



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:06 AM UTC

PDB ID : 1Q1P / pdb_00001q1p
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

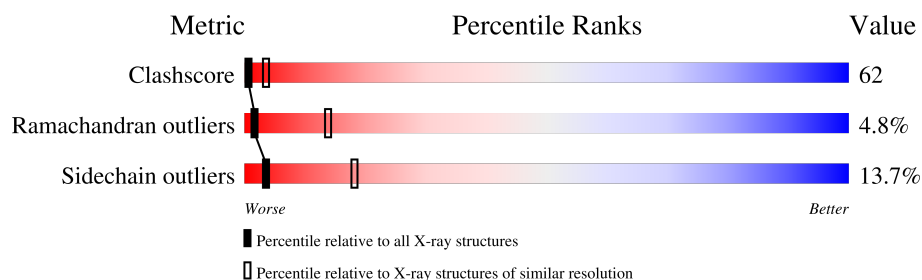
1 Overall quality at a glance

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	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (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 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 $\leq 5\%$

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 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 (CCD ID: CA) (formula: Ca).

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

- Molecule 3 is water.

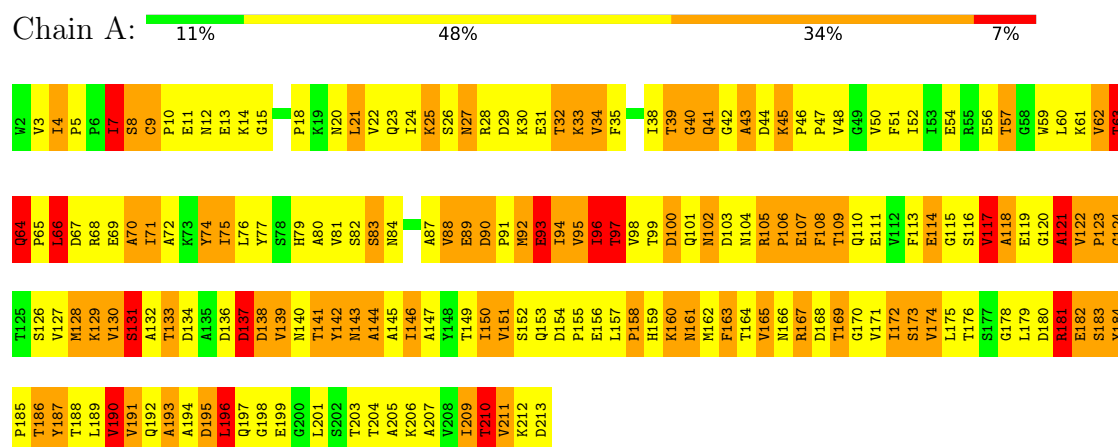
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	233	Total	O	0	0
			233	233		

3 Residue-property plots

These plots are drawn for all protein, RNA, 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: 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	2.60	113/1659 (6.8%)	1.89	51/2263 (2.3%)

