



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 02:56 PM UTC

PDB ID : 2D57 / pdb_00002d57
Title : Double layered 2D crystal structure of AQUAPORIN-4 (AQP4M23) at 3.2 Å resolution by electron crystallography
Authors : Hiroaki, Y.; Tani, K.; Kamegawa, A.; Gyobu, N.; Nishikawa, K.; Suzuki, H.; Walz, T.; Sasaki, S.; Mitsuoka, K.; Kimura, K.; Mizoguchi, A.; Fujiyoshi, Y.
Deposited on : 2005-10-29
Resolution : 3.20 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	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

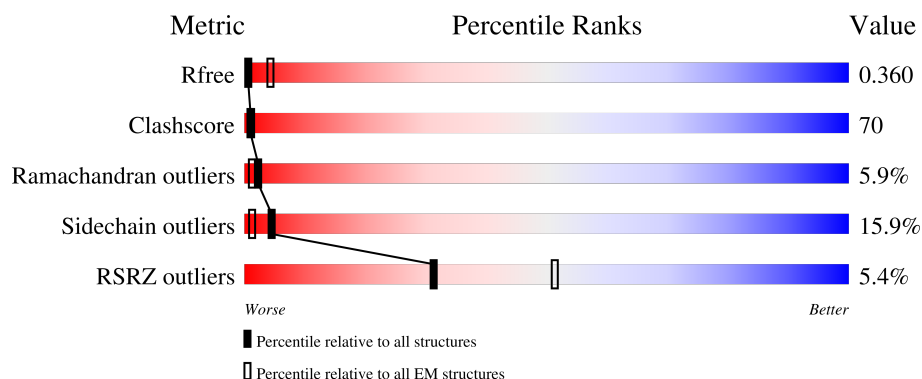
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON CRYSTALLOGRAPHY

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)	EM structures (#Entries)
R_{free}	180332	208
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102
RSRZ outliers	180361	209

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	301	4% 17% 42% 15% • 26%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1659 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-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	224	1659	1092	266	289	12	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	69.00Å 69.00Å 160.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	22.21 – 3.20 22.21 – 3.20	Depositor EDS
% Data completeness (in resolution range)	87.0 (22.21-3.20) 86.6 (22.21-3.20)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.78 (at 3.23Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.283 , 0.338 0.298 , 0.360	Depositor DCC
R_{free} test set	337 reflections (5.62%)	wwPDB-VP
Wilson B-factor (Å ²)	72.9	Xtriage
Anisotropy	0.764	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 150.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	1659	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.69	1/1702 (0.1%)	1.21	21/2328 (0.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	142	VAL	CA-CB	5.18	1.61	1.54

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	85	VAL	N-CA-C	-7.93	102.71	110.72
1	A	107	THR	N-CA-C	-7.17	103.79	112.54
1	A	165	ILE	N-CA-C	7.12	117.88	110.62
1	A	127	ILE	N-CA-C	6.30	116.78	110.23
1	A	145	LEU	N-CA-C	-6.25	104.96	112.58
1	A	191	LEU	N-CA-C	6.22	118.99	111.40
1	A	204	ALA	N-CA-C	5.98	119.84	112.54
1	A	124	LEU	N-CA-C	-5.97	104.12	111.40
1	A	167	THR	N-CA-C	-5.84	104.92	111.28
1	A	138	PRO	N-CA-C	5.48	117.39	110.70
1	A	166	ILE	N-CA-C	5.47	115.67	110.42
1	A	213	ASN	CA-C-N	5.47	126.68	119.84
1	A	213	ASN	C-N-CA	5.47	126.68	119.84
1	A	170	LEU	N-CA-C	-5.43	105.05	110.97
1	A	121	ALA	N-CA-C	-5.40	105.39	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	251	VAL	N-CA-C	5.30	120.37	109.34
1	A	194	GLY	N-CA-C	-5.26	106.40	112.50
1	A	178	CYS	N-CA-C	5.25	118.85	112.23
1	A	205	ILE	N-CA-C	5.14	120.04	109.34
1	A	133	LEU	N-CA-C	-5.14	105.76	111.36
1	A	197	VAL	N-CA-C	-5.11	105.52	110.42

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	233	TYR	Sidechain

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	1659	0	1688	234	1
All	All	1659	0	1688	234	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 70.

