



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 27, 2017 – 05:44 AM EDT

PDB ID : 1FQY
Title : STRUCTURE OF AQUAPORIN-1 AT 3.8 Å RESOLUTION BY ELECTRON CRYSTALLOGRAPHY
Authors : Murata, K.; Mitsuoka, K.; Hirai, T.; Walz, T.; Agre, P.; Heymann, J.B.; Engel, A.; Fujiyoshi, Y.
Deposited on : unknown
Resolution : 3.80 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

<http://wwpdb.org/validation/2016/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	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

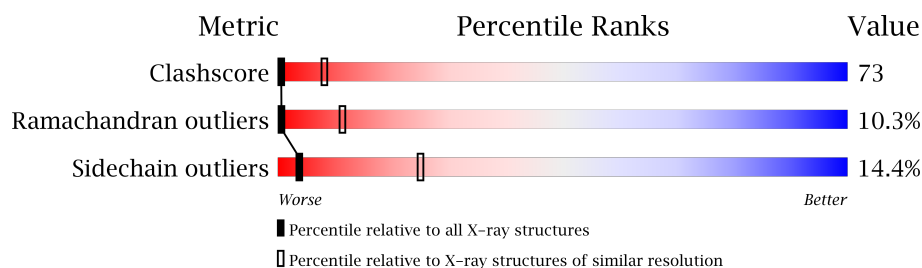
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON CRYSTALLOGRAPHY

The reported resolution of this entry is 3.80 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	112137	1030 (4.04-3.56)
Ramachandran outliers	110173	1011 (4.06-3.54)
Sidechain outliers	110143	1005 (4.06-3.54)

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. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	269	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1661 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 AQUAPORIN-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	226	1661	1077	283	296	5	0	0	0

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	96.00 Å 96.00 Å 100.00 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 3.80	Depositor
% Data completeness (in resolution range)	50.8 (6.00-3.80)	Depositor
R_{merge}	0.49	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.399 , 0.417	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1661	wwPDB-VP
Average B, all atoms (Å ²)	23.0	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	0.76	1/1693 (0.1%)	1.25	19/2308 (0.8%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	213	TRP	CB-CG	5.91	1.60	1.50

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	37	TYR	N-CA-C	10.29	138.77	111.00
1	A	195	ARG	NE-CZ-NH2	7.41	124.01	120.30
1	A	121	GLY	N-CA-C	-6.83	96.03	113.10
1	A	49	ASN	N-CA-C	6.77	129.28	111.00
1	A	232	ALA	N-CA-C	6.67	129.02	111.00
1	A	45	ALA	N-CA-C	-6.65	93.05	111.00
1	A	163	ASP	N-CA-C	6.62	128.89	111.00
1	A	195	ARG	NE-CZ-NH1	-6.55	117.02	120.30
1	A	231	LEU	CA-CB-CG	-6.40	100.59	115.30
1	A	132	GLY	N-CA-C	5.59	127.07	113.10
1	A	120	THR	N-CA-C	5.48	125.80	111.00
1	A	211	ILE	N-CA-C	-5.48	96.20	111.00
1	A	122	ASN	C-N-CA	5.42	135.25	121.70
1	A	129	LEU	CB-CG-CD2	5.37	120.14	111.00
1	A	88	GLN	N-CA-C	5.35	125.46	111.00
1	A	162	ARG	N-CA-C	5.33	125.38	111.00
1	A	40	GLY	N-CA-C	5.25	126.23	113.10
1	A	37	TYR	C-N-CD	5.22	139.35	128.40
1	A	125	GLY	N-CA-C	-5.07	100.42	113.10

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	1661	0	1712	247	0
All	All	1661	0	1712	247	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 73.