All (113) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	210	THR	CB-OG1	17.51	1.71	1.43
1	A	43	ALA	CA-C	-17.26	1.44	1.52
1	A	169	THR	CA-CB	-11.71	1.34	1.53
1	A	92	MET	SD-CE	-11.43	1.50	1.79
1	A	81	VAL	C-O	-10.28	1.13	1.24
1	A	209	ILE	C-O	-10.17	1.11	1.24
1	A	191	VAL	CA-CB	-9.82	1.42	1.54
1	A	70	ALA	CA-CB	-9.43	1.38	1.53
1	A	172	ILE	CA-CB	-9.17	1.43	1.54
1	A	174	VAL	C-O	-8.96	1.15	1.24
1	A	146	ILE	CA-CB	-8.81	1.43	1.54
1	A	129	LYS	C-O	-8.51	1.13	1.23
1	A	127	VAL	C-O	-8.37	1.15	1.23
1	A	211	VAL	CA-CB	-8.24	1.44	1.54
1	A	100	ASP	CA-C	-8.05	1.43	1.52
1	A	153	GLN	C-O	-7.99	1.14	1.23
1	A	50	VAL	CA-CB	-7.71	1.45	1.54
1	A	144	ALA	CA-C	-7.62	1.43	1.52
1	A	188	THR	C-O	-7.57	1.15	1.24
1	A	114	GLU	C-O	-7.57	1.14	1.23
1	A	211	VAL	C-O	-7.52	1.16	1.24
1	A	184	TYR	C-O	-7.44	1.16	1.24
1	A	118	ALA	CA-C	-7.40	1.44	1.52
1	A	131	SER	CA-C	7.32	1.61	1.52
1	A	165	VAL	C-O	-7.19	1.16	1.24
1	A	121	ALA	CA-CB	-7.12	1.41	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	33	LYS	CA-C	7.07	1.60	1.52
1	A	141	THR	CA-CB	-7.04	1.42	1.53
1	A	107	GLU	CA-C	7.03	1.61	1.52
1	A	117	VAL	C-O	-6.98	1.16	1.23
1	A	130	VAL	CA-C	-6.97	1.44	1.52
1	A	87	ALA	CA-C	-6.94	1.42	1.52
1	A	185	PRO	C-O	-6.90	1.15	1.24
1	A	111	GLU	CA-C	-6.85	1.43	1.52
1	A	154	ASP	C-O	-6.78	1.15	1.24
1	A	196	LEU	N-CA	-6.78	1.37	1.46
1	A	97	THR	CA-CB	-6.68	1.43	1.53
1	A	152	SER	C-O	-6.68	1.16	1.23
1	A	41	GLN	C-O	-6.65	1.15	1.24
1	A	172	ILE	C-O	-6.65	1.15	1.24
1	A	186	THR	CA-C	-6.59	1.44	1.52
1	A	64	GLN	C-O	-6.56	1.15	1.24
1	A	81	VAL	CA-C	-6.55	1.44	1.52
1	A	7	ILE	CA-CB	-6.52	1.45	1.53
1	A	9	CYS	CA-C	6.46	1.58	1.52
1	A	63	THR	CA-CB	-6.26	1.45	1.53
1	A	106	PRO	CA-CB	-6.23	1.45	1.53
1	A	169	THR	CA-C	-6.21	1.45	1.52
1	A	88	VAL	C-O	-6.15	1.18	1.24
1	A	4	ILE	CA-CB	6.14	1.62	1.54
1	A	35	PHE	CA-C	6.05	1.60	1.52
1	A	210	THR	C-O	-6.04	1.15	1.23
1	A	195	ASP	C-O	-6.03	1.15	1.23
1	A	105	ARG	CA-C	-6.02	1.46	1.52
1	A	205	ALA	C-O	-5.98	1.16	1.23
1	A	182	GLU	C-O	-5.96	1.17	1.24
