



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 06:16 PM GMT

PDB ID : 1Q1P  
Title : E-Cadherin activation  
Authors : Haussinger, D.; Stetefeld, J.  
Deposited on : 2003-07-22  
Resolution : 3.20 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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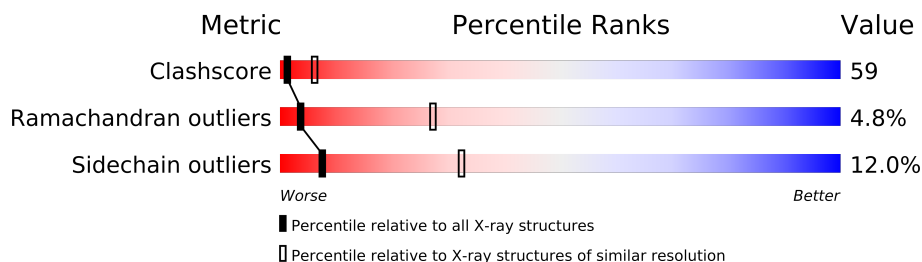
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.20 Å.

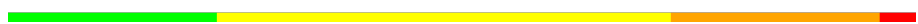
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)

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  $\geq 3$ , 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	212	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1864 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 Epithelial-cadherin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	0	0
			1628	1023	266	335	4			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Ca	0	0
			3	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	233	Total	O	0	0
			233	233		

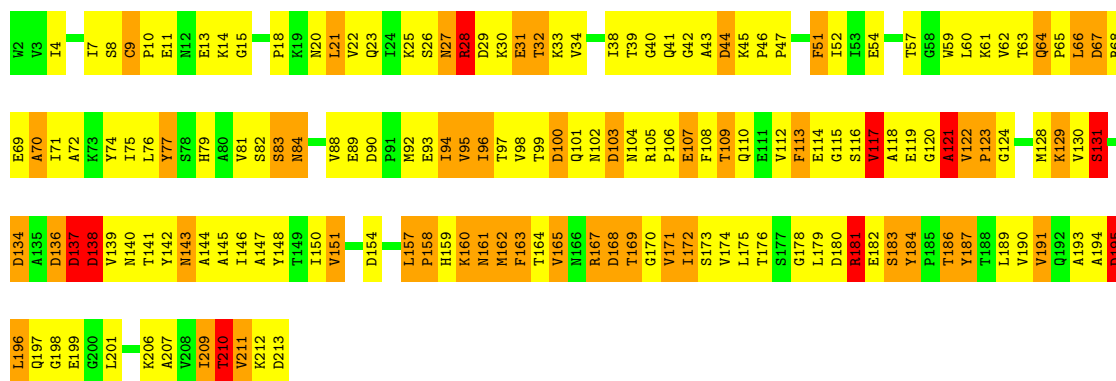
### 3 Residue-property plots

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: Epithelial-cadherin

Chain A: 



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	129.20Å 48.60Å 58.67Å 90.00° 113.93° 90.00°	Depositor
Resolution (Å)	20.00 – 3.20	Depositor
% Data completeness (in resolution range)	100.0 (20.00-3.20)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.13	Depositor
Refinement program	REFMAC 5	Depositor
R, $R_{free}$	0.259 , 0.305	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1864	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	1.97	32/1659 (1.9%)	1.54	28/2263 (1.2%)

