



Full wwPDB EM Validation Report ⓘ

Dec 13, 2022 – 12:02 AM EST

PDB ID : 1IH5
Title : CRYSTAL STRUCTURE OF AQUAPORIN-1
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Deposited on : 2001-04-18
Resolution : 3.70 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

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 : 4.02b-467
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) : 2.31.2

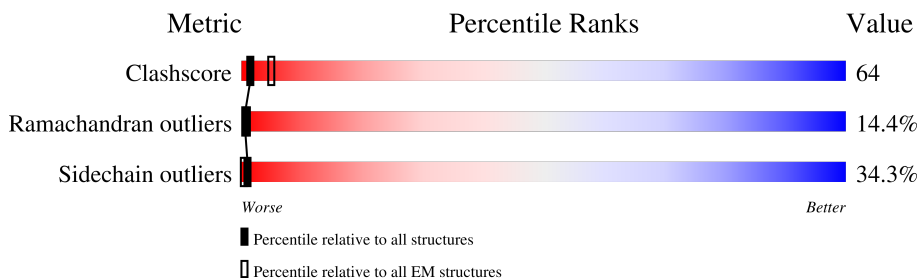
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON CRYSTALLOGRAPHY


The reported resolution of this entry is 3.70 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

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 1645 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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.

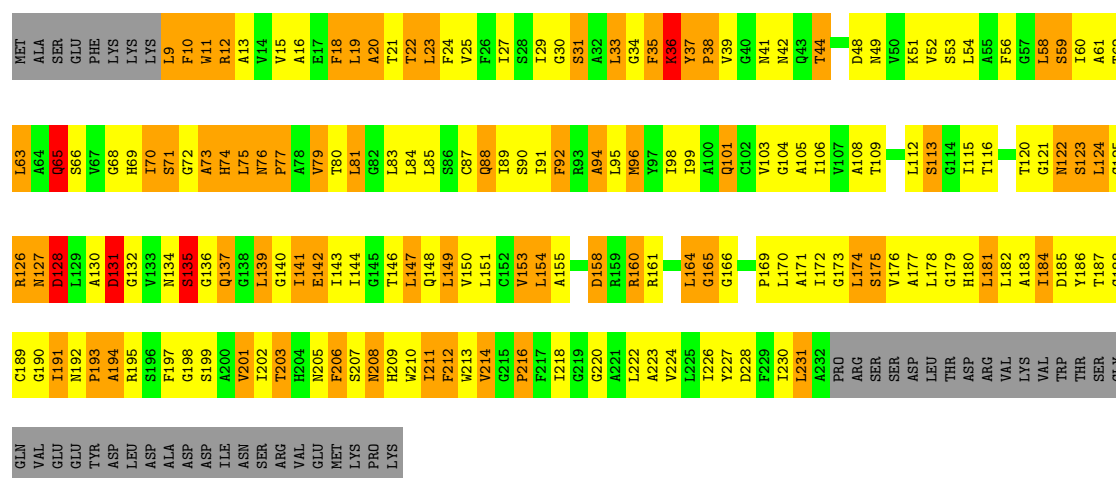
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	224	1645	1066	280	294	5	0	0

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.

• Molecule 1: AQUAPORIN-1

Chain A: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	99.58 Å 99.58 Å 100.00 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.00 – 3.70	Depositor
% Data completeness (in resolution range)	77.1 (24.00-3.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.361 , 0.458	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1645	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.32	0/1676	0.59	1/2285 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	123	SER	N-CA-C	5.67	126.30	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1645	0	1692	212	0
All	All	1645	0	1692	212	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 64.