1	A	188	THR	N-CA	-5.96	1.39	1.46
1	A	75	ILE	CA-C	-5.96	1.45	1.52
1	A	169	THR	C-O	-5.94	1.15	1.24
1	A	71	ILE	CA-C	-5.91	1.45	1.52
1	A	166	ASN	CA-C	-5.88	1.45	1.52
1	A	92	MET	CG-SD	-5.82	1.66	1.80
1	A	139	VAL	C-O	-5.77	1.17	1.23
1	A	127	VAL	CA-C	-5.72	1.46	1.52
1	A	57	THR	CA-CB	-5.71	1.46	1.54
1	A	205	ALA	CA-CB	-5.63	1.44	1.53
1	A	40	GLY	C-O	5.62	1.28	1.23
1	A	89	GLU	CA-C	-5.62	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	62	VAL	C-O	-5.61	1.18	1.24
1	A	187	TYR	CG-CD2	-5.61	1.27	1.39
1	A	187	TYR	CE1-CZ	-5.60	1.24	1.38
1	A	34	VAL	C-O	-5.58	1.18	1.24
1	A	181	ARG	CA-C	-5.58	1.45	1.52
1	A	25	LYS	C-O	-5.56	1.16	1.23
1	A	156	GLU	N-CA	-5.55	1.40	1.46
1	A	126	SER	CA-C	-5.54	1.46	1.52
1	A	163	PHE	CE1-CZ	-5.54	1.22	1.38
1	A	80	ALA	CA-CB	-5.54	1.43	1.53
1	A	149	THR	CA-CB	-5.53	1.44	1.53
1	A	129	LYS	CA-C	-5.49	1.45	1.52
1	A	8	SER	CA-C	-5.47	1.46	1.52
1	A	128	MET	CA-C	-5.42	1.45	1.52
1	A	34	VAL	CA-C	-5.41	1.46	1.52
1	A	106	PRO	C-O	-5.38	1.17	1.23
1	A	48	VAL	C-O	-5.34	1.19	1.24
1	A	9	CYS	C-O	-5.32	1.18	1.25
1	A	193	ALA	C-O	-5.31	1.17	1.24
1	A	176	THR	C-O	-5.30	1.17	1.23
1	A	117	VAL	CB-CG1	-5.30	1.35	1.52
1	A	167	ARG	CA-C	-5.26	1.45	1.52
1	A	62	VAL	CA-CB	-5.22	1.47	1.53
1	A	107	GLU	CD-OE1	5.20	1.35	1.25
1	A	137	ASP	N-CA	5.20	1.52	1.46
1	A	165	VAL	CA-C	-5.20	1.46	1.52
1	A	39	THR	CA-C	-5.20	1.46	1.52
1	A	173	SER	CA-C	5.18	1.58	1.52
1	A	152	SER	CA-C	-5.17	1.46	1.52
1	A	176	THR	CA-C	-5.17	1.46	1.52
1	A	192	GLN	CA-C	-5.16	1.46	1.52
1	A	204	THR	C-O	-5.16	1.17	1.23
1	A	209	ILE	CA-CB	-5.16	1.47	1.54
1	A	184	TYR	CA-CB	-5.15	1.47	1.53
1	A	111	GLU	N-CA	-5.15	1.39	1.45
1	A	102	ASN	CA-C	-5.11	1.46	1.52
1	A	24	ILE	C-O	-5.09	1.17	1.24
1	A	190	VAL	C-O	5.07	1.30	1.24
1	A	43	ALA	CA-CB	-5.06	1.46	1.53
1	A	66	LEU	CA-C	5.04	1.59	1.52
1	A	130	VAL	C-O	-5.04	1.18	1.24
1	A	186	THR	C-O	-5.04	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	203	THR	CA-C	5.03	1.58	1.52
1	A	181	ARG	C-O	-5.02	1.17	1.24
1	A	152	SER	N-CA	-5.02	1.40	1.46

