047:LYS:HE2	1.42	0.46
1:A:168:MET:CE	1:A:237:MET:CE	2.93	0.46
1:A:74:MET:CE	1:A:126:PHE:CE2	2.99	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: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
2:B:898:MET:HE1	2:B:933:MET:C	2.36	0.45
1:A:-1:HIS:CD2	2:B:987:ARG:CZ	2.99	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
1:A:143:GLU:O	1:A:146:THR:HG22	2.17	0.44
1:A:133:LYS:HE3	1:A:133:LYS:HB3	1.75	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
2:B:895:ASN:OD1	2:B:1024:VAL:HG21	2.17	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
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:198:VAL:HG23	1:A:240:GLU:HB3	2.01	0.42
1:A:98:ASP:C	1:A:100:TYR:H	2.22	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
1:A:61:THR:C	1:A:63:GLN:H	2.21	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
2:B:1058:TRP:NE1	3:B:123:HOH:O	2.32	0.41
1:A:28:GLU:HA	3:A:328:HOH:O	2.21	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

5.3.1 Protein backbone ⓘ

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%)	33	39
All	All	435/447 (97%)	418 (96%)	16 (4%)	1 (0%)	56	70

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	939	GLY

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	234/233 (100%)	213 (91%)	21 (9%)	14	14
2	B	150/156 (96%)	123 (82%)	27 (18%)	2	2
All	All	384/389 (99%)	336 (88%)	48 (12%)	7	6

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
2	B	1062	THR

Some 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 ⓘ

There are no RNA chains 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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.