All (247) 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:212:PHE:O	1:A:216:PRO:HD2	1.52	1.10
1:A:77:PRO:HD2	1:A:193:PRO:HD2	1.36	1.08
1:A:17:GLU:OE1	1:A:97:TYR:CD2	2.14	1.00
1:A:115:ILE:HG13	1:A:116:THR:H	1.25	0.98
1:A:149:LEU:O	1:A:153:VAL:HG23	1.67	0.94
1:A:167:SER:O	1:A:170:LEU:HG	1.67	0.94
1:A:120:THR:HA	1:A:123:SER:HB3	1.51	0.91
1:A:76:ASN:HB3	1:A:192:ASN:ND2	1.86	0.90
1:A:129:LEU:HD11	1:A:195:ARG:HE	1.38	0.89
1:A:134:ASN:HD21	1:A:137:GLN:HB2	1.38	0.88
1:A:209:HIS:HA	1:A:212:PHE:CD2	2.08	0.88
1:A:190:GLY:CA	1:A:195:ARG:NH2	2.36	0.88
1:A:51:LYS:HD3	1:A:52:VAL:H	1.39	0.84
1:A:83:LEU:HD11	1:A:92:PHE:CZ	2.11	0.84
1:A:190:GLY:HA3	1:A:195:ARG:NH2	1.92	0.84
1:A:70:ILE:HD11	1:A:161:ARG:HD3	1.59	0.84
1:A:99:ILE:O	1:A:103:VAL:HG22	1.78	0.84
1:A:120:THR:CA	1:A:123:SER:HB3	2.07	0.84
1:A:149:LEU:HD22	1:A:191:ILE:HD11	1.59	0.83
1:A:17:GLU:OE1	1:A:97:TYR:CE2	2.32	0.83
1:A:70:ILE:HD11	1:A:161:ARG:CD	2.08	0.82
1:A:48:ASP:O	1:A:51:LYS:HD2	1.78	0.82
1:A:129:LEU:HD11	1:A:189:CYS:O	1.80	0.81
1:A:190:GLY:HA3	1:A:195:ARG:HH21	1.44	0.80
1:A:61:ALA:HB2	1:A:173:GLY:HA3	1.64	0.79
1:A:77:PRO:HD2	1:A:193:PRO:CD	2.12	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:LYS:HZ3	1:A:52:VAL:HG22	1.49	0.78
1:A:83:LEU:HD21	1:A:92:PHE:CE1	2.19	0.77
1:A:190:GLY:CA	1:A:195:ARG:HH21	1.95	0.77
1:A:52:VAL:HG12	1:A:56:PHE:HE1	1.49	0.77
1:A:176:VAL:HG12	1:A:180:HIS:HE1	1.50	0.76
1:A:17:GLU:OE1	1:A:97:TYR:HD2	1.65	0.76
1:A:51:LYS:NZ	1:A:52:VAL:HG22	2.03	0.74
1:A:190:GLY:HA2	1:A:195:ARG:NH2	2.01	0.74
1:A:231:LEU:HD12	1:A:232:ALA:H	1.52	0.74
1:A:192:ASN:O	1:A:195:ARG:HD2	1.88	0.74
1:A:21:THR:O	1:A:25:VAL:HG23	1.88	0.73
1:A:168:ALA:HB3	1:A:169:PRO:HD3	1.70	0.72
1:A:83:LEU:HG	1:A:84:LEU:N	2.03	0.72
1:A:209:HIS:O	1:A:212:PHE:HB2	1.90	0.71
1:A:63:LEU:O	1:A:67:VAL:HG22	1.90	0.71
1:A:134:ASN:ND2	1:A:137:GLN:HB2	2.05	0.71
1:A:115:ILE:HG13	1:A:116:THR:N	2.05	0.71
1:A:97:TYR:O	1:A:101:GLN:HG3	1.91	0.70
1:A:51:LYS:HD3	1:A:52:VAL:N	2.06	0.70
1:A:70:ILE:HD11	1:A:161:ARG:CZ	2.20	0.70
1:A:70:ILE:HD11	1:A:161:ARG:NE	2.06	0.70
1:A:36:LYS:HA	1:A:44:THR:HG21	1.73	0.70
1:A:83:LEU:HD21	1:A:92:PHE:HE1	1.56	0.69
1:A:213:TRP:CZ3	1:A:217:PHE:HB2	2.28	0.69
1:A:116:THR:HG22	1:A:119:LEU:HG	1.74	0.69
1:A:53:SER:OG	1:A:181:LEU:HD23	1.93	0.69
1:A:129:LEU:HD11	1:A:195:ARG:NE	2.07	0.68
1:A:215:GLY:O	1:A:218:ILE:HG12	1.95	0.67
1:A:163:ASP:OD2	1:A:166:GLY:HA2	1.94	0.67
1:A:151:LEU:CD1	1:A:227:TYR:HD1	2.08	0.67
1:A:147:LEU:O	1:A:151:LEU:HB2	1.95	0.67
1:A:184:ILE:HD12	1:A:189:CYS:H	1.58	0.67
1:A:36:LYS:HA	1:A:44:THR:CG2	2.26	0.66
1:A:176:VAL:HG12	1:A:180:HIS:CE1	2.30	0.66
1:A:81:LEU:O	1:A:85:LEU:HG	1.95	0.66