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	210	THR	OG1-CB-CG2	-9.12	91.07	109.30
1	A	45	LYS	N-CA-C	8.89	116.22	108.22
1	A	131	SER	N-CA-C	8.63	123.65	109.24
1	A	40	GLY	CA-C-O	-7.84	115.73	122.16
1	A	195	ASP	N-CA-C	7.22	119.88	110.43
1	A	211	VAL	N-CA-C	7.21	118.75	109.30
1	A	169	THR	CB-CA-C	-7.16	98.41	110.44
1	A	160	LYS	N-CA-C	-7.12	99.74	110.28
1	A	186	THR	OG1-CB-CG2	-7.03	95.24	109.30
1	A	210	THR	N-CA-C	7.00	121.13	108.17
1	A	158	PRO	N-CD-CG	-6.99	95.42	103.80
1	A	146	ILE	CB-CA-C	-6.97	102.00	111.63
1	A	160	LYS	CD-CE-NZ	6.88	133.93	111.90
1	A	97	THR	N-CA-C	6.81	120.34	109.24
1	A	48	VAL	N-CA-C	6.80	118.11	108.93
1	A	169	THR	OG1-CB-CG2	-6.76	95.78	109.30
1	A	43	ALA	O-C-N	6.70	125.79	120.83
1	A	150	ILE	CA-C-N	-6.67	114.47	122.35
1	A	150	ILE	C-N-CA	-6.67	114.47	122.35
1	A	176	THR	OG1-CB-CG2	-6.63	96.03	109.30
1	A	33	LYS	O-C-N	-6.53	115.53	123.30
1	A	25	LYS	N-CA-C	6.50	118.64	108.96
1	A	96	ILE	N-CA-C	6.45	117.17	107.75
1	A	213	ASP	CA-C-O	6.34	140.01	121.00
1	A	127	VAL	N-CA-C	6.29	117.22	111.81
1	A	155	PRO	N-CD-CG	-6.02	96.58	103.80
1	A	111	GLU	N-CA-C	-5.98	106.60	114.31
1	A	33	LYS	CA-C-N	-5.92	112.73	122.67
1	A	33	LYS	C-N-CA	-5.92	112.73	122.67
1	A	107	GLU	CA-C-O	5.87	126.57	120.40
1	A	3	VAL	N-CA-C	5.86	115.68	108.53
1	A	107	GLU	N-CA-C	5.85	118.27	108.02
1	A	5	PRO	CA-C-N	5.78	127.16	120.98
1	A	5	PRO	C-N-CA	5.78	127.16	120.98
1	A	165	VAL	CB-CA-C	-5.76	101.18	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	50	VAL	N-CA-C	-5.73	105.22	113.07
1	A	141	THR	CB-CA-C	-5.70	99.72	110.16
1	A	142	TYR	N-CA-C	-5.67	106.21	113.01
1	A	12	ASN	N-CA-C	5.53	119.20	111.90
1	A	132	ALA	N-CA-C	5.42	117.42	109.24
1	A	43	ALA	CA-C-O	-5.39	116.70	119.77
1	A	74	TYR	CA-C-N	-5.38	116.13	123.12
1	A	74	TYR	C-N-CA	-5.38	116.13	123.12
1	A	93	GLU	N-CA-C	5.16	117.39	109.07
1	A	71	ILE	CB-CA-C	-5.16	102.83	111.29
1	A	7	ILE	N-CA-C	5.15	115.46	107.28
1	A	108	PHE	N-CA-C	-5.10	102.74	110.24
1	A	209	ILE	CA-C-O	-5.05	114.47	120.78
1	A	133	THR	N-CA-CB	-5.04	102.20	111.37
1	A	124	GLY	CA-C-N	5.01	127.82	120.71
1	A	124	GLY	C-N-CA	5.01	127.82	120.71