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	210	THR	CB-OG1	14.26	1.71	1.43
1	A	187	TYR	CE1-CZ	-10.57	1.24	1.38
1	A	9	CYS	CB-SG	-9.35	1.66	1.82
1	A	187	TYR	CG-CD2	-8.90	1.27	1.39
1	A	107	GLU	CD-OE1	8.71	1.35	1.25
1	A	117	VAL	CB-CG1	-8.46	1.35	1.52
1	A	163	PHE	CE1-CZ	-8.06	1.22	1.37
1	A	107	GLU	CD-OE2	7.69	1.34	1.25
1	A	187	TYR	CE2-CZ	-7.40	1.28	1.38
1	A	169	THR	CA-CB	-7.18	1.34	1.53
1	A	70	ALA	CA-CB	-6.63	1.38	1.52
1	A	131	SER	CA-CB	-6.54	1.43	1.52
1	A	148	TYR	CG-CD2	-6.50	1.30	1.39
1	A	160	LYS	CD-CE	6.33	1.67	1.51
1	A	191	VAL	CA-CB	-6.10	1.42	1.54
1	A	171	VAL	CB-CG1	-6.05	1.40	1.52
1	A	209	ILE	C-O	-5.99	1.11	1.23
1	A	211	VAL	CB-CG1	-5.77	1.40	1.52
1	A	92	MET	CG-SD	-5.75	1.66	1.81
1	A	163	PHE	CG-CD2	-5.71	1.30	1.38
1	A	51	PHE	CD1-CE1	-5.69	1.27	1.39
1	A	113	PHE	CG-CD2	-5.67	1.30	1.38
1	A	121	ALA	CA-CB	-5.24	1.41	1.52
1	A	113	PHE	CD2-CE2	-5.24	1.28	1.39
1	A	112	VAL	CB-CG1	-5.21	1.42	1.52
1	A	172	ILE	CA-CB	-5.18	1.43	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	81	VAL	C-O	-5.12	1.13	1.23
1	A	31	GLU	CD-OE1	5.06	1.31	1.25
1	A	77	TYR	CE2-CZ	-5.04	1.31	1.38
1	A	184	TYR	CE1-CZ	-5.04	1.31	1.38
1	A	77	TYR	CG-CD1	-5.04	1.32	1.39
1	A	129	LYS	C-O	-5.01	1.13	1.23

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	LYS	CD-CE-NZ	9.66	133.93	111.70
1	A	213	ASP	CA-C-O	9.48	140.01	120.10
1	A	210	THR	OG1-CB-CG2	-8.23	91.07	110.00
1	A	134	ASP	CB-CG-OD2	8.20	125.68	118.30
1	A	154	ASP	CB-CG-OD2	8.14	125.62	118.30
1	A	137	ASP	CB-CG-OD2	7.52	125.07	118.30
1	A	103	ASP	CB-CG-OD2	7.51	125.06	118.30
1	A	44	ASP	CB-CG-OD2	6.77	124.39	118.30
1	A	168	ASP	CB-CG-OD1	6.46	124.12	118.30
1	A	186	THR	OG1-CB-CG2	-6.42	95.24	110.00
1	A	169	THR	OG1-CB-CG2	-6.18	95.78	110.00
1	A	28	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	A	138	ASP	CB-CG-OD2	6.12	123.81	118.30
1	A	176	THR	OG1-CB-CG2	-6.07	96.03	110.00
1	A	137	ASP	OD1-CG-OD2	-6.05	111.80	123.30
1	A	134	ASP	OD1-CG-OD2	-5.97	111.95	123.30
1	A	167	ARG	NE-CZ-NH1	-5.83	117.39	120.30
1	A	136	ASP	CB-CG-OD2	5.75	123.47	118.30
1	A	154	ASP	OD1-CG-OD2	-5.55	112.76	123.30
1	A	157	LEU	CB-CG-CD1	-5.46	101.71	111.00
1	A	100	ASP	CB-CG-OD1	5.40	123.16	118.30
1	A	165	VAL	CB-CA-C	-5.38	101.18	111.40
1	A	137	ASP	CB-CG-OD1	5.33	123.10	118.30
1	A	168	ASP	OD1-CG-OD2	-5.21	113.40	123.30
1	A	158	PRO	N-CD-CG	-5.19	95.42	103.20
1	A	195	ASP	CB-CG-OD2	5.16	122.95	118.30
1	A	67	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	162	MET	CG-SD-CE	-5.04	92.14	100.20

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	1628	0	1595	190	1
2	A	3	0	0	0	0
3	A	233	0	0	25	0
All	All	1864	0	1595	190	1

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 59.