All (212) 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:20:ALA:HB2	1:A:63:LEU:HD11	1.30	1.11
1:A:127:ASN:ND2	1:A:199:SER:HB2	1.71	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:LEU:HA	1:A:12:ARG:HG2	1.44	0.97
1:A:127:ASN:HB3	1:A:195:ARG:HH22	1.33	0.93
1:A:131:ASP:CB	1:A:188:GLY:H	1.81	0.93
1:A:131:ASP:HB2	1:A:188:GLY:H	1.31	0.93
1:A:172:ILE:O	1:A:176:VAL:HG23	1.68	0.93
1:A:103:VAL:HA	1:A:106:ILE:HD12	1.49	0.91
1:A:160:ARG:HG2	1:A:161:ARG:H	1.34	0.91
1:A:128:ASP:HB3	1:A:189:CYS:HB2	1.52	0.89
1:A:48:ASP:HA	1:A:51:LYS:HD3	1.54	0.89
1:A:209:HIS:HB2	1:A:211:ILE:HG12	1.57	0.85
1:A:109:THR:HA	1:A:112:LEU:HD23	1.58	0.84
1:A:76:ASN:HD22	1:A:77:PRO:HD2	1.45	0.82
1:A:112:LEU:HD22	1:A:126:ARG:HH21	1.47	0.79
1:A:147:LEU:O	1:A:151:LEU:HB2	1.82	0.79
1:A:25:VAL:O	1:A:29:ILE:HG23	1.83	0.79
1:A:37:TYR:H	1:A:38:PRO:HD2	1.47	0.79
1:A:22:THR:HA	1:A:108:ALA:CB	2.13	0.78
1:A:76:ASN:ND2	1:A:77:PRO:HD2	1.99	0.78
1:A:95:LEU:O	1:A:99:ILE:HD12	1.85	0.77
1:A:99:ILE:O	1:A:103:VAL:HG23	1.85	0.77
1:A:149:LEU:HD23	1:A:149:LEU:H	1.49	0.76
1:A:134:ASN:HD21	1:A:187:THR:HG21	1.50	0.75
1:A:160:ARG:HG2	1:A:161:ARG:N	2.01	0.75
1:A:140:GLY:HA2	1:A:143:ILE:HD12	1.70	0.74
1:A:95:LEU:HA	1:A:98:ILE:HD12	1.69	0.74
1:A:109:THR:HG21	1:A:198:GLY:HA3	1.70	0.74
1:A:109:THR:CB	1:A:198:GLY:HA3	2.17	0.74
1:A:105:ALA:O	1:A:109:THR:HG23	1.87	0.73
1:A:150:VAL:O	1:A:154:LEU:HD12	1.89	0.72
1:A:112:LEU:HD12	1:A:113:SER:N	2.05	0.72
1:A:127:ASN:HB3	1:A:195:ARG:NH2	2.03	0.71
1:A:131:ASP:HB2	1:A:188:GLY:N	2.04	0.71
1:A:106:ILE:HG12	1:A:197:PHE:HE2	1.56	0.71
1:A:164:LEU:HD12	1:A:166:GLY:H	1.56	0.70
1:A:230:ILE:HG22	1:A:231:LEU:HG	1.74	0.70
1:A:109:THR:CG2	1:A:198:GLY:HA3	2.21	0.69
1:A:24:PHE:CD2	1:A:59:SER:HB2	2.27	0.69
1:A:127:ASN:CG	1:A:199:SER:HB2	2.12	0.68
1:A:126:ARG:HB3	1:A:127:ASN:ND2	2.08	0.68
1:A:109:THR:CA	1:A:112:LEU:HD23	2.24	0.67
1:A:211:ILE:O	1:A:214:VAL:HG23	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:ILE:HG22	1:A:92:PHE:H	1.59	0.67
1:A:95:LEU:HA	1:A:98:ILE:CD1	2.25	0.67
1:A:11:TRP:O	1:A:15:VAL:HG23	1.96	0.66
1:A:58:LEU:HD13	1:A:59:SER:N	2.10	0.66
1:A:126:ARG:HD2	1:A:127:ASN:ND2	2.11	0.66
1:A:31:SER:HB3	1:A:52:VAL:HG22	1.76	0.65
1:A:141:ILE:O	1:A:144:ILE:HG22	1.96	0.65
1:A:24:PHE:CE2	1:A:59:SER:HB2	2.32	0.65