All (234) 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:242:VAL:HG23	1:A:243:LEU:HD22	1.40	1.01
1:A:34:PHE:HE2	1:A:114:LYS:HG3	1.24	0.98
1:A:171:VAL:HG21	1:A:241:ALA:HA	1.49	0.92
1:A:245:GLY:O	1:A:249:GLU:HG2	1.70	0.91
1:A:99:ALA:HB1	1:A:241:ALA:HB2	1.51	0.90
1:A:66:LEU:HB3	1:A:67:PRO:HD2	1.54	0.89
1:A:98:PRO:HG2	1:A:214:PRO:HB2	1.55	0.87
1:A:59:TRP:CZ2	1:A:65:PRO:HB3	2.10	0.86
1:A:217:SER:O	1:A:220:PRO:HD2	1.78	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ALA:HB2	1:A:91:ILE:HD12	1.59	0.84
1:A:145:LEU:HD13	1:A:145:LEU:O	1.78	0.84
1:A:34:PHE:CE2	1:A:114:LYS:HG3	2.12	0.84
1:A:160:LEU:C	1:A:160:LEU:HD23	2.03	0.83
1:A:57:ILE:HD13	1:A:58:ASN:N	1.98	0.78
1:A:57:ILE:HD13	1:A:57:ILE:C	2.09	0.78
1:A:117:PHE:HA	1:A:120:THR:HG22	1.63	0.78
1:A:161:LEU:O	1:A:164:LEU:HB3	1.83	0.77
1:A:127:ILE:HG12	1:A:222:VAL:HG21	1.66	0.76
1:A:47:ILE:O	1:A:51:LEU:HB2	1.85	0.76
1:A:84:MET:HE3	1:A:84:MET:HA	1.68	0.76
1:A:167:THR:O	1:A:171:VAL:HG23	1.85	0.74
1:A:52:SER:HB3	1:A:77:PHE:CZ	2.22	0.74
1:A:128:ILE:O	1:A:132:ILE:HG23	1.87	0.74
1:A:40:ALA:CB	1:A:91:ILE:HD12	2.17	0.74
1:A:182:ARG:C	1:A:184:ASP:H	1.97	0.73
1:A:53:VAL:O	1:A:57:ILE:HG22	1.89	0.73
1:A:98:PRO:CG	1:A:214:PRO:HB2	2.18	0.72
1:A:195:PHE:O	1:A:198:ALA:HB3	1.89	0.72
1:A:230:HIS:CD2	1:A:234:TRP:HE1	2.08	0.72
1:A:50:LEU:HD23	1:A:50:LEU:C	2.15	0.72
1:A:113:ALA:O	1:A:116:VAL:HG22	1.88	0.72
1:A:117:PHE:O	1:A:120:THR:HG22	1.89	0.72
1:A:165:ILE:O	1:A:168:PHE:HB3	1.88	0.72
1:A:224:MET:SD	1:A:226:ASN:HB3	2.30	0.71
1:A:41:GLU:OE1	1:A:41:GLU:HA	1.90	0.70
1:A:66:LEU:HB2	1:A:68:VAL:HG12	1.72	0.70
1:A:221:ALA:HB1	1:A:227:TRP:CD1	2.26	0.70
1:A:135:LEU:HD13	1:A:135:LEU:C	2.16	0.70
1:A:148:THR:HG21	1:A:211:SER:HA	1.74	0.70
1:A:243:LEU:O	1:A:247:LEU:HD13	1.90	0.70
1:A:194:GLY:O	1:A:197:VAL:HB	1.92	0.69
1:A:91:ILE:HD13	1:A:91:ILE:O	1.93	0.69
1:A:221:ALA:HB1	1:A:227:TRP:HD1	1.58	0.68
