



Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 08:15 pm BST

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 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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) : 2.11

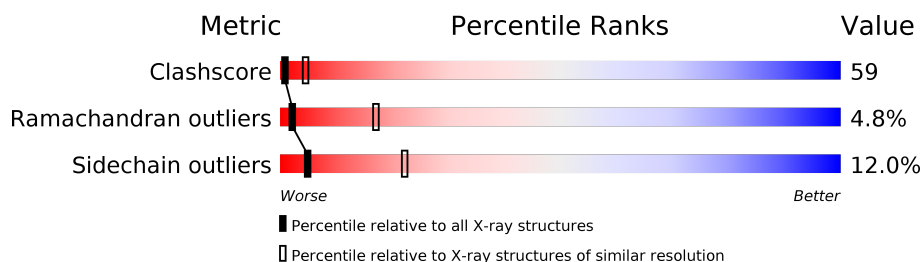
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)

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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	212	<div> <div style="width: 23%; background-color: green;"></div> <div style="width: 50%; background-color: yellow;"></div> <div style="width: 23%; background-color: orange;"></div> <div style="width: 4%; background-color: red;"></div> <div style="width: 4%; background-color: grey;"></div> </div> <div>23% 50% 23% .</div>

2 Entry composition

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

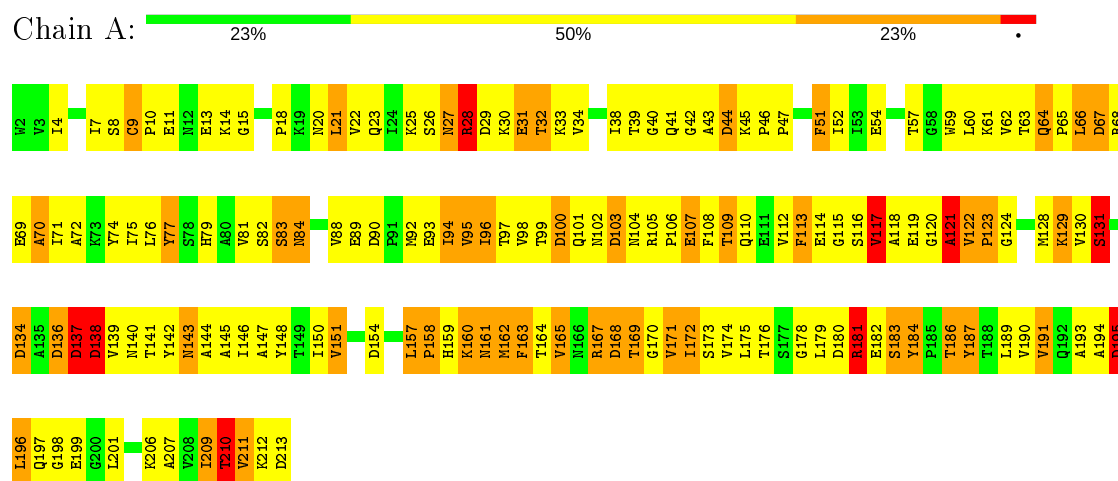
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	233	Total	O	0	0
			233	233		

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 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: Epithelial-cadherin



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	129.20 Å 48.60 Å 58.67 Å 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 5.0	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 ²)	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 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	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

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 59.