1:A:84:LEU:HD22	1:A:94:ALA:HB1	1.77	0.65
1:A:124:LEU:HG	1:A:125:GLY:H	1.62	0.64
1:A:60:ILE:HG23	1:A:74:HIS:HB3	1.78	0.64
1:A:53:SER:HB3	1:A:177:ALA:O	1.97	0.64
1:A:9:LEU:HD22	1:A:12:ARG:NH2	2.13	0.63
1:A:127:ASN:CB	1:A:195:ARG:HH22	2.09	0.63
1:A:109:THR:HB	1:A:198:GLY:HA3	1.78	0.63
1:A:149:LEU:O	1:A:153:VAL:HG23	1.99	0.63
1:A:77:PRO:HB2	1:A:193:PRO:HD2	1.81	0.63
1:A:124:LEU:HG	1:A:125:GLY:N	2.14	0.63
1:A:127:ASN:ND2	1:A:127:ASN:N	2.46	0.63
1:A:9:LEU:HA	1:A:12:ARG:CG	2.25	0.63
1:A:48:ASP:HA	1:A:51:LYS:CD	2.28	0.62
1:A:22:THR:HA	1:A:108:ALA:HB2	1.81	0.62
1:A:18:PHE:O	1:A:22:THR:OG1	2.17	0.62
1:A:75:LEU:HD13	1:A:80:THR:HG23	1.81	0.62
1:A:144:ILE:HD12	1:A:147:LEU:HD11	1.82	0.62
1:A:149:LEU:HD13	1:A:176:VAL:HG13	1.81	0.62
1:A:212:PHE:O	1:A:216:PRO:HD2	2.00	0.62
1:A:18:PHE:HA	1:A:104:GLY:HA3	1.82	0.61
1:A:178:LEU:HD23	1:A:181:LEU:HD13	1.80	0.61
1:A:146:THR:HG21	1:A:216:PRO:HB3	1.82	0.61
1:A:126:ARG:HD2	1:A:127:ASN:CG	2.21	0.61
1:A:155:ALA:HA	1:A:227:TYR:OH	2.00	0.61
1:A:33:LEU:O	1:A:37:TYR:HE1	1.84	0.61
1:A:131:ASP:HB2	1:A:187:THR:HA	1.84	0.60
1:A:147:LEU:HB3	1:A:223:ALA:HB2	1.82	0.59
1:A:36:LYS:HZ3	1:A:42:ASN:HA	1.68	0.59
1:A:208:ASN:HD22	1:A:209:HIS:N	1.99	0.59
1:A:12:ARG:HG3	1:A:13:ALA:H	1.68	0.59
1:A:48:ASP:O	1:A:51:LYS:HB2	2.03	0.59
1:A:12:ARG:HG3	1:A:13:ALA:N	2.18	0.59
1:A:76:ASN:HB3	1:A:192:ASN:ND2	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:ARG:HD2	1:A:127:ASN:OD1	2.02	0.59
1:A:29:ILE:HG13	1:A:30:GLY:N	2.18	0.58
1:A:36:LYS:NZ	1:A:42:ASN:HA	2.19	0.58
1:A:132:GLY:HA3	1:A:187:THR:OG1	2.04	0.58
1:A:134:ASN:HD21	1:A:187:THR:CG2	2.16	0.58
1:A:202:ILE:HG22	1:A:203:THR:OG1	2.05	0.57
1:A:126:ARG:HB3	1:A:127:ASN:HD21	1.69	0.57
1:A:134:ASN:ND2	1:A:187:THR:HG21	2.18	0.57
1:A:158:ASP:O	1:A:160:ARG:HD3	2.05	0.57
1:A:58:LEU:HD22	1:A:58:LEU:O	2.05	0.56
1:A:41:ASN:ND2	1:A:42:ASN:H	2.03	0.56
1:A:220:GLY:O	1:A:224:VAL:HG23	2.06	0.55
1:A:164:LEU:HD12	1:A:165:GLY:H	1.72	0.54
1:A:116:THR:O	1:A:120:THR:OG1	2.23	0.54
1:A:63:LEU:HB3	1:A:65:GLN:HG3	1.90	0.54
1:A:70:ILE:CD1	1:A:71:SER:H	2.21	0.54
1:A:208:ASN:C	1:A:210:TRP:H	2.11	0.54
1:A:63:LEU:CB	1:A:65:GLN:HG3	2.38	0.53
1:A:20:ALA:HB1	1:A:24:PHE:CZ	2.44	0.53
1:A:209:HIS:HB2	1:A:211:ILE:CG1	2.34	0.53
1:A:76:ASN:O	1:A:79:VAL:HG23	2.09	0.53
1:A:84:LEU:O	1:A:88:GLN:HB2	2.09	0.53