1:A:31:THR:O	1:A:33:ALA:N	2.27	0.68
1:A:144:GLY:O	1:A:147:VAL:HG13	1.94	0.68
1:A:166:ILE:HB	1:A:212:MET:CE	2.23	0.68
1:A:57:ILE:O	1:A:60:GLY:N	2.26	0.68
1:A:35:TRP:HA	1:A:35:TRP:CE3	2.29	0.67
1:A:65:PRO:O	1:A:66:LEU:HD23	1.95	0.67
1:A:235:VAL:HG23	1:A:236:GLY:N	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:LEU:O	1:A:174:ILE:HD12	1.95	0.66
1:A:231:TRP:HE3	1:A:235:VAL:HG11	1.59	0.66
1:A:117:PHE:CA	1:A:120:THR:HG22	2.28	0.64
1:A:174:ILE:O	1:A:178:CYS:SG	2.55	0.64
1:A:102:VAL:O	1:A:105:VAL:HG12	1.98	0.63
1:A:35:TRP:HA	1:A:35:TRP:HE3	1.62	0.63
1:A:160:LEU:HD23	1:A:161:LEU:N	2.13	0.63
1:A:166:ILE:HB	1:A:212:MET:HE2	1.79	0.63
1:A:124:LEU:O	1:A:128:ILE:HG22	1.99	0.63
1:A:227:TRP:HB3	1:A:230:HIS:HB2	1.79	0.63
1:A:69:ASP:O	1:A:73:ILE:HG13	1.99	0.63
1:A:97:ASN:HB2	1:A:213:ASN:HD21	1.64	0.62
1:A:97:ASN:HB2	1:A:213:ASN:ND2	2.14	0.62
1:A:96:ILE:HG12	1:A:96:ILE:O	2.00	0.61
1:A:34:PHE:HE2	1:A:114:LYS:CG	2.07	0.61
1:A:95:HIS:ND1	1:A:104:MET:HG3	2.15	0.61
1:A:49:VAL:HG23	1:A:50:LEU:H	1.67	0.60
1:A:141:VAL:HG22	1:A:145:LEU:HB2	1.82	0.60
1:A:95:HIS:CE1	1:A:104:MET:HG3	2.37	0.59
1:A:141:VAL:CG2	1:A:145:LEU:HB2	2.31	0.59
1:A:97:ASN:HB3	1:A:100:VAL:CG2	2.32	0.59
1:A:166:ILE:HA	1:A:169:GLN:NE2	2.17	0.59
1:A:34:PHE:HE1	1:A:35:TRP:CZ3	2.21	0.59
1:A:144:GLY:O	1:A:145:LEU:HB3	2.01	0.59
1:A:149:THR:O	1:A:151:HIS:N	2.36	0.59
1:A:188:SER:HB3	1:A:191:LEU:HD12	1.83	0.59
1:A:219:GLY:O	1:A:222:VAL:HG23	2.02	0.58
1:A:127:ILE:CG1	1:A:222:VAL:HG21	2.33	0.58
1:A:235:VAL:HG23	1:A:236:GLY:H	1.66	0.58
1:A:97:ASN:HB3	1:A:100:VAL:HG23	1.86	0.58
1:A:54:GLY:O	1:A:57:ILE:HG23	2.04	0.58
1:A:98:PRO:CB	1:A:214:PRO:HB2	2.34	0.58
1:A:59:TRP:O	1:A:61:GLY:N	2.32	0.57
1:A:149:THR:OG1	1:A:228:GLU:HB3	2.05	0.56
1:A:150:VAL:N	1:A:233:TYR:OH	2.39	0.55
1:A:239:ILE:O	1:A:242:VAL:HG22	2.07	0.55
1:A:49:VAL:HG23	1:A:50:LEU:N	2.21	0.55
1:A:117:PHE:C	1:A:120:THR:HG22	2.31	0.55