1:A:80:THR:O	1:A:83:LEU:HD23	1.96	0.65
1:A:76:ASN:O	1:A:79:VAL:HG22	1.97	0.65
1:A:128:ASP:C	1:A:129:LEU:HD23	2.17	0.65
1:A:85:LEU:N	1:A:85:LEU:HD23	2.09	0.65
1:A:141:ILE:HG13	1:A:142:GLU:N	2.11	0.65
1:A:172:ILE:O	1:A:176:VAL:HG23	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:VAL:O	1:A:56:PHE:HD1	1.81	0.63
1:A:166:GLY:O	1:A:170:LEU:HD23	1.98	0.63
1:A:217:PHE:O	1:A:221:ALA:N	2.32	0.63
1:A:149:LEU:HD22	1:A:191:ILE:CD1	2.28	0.63
1:A:226:ILE:O	1:A:230:ILE:HG12	1.99	0.62
1:A:74:HIS:O	1:A:75:LEU:HD23	2.00	0.62
1:A:209:HIS:HA	1:A:212:PHE:CG	2.34	0.62
1:A:210:TRP:C	1:A:212:PHE:N	2.46	0.61
1:A:105:ALA:O	1:A:108:ALA:HB3	2.01	0.61
1:A:190:GLY:HA2	1:A:195:ARG:CZ	2.31	0.61
1:A:89:ILE:HA	1:A:92:PHE:HB2	1.83	0.61
1:A:231:LEU:HD12	1:A:232:ALA:N	2.16	0.60
1:A:180:HIS:HA	1:A:183:ALA:HB3	1.82	0.60
1:A:214:VAL:O	1:A:218:ILE:HG12	2.02	0.60
1:A:83:LEU:HD11	1:A:92:PHE:HZ	1.63	0.59
1:A:208:ASN:O	1:A:210:TRP:N	2.35	0.59
1:A:134:ASN:OD1	1:A:135:SER:N	2.35	0.59
1:A:151:LEU:HD11	1:A:227:TYR:HD1	1.67	0.59
1:A:213:TRP:O	1:A:213:TRP:HE3	1.86	0.59
1:A:121:GLY:C	1:A:123:SER:H	2.05	0.59
1:A:91:ILE:HG12	1:A:91:ILE:O	2.03	0.59
1:A:156:THR:HG21	1:A:168:ALA:HB1	1.83	0.59
1:A:210:TRP:CZ3	1:A:213:TRP:HD1	2.21	0.59
1:A:192:ASN:O	1:A:195:ARG:NH1	2.36	0.58
1:A:96:MET:O	1:A:99:ILE:HG22	2.03	0.58
1:A:167:SER:HA	1:A:170:LEU:HD21	1.86	0.58
1:A:170:LEU:O	1:A:174:LEU:HG	2.03	0.58
1:A:176:VAL:HG13	1:A:191:ILE:HD13	1.85	0.58
1:A:210:TRP:HZ3	1:A:213:TRP:HD1	1.50	0.58
1:A:129:LEU:HD13	1:A:188:GLY:O	2.03	0.57
1:A:189:CYS:O	1:A:189:CYS:SG	2.62	0.57
1:A:80:THR:HG21	1:A:94:ALA:HB1	1.85	0.57
1:A:33:LEU:HD21	1:A:125:GLY:HA2	1.87	0.56
1:A:167:SER:HA	1:A:170:LEU:CD2	2.35	0.56
1:A:86:SER:OG	1:A:87:CYS:N	2.39	0.56
1:A:12:ARG:HA	1:A:15:VAL:CG2	2.36	0.56
1:A:163:ASP:HB2	1:A:166:GLY:H	1.71	0.56
1:A:206:PHE:HB3	1:A:208:ASN:HB2	1.88	0.56
1:A:206:PHE:C	1:A:208:ASN:H	2.09	0.55
1:A:168:ALA:O	1:A:171:ALA:HB3	2.07	0.55
1:A:151:LEU:HD12	1:A:227:TYR:CD1	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:GLU:HG3	1:A:190:GLY:O	2.08	0.54
1:A:145:GLY:O	1:A:148:GLN:HG2	2.07	0.54
1:A:197:PHE:O	1:A:201:VAL:HG23	2.07	0.54
1:A:226:ILE:HA	1:A:229:PHE:CE2	2.42	0.54
1:A:129:LEU:CD1	1:A:189:CYS:O	2.54	0.54
1:A:129:LEU:CD1	1:A:195:ARG:HH21	2.20	0.54
1:A:31:SER:O	1:A:35:PHE:HD1	1.91	0.53
1:A:147:LEU:HD13	1:A:219:GLY:O	2.07	0.53
1:A:149:LEU:HD13	1:A:176:VAL:HG22	1.90	0.53
1:A:109:THR:HG21	1:A:198:GLY:O	2.09	0.53
1:A:228:ASP:OD1	1:A:233:PRO:HD2	2.08	0.53
1:A:209:HIS:CD2	1:A:210:TRP:CD1	2.97	0.52
1:A:36:LYS:O	1:A:36:LYS:HG2	2.09	0.52
1:A:206:PHE:HB3	1:A:208:ASN:CB	2.40	0.52
1:A:70:ILE:CD1	1:A:161:ARG:HD3	2.36	0.52