1:A:209:HIS:C	1:A:211:ILE:N	2.61	0.52
1:A:190:GLY:HA2	1:A:195:ARG:HD3	1.92	0.52
1:A:35:PHE:O	1:A:37:TYR:HD1	1.93	0.52
1:A:183:ALA:C	1:A:185:ASP:H	2.13	0.51
1:A:9:LEU:C	1:A:11:TRP:H	2.14	0.51
1:A:35:PHE:O	1:A:35:PHE:HD1	1.94	0.51
1:A:61:ALA:HA	1:A:65:GLN:HE22	1.74	0.51
1:A:135:SER:C	1:A:137:GLN:H	2.14	0.51
1:A:142:GLU:OE2	1:A:191:ILE:HA	2.11	0.51
1:A:20:ALA:CB	1:A:63:LEU:HD11	2.20	0.51
1:A:81:LEU:O	1:A:85:LEU:HG	2.11	0.50
1:A:33:LEU:O	1:A:35:PHE:N	2.44	0.50
1:A:146:THR:O	1:A:150:VAL:HG23	2.11	0.50
1:A:178:LEU:CD2	1:A:181:LEU:HD13	2.41	0.50
1:A:75:LEU:O	1:A:101:GLN:HG3	2.12	0.50
1:A:22:THR:HA	1:A:108:ALA:CA	2.41	0.49
1:A:127:ASN:HD21	1:A:199:SER:HB2	1.71	0.49
1:A:89:ILE:HG22	1:A:90:SER:N	2.28	0.49
1:A:58:LEU:HD22	1:A:58:LEU:C	2.32	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:ILE:HG22	1:A:231:LEU:N	2.27	0.49
1:A:209:HIS:C	1:A:211:ILE:H	2.16	0.49
1:A:49:ASN:HA	1:A:52:VAL:HG23	1.95	0.49
1:A:22:THR:HA	1:A:108:ALA:HA	1.93	0.49
1:A:127:ASN:N	1:A:127:ASN:HD22	2.10	0.48
1:A:191:ILE:HG22	1:A:192:ASN:OD1	2.13	0.48
1:A:23:LEU:O	1:A:27:ILE:HG12	2.12	0.48
1:A:171:ALA:O	1:A:174:LEU:HD23	2.13	0.48
1:A:37:TYR:N	1:A:38:PRO:HD2	2.23	0.48
1:A:135:SER:OG	1:A:136:GLY:N	2.47	0.48
1:A:62:THR:O	1:A:62:THR:HG22	2.14	0.48
1:A:149:LEU:HD23	1:A:149:LEU:N	2.23	0.48
1:A:131:ASP:O	1:A:187:THR:HG23	2.14	0.47
1:A:96:MET:SD	1:A:96:MET:N	2.82	0.47
1:A:181:LEU:HD23	1:A:182:LEU:N	2.29	0.47
1:A:58:LEU:HD22	1:A:62:THR:HG1	1.79	0.47
1:A:61:ALA:HA	1:A:65:GLN:NE2	2.29	0.47
1:A:184:ILE:HG22	1:A:184:ILE:O	2.13	0.47
1:A:126:ARG:NH1	1:A:127:ASN:OD1	2.47	0.47
1:A:29:ILE:HG22	1:A:126:ARG:CZ	2.46	0.46
1:A:126:ARG:HD2	1:A:127:ASN:HD21	1.78	0.46
1:A:227:TYR:HA	1:A:230:ILE:HD12	1.97	0.46
1:A:29:ILE:CG2	1:A:126:ARG:CZ	2.93	0.46
1:A:192:ASN:HB3	1:A:193:PRO:HD2	1.98	0.46
1:A:193:PRO:O	1:A:194:ALA:C	2.53	0.46
1:A:218:ILE:O	1:A:222:LEU:HG	2.16	0.46
1:A:77:PRO:HB2	1:A:193:PRO:HG2	1.97	0.46
1:A:127:ASN:CG	1:A:199:SER:CB	2.83	0.46
1:A:176:VAL:HG12	1:A:180:HIS:CE1	2.51	0.46
1:A:41:ASN:CG	1:A:42:ASN:H	2.20	0.45
1:A:121:GLY:O	1:A:122:ASN:C	2.54	0.45
1:A:151:LEU:HD21	1:A:227:TYR:HD1	1.79	0.45
1:A:148:GLN:NE2	1:A:175:SER:O	2.49	0.45
1:A:139:LEU:O	1:A:143:ILE:HG13	2.17	0.45
1:A:70:ILE:HD12	1:A:71:SER:H	1.81	0.45