All (190) 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: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:HG12	1:A:190:VAL:O	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	Interatomic distance (Å)	Clash overlap (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:104:ASN:HB2	1:A:136:ASP:OD2	1.92	0.70
1:A:165:VAL:O	1:A:165:VAL:CG1	2.40	0.70
1:A:128:MET:HG3	1:A:172:ILE:HD12	1.74	0.69
1:A:195:ASP:O	1:A:196:LEU:CB	2.39	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:167:ARG:HH11	1:A:167:ARG:HB3	1.62	0.64
1:A:39:THR:HG23	1:A:79:HIS:NE2	2.12	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:22:VAL:HG22	1:A:23:GLN:H	1.66	0.60
1:A:39:THR:CA	1:A:44:ASP:OD1	2.47	0.60
1:A:151:VAL:CG2	1:A:190:VAL:HG12	2.32	0.60
1:A:142:TYR:O	1:A:145:ALA:N	2.30	0.59
1:A:64:GLN:HB2	1:A:65:PRO:CD	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:LEU:HD22	1:A:211:VAL:HG21	1.84	0.58
1:A:181:ARG:NE	3:A:816:HOH:O	2.36	0.57
1:A:110:GLN:HB2	1:A:113:PHE:CE2	2.39	0.57
1:A:122:VAL:O	1:A:124:GLY:N	2.37	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:163:PHE:CZ	1:A:209:ILE:HG21	2.41	0.55
1:A:28:ARG:HG2	1:A:28:ARG:HH11	1.71	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:130:VAL:O	1:A:130:VAL:HG23	2.07	0.54
1:A:28:ARG:HD2	1:A:28:ARG:N	2.18	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:68:ARG:CD	1:A:100:ASP:HB2	2.37	0.51
1:A:117:VAL:HG11	1:A:179:LEU:HD13	1.92	0.51
1:A:138:ASP:HA	1:A:144:ALA:HB3	1.93	0.51
1:A:102:ASN:OD1	1:A:143:ASN:O	2.29	0.51
1:A:22:VAL:HG22	1:A:23:GLN:N	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:GLU:O	1:A:65:PRO:HG3	2.11	0.50
1:A:209:ILE:O	1:A:209:ILE:HG22	2.11	0.50
1:A:39:THR:CG2	1:A:79:HIS:NE2	2.75	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:41:GLN:HG2	1:A:46:PRO:O	2.13	0.49
1:A:72:ALA:O	1:A:98:VAL:HG23	2.13	0.49
1:A:40:GLY:N	1:A:44:ASP:OD1	2.45	0.48
1:A:30:LYS:HB3	3:A:847:HOH:O	2.12	0.48
1:A:60:LEU:HD11	1:A:94:ILE:HD13	1.96	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:105:ARG:HG2	1:A:201:LEU:HD13	1.96	0.47
1:A:117:VAL:HG22	1:A:118:ALA:H	1.80	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:114:GLU:CD	3:A:807:HOH:O	2.54	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: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:167:ARG:CG	1:A:168:ASP:N	2.79	0.45
1:A:163:PHE:CE1	1:A:209:ILE:HD13	2.51	0.45
1:A:76:LEU:HD23	1:A:76:LEU:HA	1.69	0.45
1:A:158:PRO:O	1:A:159:HIS:CG	2.70	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: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:107:GLU:HG2	3:A:746:HOH:O	2.14	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:LYS:HG3	1:A:26:SER:H	1.82	0.44
1:A:137:ASP:C	1:A:139:VAL:H	2.20	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
1:A:137:ASP:C	1:A:139:VAL:N	2.71	0.43
1:A:184:TYR:HB2	3:A:711:HOH:O	2.17	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:158:PRO:C	1:A:159:HIS:ND1	2.72	0.42
1:A:196:LEU:O	1:A:197:GLN:HB2	2.19	0.42
1:A:14:LYS:O	1:A:15:GLY:C	2.58	0.42
1:A:38:ILE:HG21	1:A:38:ILE:HD13	1.69	0.42
1:A:109:THR:CG2	1:A:131:SER:O	2.38	0.42
1:A:21:LEU:HD11	1:A:51:PHE:CE1	2.51	0.42
1:A:82:SER:C	1:A:84:ASN:N	2.73	0.42
1:A:163:PHE:N	1:A:163:PHE:CD2	2.87	0.42
1:A:77:TYR:CE1	1:A:93:GLU:HB2	2.55	0.42
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:43:ALA:HB2	1:A:76:LEU:HD21	2.02	0.41
1:A:102:ASN:HB2	1:A:143:ASN:OD1	2.20	0.41
1:A:105:ARG:NH1	1:A:105:ARG:HG2	2.36	0.41
1:A:31:GLU:HB2	3:A:751:HOH:O	2.08	0.41
1:A:82:SER:O	1:A:83:SER:C	2.59	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:NH1	1:A:167:ARG:CB	2.84	0.41
1:A:103:ASP:OD1	1:A:103:ASP:N	2.54	0.41
1:A:194:ALA:O	1:A:198:GLY:HA2	2.21	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:119:GLU:N	1:A:212:LYS:O	2.48	0.41
1:A:68:ARG:HG3	1:A:98:VAL:O	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:SER:O	1:A:164:THR:OG1[3_444]	1.96	0.24

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	210/212 (99%)	176 (84%)	24 (11%)	10 (5%)	2 17

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%)	5 22

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 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](#)

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.

No monomer is involved in short contacts.

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.