1:A:130:ALA:HB2	1:A:212:PHE:CZ	2.44	0.52
1:A:26:PHE:CZ	1:A:115:ILE:HD11	2.45	0.52
1:A:129:LEU:HD22	1:A:188:GLY:C	2.31	0.51
1:A:149:LEU:HG	1:A:150:VAL:N	2.24	0.51
1:A:70:ILE:CD1	1:A:161:ARG:NH1	2.74	0.51
1:A:206:PHE:C	1:A:208:ASN:N	2.64	0.51
1:A:33:LEU:HD12	1:A:112:LEU:HD21	1.93	0.50
1:A:28:SER:HB2	1:A:56:PHE:CD2	2.46	0.50
1:A:51:LYS:O	1:A:54:LEU:HB2	2.11	0.50
1:A:220:GLY:HA2	1:A:223:ALA:HB3	1.94	0.50
1:A:220:GLY:O	1:A:223:ALA:HB3	2.12	0.50
1:A:174:LEU:O	1:A:177:ALA:HB3	2.12	0.49
1:A:200:ALA:HB1	1:A:204:HIS:CD2	2.48	0.49
1:A:209:HIS:HA	1:A:212:PHE:CE2	2.44	0.49
1:A:44:THR:HG23	1:A:47:GLN:H	1.78	0.49
1:A:106:ILE:HD12	1:A:201:VAL:HG21	1.94	0.49
1:A:52:VAL:O	1:A:56:PHE:CD1	2.64	0.49
1:A:26:PHE:HZ	1:A:115:ILE:HD11	1.76	0.49
1:A:12:ARG:HA	1:A:15:VAL:HG22	1.94	0.49
1:A:139:LEU:HD22	1:A:211:ILE:CG2	2.43	0.49
1:A:183:ALA:HB1	1:A:189:CYS:HA	1.94	0.49
1:A:151:LEU:CD1	1:A:227:TYR:CD1	2.93	0.48
1:A:200:ALA:HB1	1:A:204:HIS:HB3	1.95	0.48
1:A:13:ALA:O	1:A:16:ALA:HB3	2.14	0.48
1:A:23:LEU:O	1:A:27:ILE:HG13	2.12	0.48
1:A:80:THR:CG2	1:A:94:ALA:HB1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:TRP:C	1:A:212:PHE:H	2.14	0.48
1:A:70:ILE:CD1	1:A:161:ARG:CZ	2.89	0.48
1:A:70:ILE:HD11	1:A:161:ARG:NH1	2.29	0.48
1:A:48:ASP:O	1:A:51:LYS:CD	2.56	0.48
1:A:51:LYS:HD3	1:A:52:VAL:HG23	1.96	0.48
1:A:69:HIS:CG	1:A:70:ILE:H	2.32	0.48
1:A:120:THR:HA	1:A:123:SER:CB	2.35	0.48
1:A:134:ASN:HD21	1:A:138:GLY:N	2.12	0.47
1:A:37:TYR:O	1:A:38:PRO:C	2.50	0.47
1:A:180:HIS:O	1:A:184:ILE:HB	2.14	0.47
1:A:120:THR:CB	1:A:123:SER:HB3	2.44	0.47
1:A:80:THR:O	1:A:83:LEU:HB3	2.14	0.47
1:A:212:PHE:O	1:A:216:PRO:CD	2.43	0.47
1:A:124:LEU:HD23	1:A:126:ARG:HG3	1.97	0.47
1:A:172:ILE:O	1:A:175:SER:HB3	2.14	0.47
1:A:210:TRP:CZ3	1:A:213:TRP:CD1	3.02	0.47
1:A:48:ASP:OD1	1:A:51:LYS:HD2	2.15	0.47
1:A:129:LEU:O	1:A:131:ASP:N	2.48	0.47
1:A:140:GLY:O	1:A:143:ILE:HG12	2.15	0.47
1:A:129:LEU:CD1	1:A:195:ARG:NH2	2.79	0.46
1:A:69:HIS:CG	1:A:70:ILE:N	2.83	0.46
1:A:17:GLU:CD	1:A:97:TYR:CE2	2.89	0.46
1:A:26:PHE:HE1	1:A:112:LEU:CD1	2.29	0.46
1:A:141:ILE:CG1	1:A:142:GLU:N	2.78	0.46
1:A:200:ALA:O	1:A:204:HIS:HD2	1.98	0.46
1:A:25:VAL:HA	1:A:28:SER:OG	2.16	0.46
1:A:222:LEU:O	1:A:226:ILE:HG23	2.16	0.46
1:A:151:LEU:HD12	1:A:227:TYR:HD1	1.76	0.46
1:A:210:TRP:HZ3	1:A:213:TRP:CD1	2.30	0.46
1:A:37:TYR:HB2	1:A:119:LEU:HD22	1.98	0.45
1:A:26:PHE:HZ	1:A:115:ILE:CD1	2.30	0.45
1:A:129:LEU:HD12	1:A:195:ARG:NH2	2.31	0.45
1:A:147:LEU:CD1	1:A:223:ALA:HB2	2.46	0.45
1:A:77:PRO:HD2	1:A:193:PRO:CG	2.47	0.45
1:A:127:ASN:C	1:A:129:LEU:N	2.70	0.45
1:A:12:ARG:O	1:A:16:ALA:N	2.37	0.45
1:A:50:VAL:HG23	1:A:51:LYS:N	2.32	0.44