1:A:208:ASN:HD22	1:A:209:HIS:H	1.63	0.45
1:A:174:LEU:O	1:A:177:ALA:HB3	2.18	0.45
1:A:126:ARG:C	1:A:127:ASN:ND2	2.71	0.44
1:A:131:ASP:HB2	1:A:187:THR:CA	2.47	0.44
1:A:83:LEU:O	1:A:87:CYS:SG	2.76	0.44
1:A:115:ILE:HD12	1:A:116:THR:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:SER:HB3	1:A:177:ALA:CA	2.48	0.44
1:A:68:GLY:C	1:A:69:HIS:CD2	2.91	0.44
1:A:79:VAL:CG2	1:A:192:ASN:HD21	2.31	0.44
1:A:173:GLY:O	1:A:177:ALA:HB2	2.18	0.44
1:A:209:HIS:O	1:A:211:ILE:N	2.51	0.44
1:A:191:ILE:HG22	1:A:192:ASN:N	2.32	0.44
1:A:36:LYS:CD	1:A:44:THR:H	2.31	0.43
1:A:24:PHE:CD2	1:A:24:PHE:N	2.84	0.43
1:A:210:TRP:O	1:A:213:TRP:N	2.40	0.43
1:A:33:LEU:O	1:A:37:TYR:CE1	2.67	0.43
1:A:211:ILE:HA	1:A:214:VAL:CG2	2.48	0.43
1:A:81:LEU:CD2	1:A:85:LEU:HD11	2.49	0.43
1:A:135:SER:O	1:A:137:GLN:N	2.49	0.43
1:A:148:GLN:OE1	1:A:179:GLY:CA	2.67	0.43
1:A:112:LEU:HD12	1:A:112:LEU:C	2.38	0.42
1:A:60:ILE:O	1:A:63:LEU:HB2	2.19	0.42
1:A:115:ILE:H	1:A:115:ILE:HG13	1.67	0.42
1:A:77:PRO:HB2	1:A:193:PRO:CD	2.48	0.42
1:A:19:LEU:O	1:A:22:THR:OG1	2.38	0.42
1:A:29:ILE:HG13	1:A:30:GLY:H	1.84	0.42
1:A:59:SER:O	1:A:63:LEU:HD23	2.20	0.42
1:A:109:THR:O	1:A:112:LEU:CD2	2.67	0.42
1:A:131:ASP:OD2	1:A:212:PHE:HE2	2.03	0.42
1:A:174:LEU:HD23	1:A:175:SER:N	2.34	0.42
1:A:65:GLN:CB	1:A:73:ALA:HA	2.50	0.42
1:A:22:THR:CG2	1:A:108:ALA:HA	2.50	0.42
1:A:42:ASN:N	1:A:42:ASN:OD1	2.52	0.42
1:A:124:LEU:CG	1:A:125:GLY:N	2.82	0.42
1:A:120:THR:HG21	1:A:124:LEU:HB2	2.02	0.41
1:A:201:VAL:HG12	1:A:202:ILE:CD1	2.50	0.41
1:A:201:VAL:HG12	1:A:202:ILE:HD12	2.02	0.41
1:A:201:VAL:HG12	1:A:202:ILE:N	2.35	0.41
1:A:35:PHE:C	1:A:36:LYS:HG2	2.38	0.41
1:A:127:ASN:OD1	1:A:195:ARG:NH1	2.53	0.41
1:A:53:SER:CB	1:A:177:ALA:O	2.65	0.41
1:A:147:LEU:H	1:A:147:LEU:HG	1.68	0.41
1:A:201:VAL:HG12	1:A:202:ILE:HG13	2.02	0.41
1:A:76:ASN:O	1:A:77:PRO:C	2.59	0.41
1:A:79:VAL:O	1:A:83:LEU:HG	2.21	0.41
1:A:16:ALA:O	1:A:19:LEU:HB3	2.21	0.40
1:A:61:ALA:C	1:A:63:LEU:H	2.24	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:LEU:HD22	1:A:94:ALA:CB	2.50	0.40
1:A:130:ALA:O	1:A:131:ASP:O	2.40	0.40
1:A:140:GLY:O	1:A:143:ILE:HB	2.21	0.40
1:A:222:LEU:O	1:A:226:ILE:HD12	2.21	0.40
1:A:131:ASP:HB3	1:A:188:GLY:H	1.79	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 PDB entries followed by that with respect to all EM entries.