All (190) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:210:THR:OG1	1:A:210:THR:CB	1.71	1.36
1:A:109:THR:HG23	1:A:131:SER:O	1.43	1.18
1:A:28:ARG:NH1	1:A:88:VAL:HB	1.72	1.04
1:A:11:GLU:OE2	1:A:101:GLN:N	1.95	0.98
1:A:13:GLU:OE1	3:A:824:HOH:O	1.81	0.97
1:A:31:GLU:HB3	3:A:751:HOH:O	1.67	0.94
1:A:39:THR:HA	1:A:44:ASP:OD1	1.73	0.89
1:A:129:LYS:HG3	1:A:170:GLY:O	1.74	0.86
1:A:25:LYS:HE3	1:A:29:ASP:OD1	1.76	0.86
1:A:165:VAL:O	1:A:165:VAL:HG13	1.76	0.86
1:A:32:THR:OG1	1:A:33:LYS:N	2.01	0.85
1:A:186:THR:HG22	1:A:210:THR:OG1	1.77	0.84
1:A:210:THR:OG1	1:A:210:THR:CG2	2.25	0.83
1:A:142:TYR:O	1:A:144:ALA:N	2.12	0.82
1:A:183:SER:C	1:A:184:TYR:CD1	2.52	0.82
1:A:189:LEU:HB2	1:A:207:ALA:HB3	1.63	0.81
1:A:122:VAL:HG23	1:A:123:PRO:HD2	1.63	0.81
1:A:210:THR:O	1:A:210:THR:HG22	1.78	0.80
1:A:120:GLY:O	1:A:121:ALA:O	1.98	0.80
1:A:75:ILE:O	3:A:773:HOH:O	2.00	0.79
1:A:134:ASP:OD2	1:A:144:ALA:HA	1.82	0.79
1:A:190:VAL:O	1:A:190:VAL:HG12	1.81	0.79
1:A:28:ARG:HH11	1:A:88:VAL:HB	1.44	0.79
1:A:28:ARG:H	1:A:28:ARG:HD2	1.49	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:67:ASP:OD1	1:A:69:GLU:HB2	1.85	0.77
1:A:184:TYR:N	1:A:184:TYR:CD1	2.47	0.77
1:A:206:LYS:HD2	3:A:715:HOH:O	1.84	0.76
1:A:107:GLU:HG3	3:A:746:HOH:O	1.86	0.75
1:A:68:ARG:HD3	1:A:100:ASP:HB2	1.69	0.75
1:A:31:GLU:CB	3:A:751:HOH:O	2.28	0.74
1:A:119:GLU:O	1:A:120:GLY:C	2.25	0.73
1:A:183:SER:C	1:A:184:TYR:HD1	1.93	0.72
1:A:151:VAL:HG23	1:A:190:VAL:HG12	1.71	0.71
1:A:165:VAL:O	1:A:165:VAL:CG1	2.40	0.70
1:A:104:ASN:HB2	1:A:136:ASP:OD2	1.92	0.70
1:A:195:ASP:O	1:A:196:LEU:CB	2.39	0.69
1:A:128:MET:HG3	1:A:172:ILE:HD12	1.74	0.69
1:A:107:GLU:CG	3:A:746:HOH:O	2.40	0.69
1:A:210:THR:C	3:A:726:HOH:O	2.30	0.68
1:A:178:GLY:O	1:A:179:LEU:C	2.31	0.68
1:A:82:SER:O	1:A:84:ASN:N	2.27	0.68
1:A:54:GLU:OE1	1:A:61:LYS:HE3	1.93	0.67
1:A:183:SER:O	1:A:184:TYR:HD1	1.78	0.67
1:A:163:PHE:CE1	1:A:209:ILE:HG21	2.30	0.66
1:A:195:ASP:O	1:A:196:LEU:HB2	1.97	0.65
1:A:39:THR:HG23	1:A:79:HIS:NE2	2.12	0.64
1:A:167:ARG:HH11	1:A:167:ARG:HB3	1.62	0.64
1:A:38:ILE:HG13	1:A:43:ALA:HB1	1.80	0.64
1:A:25:LYS:CG	1:A:26:SER:H	2.10	0.63
1:A:107:GLU:O	1:A:108:PHE:C	2.34	0.63
1:A:199:GLU:HG3	3:A:841:HOH:O	1.97	0.63
1:A:25:LYS:CG	1:A:26:SER:N	2.62	0.62