1:A:156:ALA:O	1:A:160:LEU:HB3	2.07	0.55
1:A:183:THR:O	1:A:183:THR:HG22	2.06	0.55
1:A:162:VAL:O	1:A:165:ILE:HG22	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:HIS:O	1:A:152:GLY:C	2.49	0.55
1:A:233:TYR:O	1:A:237:PRO:HD2	2.06	0.55
1:A:170:LEU:HA	1:A:196:SER:OG	2.07	0.55
1:A:59:TRP:C	1:A:61:GLY:H	2.13	0.55
1:A:131:GLY:O	1:A:134:TYR:HB3	2.06	0.55
1:A:201:HIS:O	1:A:202:LEU:C	2.49	0.55
1:A:52:SER:HB3	1:A:77:PHE:CE2	2.42	0.54
1:A:91:ILE:HD13	1:A:91:ILE:C	2.33	0.54
1:A:149:THR:O	1:A:150:VAL:C	2.50	0.54
1:A:201:HIS:O	1:A:205:ILE:HG13	2.08	0.53
1:A:231:TRP:CE3	1:A:235:VAL:HG11	2.43	0.53
1:A:232:ILE:HA	1:A:235:VAL:HG22	1.91	0.53
1:A:196:SER:HA	1:A:199:ILE:HD11	1.90	0.53
1:A:130:ALA:O	1:A:133:LEU:HB3	2.09	0.53
1:A:228:GLU:OE1	1:A:228:GLU:HA	2.08	0.53
1:A:231:TRP:O	1:A:235:VAL:HG22	2.09	0.53
1:A:229:ASN:OD1	1:A:229:ASN:O	2.27	0.53
1:A:100:VAL:O	1:A:104:MET:HG2	2.08	0.53
1:A:148:THR:HG23	1:A:216:ARG:NH2	2.24	0.52
1:A:45:MET:HE2	1:A:215:ALA:CB	2.40	0.52
1:A:182:ARG:O	1:A:184:ASP:N	2.42	0.52
1:A:160:LEU:C	1:A:160:LEU:CD2	2.76	0.52
1:A:165:ILE:HG23	1:A:166:ILE:N	2.25	0.52
1:A:105:VAL:HG23	1:A:110:ILE:O	2.10	0.51
1:A:138:PRO:HG2	1:A:139:PRO:HD3	1.91	0.51
1:A:195:PHE:O	1:A:199:ILE:HG12	2.10	0.51
1:A:201:HIS:HB3	1:A:205:ILE:HD11	1.90	0.51
1:A:97:ASN:C	1:A:97:ASN:OD1	2.52	0.51
1:A:50:LEU:HD12	1:A:132:ILE:HD11	1.92	0.51
1:A:182:ARG:C	1:A:184:ASP:N	2.66	0.51
1:A:78:GLY:HA2	1:A:197:VAL:CG1	2.40	0.51
1:A:117:PHE:HA	1:A:120:THR:CG2	2.36	0.51
1:A:232:ILE:HA	1:A:235:VAL:CG2	2.39	0.51
1:A:243:LEU:HD22	1:A:243:LEU:N	2.26	0.50
1:A:168:PHE:CG	1:A:244:ALA:HB2	2.46	0.50
1:A:90:HIS:ND1	1:A:90:HIS:N	2.58	0.50
1:A:196:SER:O	1:A:199:ILE:HG13	2.12	0.50
1:A:243:LEU:HD22	1:A:243:LEU:H	1.77	0.50
1:A:71:VAL:CG1	1:A:72:LEU:N	2.75	0.49
1:A:34:PHE:HE1	1:A:35:TRP:HZ3	1.60	0.49
1:A:155:THR:O	1:A:157:GLY:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:ALA:HA	1:A:248:TYR:CZ	2.47	0.49