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	222/269 (82%)	151 (68%)	39 (18%)	32 (14%)	0 3

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	TRP
1	A	44	THR
1	A	65	GLN
1	A	71	SER
1	A	77	PRO
1	A	94	ALA
1	A	113	SER
1	A	131	ASP
1	A	194	ALA
1	A	206	PHE
1	A	207	SER
1	A	34	GLY
1	A	36	LYS
1	A	158	ASP
1	A	191	ILE
1	A	205	ASN

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Mol	Chain	Res	Type
1	A	10	PHE
1	A	20	ALA
1	A	122	ASN
1	A	135	SER
1	A	193	PRO
1	A	72	GLY
1	A	73	ALA
1	A	165	GLY
1	A	184	ILE
1	A	37	TYR
1	A	128	ASP
1	A	186	TYR
1	A	216	PRO
1	A	39	VAL
1	A	38	PRO
1	A	169	PRO

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 PDB entries followed by that with respect to all EM entries.

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	172/214 (80%)	113 (66%)	59 (34%)	0 1

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	10	PHE
1	A	12	ARG
1	A	18	PHE
1	A	19	LEU
1	A	21	THR
1	A	22	THR
1	A	23	LEU
1	A	31	SER
1	A	33	LEU

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Mol	Chain	Res	Type
1	A	35	PHE
1	A	36	LYS
1	A	54	LEU
1	A	56	PHE
1	A	58	LEU
1	A	59	SER
1	A	63	LEU
1	A	65	GLN
1	A	66	SER
1	A	70	ILE
1	A	74	HIS
1	A	75	LEU
1	A	76	ASN
1	A	79	VAL
1	A	81	LEU
1	A	88	GLN
1	A	92	PHE
1	A	96	MET
1	A	101	GLN
1	A	123	SER
1	A	124	LEU
1	A	126	ARG
1	A	127	ASN
1	A	128	ASP
1	A	131	ASP
1	A	135	SER
1	A	137	GLN
1	A	139	LEU
1	A	141	ILE
1	A	142	GLU
1	A	147	LEU
1	A	149	LEU
1	A	153	VAL
1	A	154	LEU
1	A	160	ARG
1	A	164	LEU
1	A	170	LEU
1	A	174	LEU
1	A	175	SER
1	A	181	LEU
1	A	201	VAL
1	A	203	THR

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Mol	Chain	Res	Type
1	A	206	PHE
1	A	208	ASN
1	A	211	ILE
1	A	212	PHE
1	A	214	VAL
1	A	228	ASP
1	A	231	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	43	GLN
1	A	69	HIS
1	A	74	HIS
1	A	76	ASN
1	A	101	GLN
1	A	134	ASN
1	A	208	ASN
1	A	209	HIS

5.3.3 RNA [i](#)

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 monosaccharides 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.