1:A:150:ILE:HG21	1:A:189:LEU:HD22	1.82	0.62
1:A:25:LYS:HG2	1:A:26:SER:N	2.15	0.62
1:A:18:PRO:HB3	1:A:63:THR:HG22	1.82	0.61
1:A:51:PHE:CZ	1:A:96:ILE:HD12	2.36	0.61
1:A:88:VAL:HG23	1:A:89:GLU:HG2	1.82	0.61
1:A:104:ASN:HB2	1:A:136:ASP:CG	2.20	0.61
1:A:39:THR:CA	1:A:44:ASP:OD1	2.47	0.60
1:A:22:VAL:HG22	1:A:23:GLN:H	1.66	0.60
1:A:151:VAL:CG2	1:A:190:VAL:HG12	2.32	0.60
1:A:64:GLN:HB2	1:A:65:PRO:CD	2.32	0.59
1:A:142:TYR:O	1:A:145:ALA:N	2.30	0.59
1:A:128:MET:CG	1:A:172:ILE:HD12	2.32	0.59
1:A:104:ASN:HB2	1:A:136:ASP:OD1	2.03	0.59
1:A:179:LEU:HD22	1:A:211:VAL:HG21	1.84	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:181:ARG:NE	3:A:816:HOH:O	2.36	0.57
1:A:122:VAL:O	1:A:124:GLY:N	2.37	0.57
1:A:110:GLN:HB2	1:A:113:PHE:CE2	2.39	0.57
1:A:167:ARG:HH11	1:A:167:ARG:CB	2.18	0.57
1:A:26:SER:O	1:A:28:ARG:N	2.38	0.56
1:A:7:ILE:HD12	1:A:94:ILE:HG23	1.87	0.56
1:A:21:LEU:HD11	1:A:51:PHE:HE1	1.70	0.56
1:A:115:GLY:HA3	1:A:128:MET:SD	2.46	0.56
1:A:38:ILE:HD12	1:A:76:LEU:HD13	1.87	0.56
1:A:28:ARG:HG2	1:A:28:ARG:HH11	1.71	0.55
1:A:163:PHE:CZ	1:A:209:ILE:HG21	2.41	0.55
1:A:20:ASN:HB3	1:A:59:TRP:CZ3	2.42	0.55
1:A:151:VAL:HG23	1:A:190:VAL:O	2.07	0.54
1:A:179:LEU:HD22	1:A:211:VAL:CG2	2.36	0.54
1:A:137:ASP:CG	1:A:140:ASN:H	2.10	0.54
1:A:28:ARG:HD2	1:A:28:ARG:N	2.18	0.54
1:A:130:VAL:HG23	1:A:130:VAL:O	2.07	0.54
1:A:108:PHE:CZ	1:A:193:ALA:N	2.76	0.53
1:A:54:GLU:HB2	1:A:57:THR:OG1	2.07	0.53
1:A:62:VAL:HG13	1:A:62:VAL:O	2.08	0.53
1:A:137:ASP:OD2	1:A:140:ASN:N	2.42	0.53
1:A:100:ASP:CG	1:A:101:GLN:N	2.62	0.53
1:A:182:GLU:OE2	3:A:813:HOH:O	2.19	0.53
1:A:129:LYS:HG3	1:A:170:GLY:C	2.28	0.52
1:A:162:MET:O	1:A:175:LEU:HB3	2.08	0.52
1:A:122:VAL:HG23	1:A:123:PRO:CD	2.38	0.52
1:A:8:SER:HA	1:A:97:THR:O	2.09	0.52
1:A:180:ASP:O	1:A:182:GLU:N	2.42	0.52
1:A:206:LYS:CD	3:A:715:HOH:O	2.49	0.52
1:A:146:ILE:CG2	1:A:147:ALA:N	2.72	0.51
1:A:30:LYS:HG2	3:A:776:HOH:O	2.09	0.51
1:A:117:VAL:HG11	1:A:179:LEU:HD13	1.92	0.51
1:A:68:ARG:CD	1:A:100:ASP:HB2	2.37	0.51
1:A:138:ASP:HA	1:A:144:ALA:HB3	1.93	0.51
1:A:22:VAL:HG22	1:A:23:GLN:N	2.26	0.51
1:A:102:ASN:OD1	1:A:143:ASN:O	2.29	0.51
1:A:211:VAL:N	3:A:726:HOH:O	2.43	0.51
1:A:164:THR:HB	1:A:175:LEU:HD13	1.94	0.50