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	201	1
2	A	3	0	0	0	0
3	A	233	0	0	25	0
All	All	1864	0	1595	201	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 62.

All (201) 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:CB	1:A:210:THR:OG1	1.71	1.36

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:183:SER:C	1:A:184:TYR:CD1	2.52	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: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:HG22	1:A:210:THR:O	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:119:GLU:O	1:A:120:GLY:C	2.25	0.77
1:A:28:ARG:H	1:A:28:ARG:HD2	1.49	0.77
1:A:67:ASP:OD1	1:A:69:GLU:HB2	1.85	0.77
1:A:183:SER:C	1:A:184:TYR:HD1	1.93	0.77
1:A:184:TYR:CD1	1:A:184:TYR:N	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:178:GLY:O	1:A:179:LEU:C	2.31	0.73
1:A:210:THR:C	3:A:726:HOH:O	2.30	0.73
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:82:SER:O	1:A:84:ASN:N	2.27	0.68
1:A:107:GLU:O	1:A:108:PHE:C	2.34	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:104:ASN:HB2	1:A:136:ASP:CG	2.20	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: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: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: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:137:ASP:CG	1:A:140:ASN:H	2.10	0.58
1:A:179:LEU:HD22	1:A:211:VAL:HG21	1.84	0.58
1:A:100:ASP:CG	1:A:101:GLN:N	2.62	0.57
1:A:181:ARG:NE	3:A:816:HOH:O	2.36	0.57
1:A:129:LYS:HG3	1:A:170:GLY:C	2.28	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:7:ILE:HD12	1:A:94:ILE:HG23	1.87	0.56
1:A:26:SER:O	1:A:28:ARG:N	2.38	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:HH11	1:A:28:ARG:HG2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:ASN:C	1:A:201:LEU:HD12	2.32	0.54
1:A:28:ARG:HD2	1:A:28:ARG:N	2.18	0.54
1:A:130:VAL:O	1:A:130:VAL:HG23	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:O	1:A:62:VAL:HG13	2.08	0.53
1:A:173:SER:O	1:A:174:VAL:C	2.50	0.53
1:A:27:ASN:C	1:A:29:ASP:H	2.17	0.53
1:A:137:ASP:OD2	1:A:140:ASN:N	2.42	0.53
1:A:182:GLU:OE2	3:A:813:HOH:O	2.19	0.53
1:A:109:THR:HG23	1:A:131:SER:C	2.32	0.52
1:A:162:MET:O	1:A:175:LEU:HB3	2.08	0.52
1:A:8:SER:HA	1:A:97:THR:O	2.09	0.52
1:A:122:VAL:HG23	1:A:123:PRO:CD	2.38	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:210:THR:CB	1:A:210:THR:HG1	2.15	0.52
1:A:30:LYS:HG2	3:A:776:HOH:O	2.09	0.51
1:A:146:ILE:CG2	1:A:147:ALA:N	2.72	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: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:114:GLU:CD	3:A:807:HOH:O	2.54	0.50
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
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:181:ARG:HG3	1:A:181:ARG:HH11	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:44:ASP:O	1:A:45:LYS:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ASP:C	1:A:139:VAL:N	2.71	0.48
1:A:137:ASP:C	1:A:139:VAL:H	2.20	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:158:PRO:C	1:A:159:HIS:ND1	2.72	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:14:LYS:O	1:A:15:GLY:C	2.58	0.47
1:A:82:SER:C	1:A:84:ASN:N	2.73	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:82:SER:O	1:A:83:SER:C	2.59	0.46
1:A:140:ASN:C	1:A:141:THR:HG23	2.40	0.46
1:A:160:LYS:O	1:A:161:ASN:HB2	2.16	0.46
1:A:70:ALA:C	1:A:71:ILE:HG13	2.41	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: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: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:187:TYR:HE1	3:A:711:HOH:O	1.98	0.45
1:A:108:PHE:CZ	1:A:193:ALA:HB2	2.51	0.45
1:A:95:VAL:O	1:A:95:VAL:HG12	2.16	0.45
1:A:142:TYR:O	1:A:143:ASN:C	2.56	0.45
1:A:181:ARG:CD	3:A:816:HOH:O	2.65	0.45
1:A:122:VAL:O	1:A:123:PRO:C	2.58	0.44
1:A:140:ASN:C	1:A:141:THR:CG2	2.90	0.44
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:180:ASP:O	1:A:181:ARG:C	2.60	0.44
1:A:82:SER:C	1:A:84:ASN:H	2.24	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:94:ILE:O	1:A:94:ILE:HG22	2.15	0.44
1:A:108:PHE:HZ	1:A:193:ALA:N	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ASP:O	1:A:91:PRO:C	2.60	0.44
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:10:PRO:HA	1:A:99:THR:OG1	2.19	0.43
1:A:76:LEU:HG	1:A:96:ILE:HD11	2.01	0.43
1:A:52:ILE:HG13	1:A:61:LYS:HB2	2.01	0.43
1:A:150:ILE:HG21	1:A:189:LEU:CD2	2.48	0.43
1:A:142:TYR:C	1:A:144:ALA:H	2.27	0.42
1:A:196:LEU:O	1:A:197:GLN:HB2	2.19	0.42
1:A:38:ILE:HG21	1:A:38:ILE:HD13	1.69	0.42
1:A:21:LEU:HD11	1:A:51:PHE:CE1	2.51	0.42
1:A:109:THR:CG2	1:A:131:SER:O	2.38	0.42
1:A:77:TYR:CE1	1:A:93:GLU:HB2	2.55	0.42
1:A:163:PHE:CD2	1:A:163:PHE:N	2.87	0.42
1:A:43:ALA:HB2	1:A:76:LEU:HD21	2.02	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:45:LYS:O	1:A:46:PRO:C	2.62	0.41
1:A:102:ASN:HB2	1:A:143:ASN:OD1	2.20	0.41
1:A:105:ARG:HG2	1:A:105:ARG:NH1	2.36	0.41
1:A:25:LYS:HG2	1:A:26:SER:H	1.77	0.41
1:A:167:ARG:CB	1:A:167:ARG:NH1	2.84	0.41
1:A:9:CYS:N	1:A:97:THR:O	2.47	0.41
1:A:103:ASP:N	1:A:103:ASP:OD1	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:68:ARG:HG3	1:A:98:VAL:O	2.20	0.41
1:A:92:MET:HE2	1:A:92:MET:HB3	1.78	0.41
1:A:119:GLU:N	1:A:212:LYS:O	2.48	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
1:A:23:GLN:HE21	1:A:59:TRP:NE1	2.20	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 14

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 [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	183/183 (100%)	158 (86%)	25 (14%)	3 18

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	7	ILE
1	A	32	THR
1	A	34	VAL
1	A	56	GLU
1	A	63	THR
1	A	66	LEU
1	A	90	ASP
1	A	93	GLU
1	A	94	ILE
1	A	95	VAL
1	A	96	ILE
1	A	97	THR
1	A	109	THR
1	A	117	VAL
1	A	122	VAL
1	A	131	SER
1	A	133	THR
1	A	138	ASP
1	A	151	VAL
1	A	183	SER
1	A	190	VAL
1	A	191	VAL
1	A	196	LEU
1	A	210	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 [i](#)

There are no oligosaccharides 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.