1:A:60:ILE:HG23	1:A:75:LEU:CD1	2.48	0.44
1:A:82:GLY:HA2	1:A:224:VAL:HG21	1.99	0.44
1:A:121:GLY:C	1:A:123:SER:N	2.71	0.44
1:A:180:HIS:O	1:A:181:LEU:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:HIS:C	1:A:212:PHE:HB2	2.38	0.44
1:A:106:ILE:HG23	1:A:201:VAL:HG21	2.00	0.44
1:A:156:THR:HG21	1:A:168:ALA:CB	2.46	0.44
1:A:67:VAL:O	1:A:68:GLY:C	2.56	0.44
1:A:184:ILE:CD1	1:A:189:CYS:HB3	2.48	0.44
1:A:69:HIS:CD2	1:A:70:ILE:H	2.36	0.44
1:A:218:ILE:HA	1:A:221:ALA:CB	2.49	0.43
1:A:200:ALA:O	1:A:202:ILE:N	2.51	0.43
1:A:187:THR:O	1:A:188:GLY:O	2.36	0.43
1:A:30:GLY:O	1:A:34:GLY:N	2.49	0.43
1:A:146:THR:HG23	1:A:150:VAL:HG23	2.00	0.43
1:A:220:GLY:HA2	1:A:223:ALA:CB	2.48	0.43
1:A:65:GLN:HB3	1:A:65:GLN:HE21	1.61	0.43
1:A:81:LEU:HA	1:A:81:LEU:HD23	1.93	0.43
1:A:91:ILE:CG1	1:A:91:ILE:O	2.66	0.43
1:A:124:LEU:HG	1:A:126:ARG:HA	2.01	0.43
1:A:12:ARG:O	1:A:15:VAL:HG23	2.19	0.43
1:A:151:LEU:HA	1:A:151:LEU:HD12	1.90	0.43
1:A:83:LEU:HD11	1:A:92:PHE:CE1	2.50	0.42
1:A:176:VAL:O	1:A:180:HIS:ND1	2.52	0.42
1:A:24:PHE:HB2	1:A:63:LEU:HD13	2.01	0.42
1:A:71:SER:OG	1:A:72:GLY:N	2.52	0.42
1:A:84:LEU:O	1:A:86:SER:N	2.52	0.42
1:A:146:THR:O	1:A:146:THR:CG2	2.67	0.42
1:A:184:ILE:CG2	1:A:185:ASP:N	2.83	0.42
1:A:115:ILE:CG1	1:A:116:THR:H	2.09	0.42
1:A:60:ILE:HG23	1:A:75:LEU:HD11	2.02	0.42
1:A:17:GLU:CD	1:A:97:TYR:HE2	2.23	0.42
1:A:149:LEU:HD22	1:A:191:ILE:CG1	2.50	0.42
1:A:19:LEU:O	1:A:22:THR:HB	2.19	0.42
1:A:218:ILE:HA	1:A:221:ALA:HB3	2.01	0.42
1:A:229:PHE:CD1	1:A:229:PHE:C	2.93	0.42
1:A:76:ASN:HA	1:A:77:PRO:HD3	1.76	0.42
1:A:213:TRP:O	1:A:215:GLY:N	2.53	0.41
1:A:144:ILE:O	1:A:147:LEU:HB3	2.20	0.41
1:A:147:LEU:HD13	1:A:223:ALA:HB2	2.01	0.41
1:A:129:LEU:CD1	1:A:195:ARG:NE	2.79	0.41
1:A:200:ALA:HB1	1:A:204:HIS:CG	2.55	0.41
1:A:230:ILE:HD13	1:A:230:ILE:HA	1.86	0.41
1:A:28:SER:HB2	1:A:56:PHE:CE2	2.55	0.41
1:A:87:CYS:O	1:A:88:GLN:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:THR:O	1:A:112:LEU:HB3	2.19	0.41
1:A:27:ILE:O	1:A:30:GLY:N	2.53	0.41
1:A:126:ARG:O	1:A:128:ASP:N	2.54	0.41
1:A:24:PHE:CD2	1:A:25:VAL:HG22	2.55	0.41
1:A:37:TYR:CB	1:A:119:LEU:HD22	2.51	0.41
1:A:37:TYR:CD2	1:A:38:PRO:HD3	2.56	0.41
1:A:149:LEU:O	1:A:152:CYS:SG	2.63	0.41
1:A:127:ASN:O	1:A:129:LEU:N	2.53	0.41
1:A:231:LEU:HA	1:A:231:LEU:HD12	1.62	0.41
1:A:200:ALA:CB	1:A:204:HIS:HB3	2.51	0.40
1:A:139:LEU:HD22	1:A:211:ILE:HG21	2.01	0.40
1:A:163:ASP:CG	1:A:166:GLY:HA2	2.41	0.40
1:A:208:ASN:O	1:A:211:ILE:N	2.54	0.40
1:A:208:ASN:ND2	1:A:212:PHE:CE1	2.89	0.40
1:A:35:PHE:CZ	1:A:51:LYS:HE3	2.56	0.40
1:A:65:GLN:O	1:A:65:GLN:HG2	2.21	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	224/269 (83%)	142 (63%)	59 (26%)	23 (10%)	0	11