1:A:146:ILE:HG22	1:A:147:ALA:N	2.25	0.50
1:A:137:ASP:OD2	1:A:140:ASN:HB2	2.12	0.50
1:A:13:GLU:O	1:A:65:PRO:HG3	2.11	0.50
1:A:39:THR:CG2	1:A:79:HIS:NE2	2.75	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:209:ILE:O	1:A:209:ILE:HG22	2.11	0.50
1:A:129:LYS:HD2	1:A:169:THR:O	2.12	0.49
1:A:104:ASN:C	1:A:201:LEU:HD12	2.32	0.49
1:A:181:ARG:HH11	1:A:181:ARG:HG3	1.78	0.49
1:A:21:LEU:HB2	1:A:60:LEU:HB3	1.94	0.49
1:A:72:ALA:O	1:A:98:VAL:HG23	2.13	0.49
1:A:41:GLN:HG2	1:A:46:PRO:O	2.13	0.49
1:A:40:GLY:N	1:A:44:ASP:OD1	2.45	0.48
1:A:60:LEU:HD11	1:A:94:ILE:HD13	1.96	0.48
1:A:30:LYS:HB3	3:A:847:HOH:O	2.12	0.48
1:A:173:SER:O	1:A:174:VAL:C	2.50	0.48
1:A:44:ASP:O	1:A:45:LYS:HG3	2.13	0.48
1:A:27:ASN:C	1:A:29:ASP:H	2.17	0.48
1:A:68:ARG:HD3	1:A:100:ASP:CB	2.41	0.47
1:A:60:LEU:O	1:A:61:LYS:HG3	2.14	0.47
1:A:117:VAL:HG22	1:A:118:ALA:H	1.80	0.47
1:A:105:ARG:HG2	1:A:201:LEU:HD13	1.96	0.47
1:A:116:SER:N	3:A:734:HOH:O	2.16	0.47
1:A:167:ARG:CG	1:A:168:ASP:H	2.28	0.47
1:A:181:ARG:HB2	1:A:211:VAL:HG12	1.97	0.46
1:A:160:LYS:O	1:A:161:ASN:HB2	2.16	0.46
1:A:11:GLU:OE2	1:A:100:ASP:HA	2.16	0.46
1:A:102:ASN:OD1	1:A:143:ASN:HB3	2.15	0.46
1:A:114:GLU:CD	3:A:807:HOH:O	2.54	0.46
1:A:42:GLY:HA2	1:A:47:PRO:HG2	1.98	0.45
1:A:66:LEU:HD22	1:A:74:TYR:CE1	2.51	0.45
1:A:76:LEU:HD23	1:A:76:LEU:HA	1.69	0.45
1:A:163:PHE:CE1	1:A:209:ILE:HD13	2.51	0.45
1:A:167:ARG:CG	1:A:168:ASP:N	2.79	0.45
1:A:187:TYR:HE1	3:A:711:HOH:O	1.98	0.45
1:A:7:ILE:HA	3:A:826:HOH:O	2.17	0.45
1:A:158:PRO:O	1:A:159:HIS:CG	2.70	0.45
1:A:108:PHE:CZ	1:A:193:ALA:HB2	2.51	0.45
1:A:95:VAL:HG12	1:A:95:VAL:O	2.16	0.45
1:A:181:ARG:CD	3:A:816:HOH:O	2.65	0.45
1:A:150:ILE:CG2	1:A:189:LEU:HD22	2.46	0.44
1:A:18:PRO:HB3	1:A:63:THR:CG2	2.47	0.44
1:A:130:VAL:O	1:A:130:VAL:CG2	2.65	0.44
1:A:25:LYS:HG3	1:A:26:SER:H	1.82	0.44
1:A:107:GLU:HG2	3:A:746:HOH:O	2.14	0.44
1:A:108:PHE:HZ	1:A:193:ALA:N	2.16	0.44
1:A:94:ILE:HG22	1:A:94:ILE:O	2.15	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:137:ASP:C	1:A:139:VAL:H	2.20	0.44
1:A:184:TYR:HB2	3:A:711:HOH:O	2.17	0.43
1:A:137:ASP:C	1:A:139:VAL:N	2.71	0.43
1:A:7:ILE:O	1:A:96:ILE:HA	2.18	0.43
1:A:106:PRO:HG2	1:A:195:ASP:HB3	2.00	0.43
1:A:51:PHE:CE2	1:A:96:ILE:HD12	2.53	0.43
1:A:76:LEU:HG	1:A:96:ILE:HD11	2.01	0.43
1:A:10:PRO:HA	1:A:99:THR:OG1	2.19	0.43
1:A:150:ILE:HG21	1:A:189:LEU:CD2	2.48	0.43
1:A:52:ILE:HG13	1:A:61:LYS:HB2	2.01	0.43
1:A:196:LEU:O	1:A:197:GLN:HB2	2.19	0.42
1:A:158:PRO:C	1:A:159:HIS:ND1	2.72	0.42
1:A:38:ILE:HG21	1:A:38:ILE:HD13	1.69	0.42
1:A:14:LYS:O	1:A:15:GLY:C	2.58	0.42
1:A:109:THR:CG2	1:A:131:SER:O	2.38	0.42
1:A:82:SER:C	1:A:84:ASN:N	2.73	0.42
1:A:21:LEU:HD11	1:A:51:PHE:CE1	2.51	0.42
1:A:163:PHE:CD2	1:A:163:PHE:N	2.87	0.42
1:A:77:TYR:CE1	1:A:93:GLU:HB2	2.55	0.42
1:A:43:ALA:HB2	1:A:76:LEU:HD21	2.02	0.41
1:A:140:ASN:C	1:A:141:THR:HG23	2.40	0.41
1:A:159:HIS:CE1	3:A:876:HOH:O	2.73	0.41
1:A:31:GLU:HB2	3:A:751:HOH:O	2.08	0.41
1:A:105:ARG:NH1	1:A:105:ARG:HG2	2.36	0.41
1:A:82:SER:O	1:A:83:SER:C	2.59	0.41
1:A:102:ASN:HB2	1:A:143:ASN:OD1	2.20	0.41
1:A:25:LYS:HG2	1:A:26:SER:H	1.77	0.41
1:A:70:ALA:C	1:A:71:ILE:HG13	2.41	0.41
1:A:167:ARG:CB	1:A:167:ARG:NH1	2.84	0.41
1:A:211:VAL:HA	3:A:726:HOH:O	2.19	0.41
1:A:9:CYS:N	1:A:97:THR:O	2.47	0.41
1:A:194:ALA:O	1:A:198:GLY:HA2	2.21	0.41
1:A:103:ASP:OD1	1:A:103:ASP:N	2.54	0.41
1:A:68:ARG:HG3	1:A:98:VAL:O	2.20	0.41
1:A:119:GLU:N	1:A:212:LYS:O	2.48	0.41
1:A:82:SER:C	1:A:84:ASN:H	2.24	0.41
1:A:164:THR:CB	1:A:175:LEU:HD13	2.51	0.41
1:A:183:SER:O	1:A:184:TYR:CD1	2.63	0.40
1:A:129:LYS:HD3	1:A:171:VAL:HG22	2.02	0.40
1:A:157:LEU:HB2	1:A:184:TYR:CE2	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:83:SER:O	1:A:164:THR:OG1[3.444]	1.96	0.24

## 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	210/212 (99%)	176 (84%)	24 (11%)	10 (5%)	4	27

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	121	ALA
1	A	143	ASN
1	A	21	LEU
1	A	83	SER
1	A	137	ASP
1	A	181	ARG
1	A	123	PRO
1	A	161	ASN
1	A	64	GLN

### 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	183/183 (100%)	161 (88%)	22 (12%)	7	32

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	28	ARG
1	A	32	THR
1	A	34	VAL
1	A	66	LEU
1	A	84	ASN
1	A	90	ASP
1	A	94	ILE
1	A	95	VAL
1	A	96	ILE
1	A	109	THR
1	A	117	VAL
1	A	122	VAL
1	A	131	SER
1	A	138	ASP
1	A	151	VAL
1	A	181	ARG
1	A	183	SER
1	A	191	VAL
1	A	195	ASP
1	A	196	LEU
1	A	210	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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.