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	GLY
1	A	126	ARG
1	A	158	ASP
1	A	188	GLY
1	A	39	VAL

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Mol	Chain	Res	Type
1	A	48	ASP
1	A	68	GLY
1	A	74	HIS
1	A	130	ALA
1	A	132	GLY
1	A	161	ARG
1	A	201	VAL
1	A	209	HIS
1	A	86	SER
1	A	184	ILE
1	A	85	LEU
1	A	123	SER
1	A	171	ALA
1	A	183	ALA
1	A	213	TRP
1	A	214	VAL
1	A	141	ILE
1	A	72	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	174/214 (81%)	149 (86%)	25 (14%)	4 25

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

Mol	Chain	Res	Type
1	A	25	VAL
1	A	36	LYS
1	A	38	PRO
1	A	41	ASN
1	A	51	LYS
1	A	75	LEU
1	A	83	LEU
1	A	87	CYS

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Mol	Chain	Res	Type
1	A	93	ARG
1	A	103	VAL
1	A	107	VAL
1	A	122	ASN
1	A	127	ASN
1	A	129	LEU
1	A	142	GLU
1	A	143	ILE
1	A	147	LEU
1	A	169	PRO
1	A	181	LEU
1	A	195	ARG
1	A	197	PHE
1	A	203	THR
1	A	208	ASN
1	A	213	TRP
1	A	233	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	65	GLN
1	A	69	HIS
1	A	137	GLN
1	A	192	ASN
1	A	204	HIS
1	A	208	ASN
1	A	209	HIS

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 carbohydrates 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.