1:A:247:LEU:HD12	1:A:247:LEU:N	2.27	0.49
1:A:83:THR:O	1:A:86:GLN:HB2	2.12	0.49
1:A:238:ILE:O	1:A:241:ALA:HB3	2.12	0.49
1:A:230:HIS:CD2	1:A:234:TRP:NE1	2.80	0.49
1:A:135:LEU:HD22	1:A:135:LEU:O	2.12	0.49
1:A:239:ILE:HA	1:A:242:VAL:HG22	1.94	0.49
1:A:132:ILE:O	1:A:136:VAL:HG23	2.14	0.48
1:A:242:VAL:HG23	1:A:243:LEU:N	2.29	0.48
1:A:171:VAL:O	1:A:175:PHE:HD1	1.96	0.48
1:A:52:SER:HB3	1:A:77:PHE:CE1	2.48	0.48
1:A:141:VAL:O	1:A:143:GLY:N	2.47	0.48
1:A:34:PHE:CE2	1:A:114:LYS:HE3	2.49	0.48
1:A:128:ILE:HG23	1:A:129:GLY:N	2.29	0.48
1:A:54:GLY:HA2	1:A:57:ILE:CG2	2.43	0.47
1:A:57:ILE:HD13	1:A:58:ASN:CA	2.43	0.47
1:A:98:PRO:HB2	1:A:214:PRO:HB2	1.96	0.47
1:A:166:ILE:HA	1:A:169:GLN:HE21	1.77	0.47
1:A:174:ILE:HG13	1:A:193:ILE:HG12	1.97	0.47
1:A:197:VAL:HG13	1:A:201:HIS:CE1	2.49	0.47
1:A:71:VAL:HG13	1:A:72:LEU:N	2.30	0.47
1:A:128:ILE:HG23	1:A:129:GLY:H	1.79	0.47
1:A:242:VAL:CG2	1:A:243:LEU:HD22	2.29	0.47
1:A:127:ILE:CD1	1:A:222:VAL:HG21	2.44	0.47
1:A:64:ASN:O	1:A:66:LEU:HG	2.14	0.47
1:A:66:LEU:HB3	1:A:67:PRO:CD	2.33	0.47
1:A:88:PHE:HA	1:A:91:ILE:HG22	1.96	0.47
1:A:164:LEU:O	1:A:240:GLY:HA3	2.15	0.47
1:A:88:PHE:N	1:A:88:PHE:CD1	2.83	0.47
1:A:231:TRP:O	1:A:235:VAL:HG13	2.15	0.47
1:A:235:VAL:CG2	1:A:236:GLY:N	2.78	0.47
1:A:237:PRO:O	1:A:241:ALA:HB2	2.15	0.47
1:A:84:MET:HE2	1:A:88:PHE:HE1	1.80	0.46
1:A:142:VAL:C	1:A:144:GLY:H	2.23	0.46
1:A:88:PHE:CA	1:A:91:ILE:HG22	2.45	0.46
1:A:148:THR:HG21	1:A:211:SER:CA	2.43	0.46
1:A:239:ILE:O	1:A:243:LEU:HD23	2.14	0.46
1:A:45:MET:HE2	1:A:215:ALA:HB3	1.97	0.46
1:A:171:VAL:HG13	1:A:175:PHE:CE1	2.51	0.46
1:A:83:THR:O	1:A:87:CYS:N	2.45	0.46
1:A:46:LEU:HA	1:A:125:GLY:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:THR:O	1:A:40:ALA:C	2.56	0.45
1:A:148:THR:O	1:A:233:TYR:CE2	2.69	0.45
1:A:217:SER:C	1:A:220:PRO:HD2	2.39	0.45
1:A:228:GLU:HG3	1:A:229:ASN:HD22	1.81	0.45
1:A:247:LEU:N	1:A:247:LEU:CD1	2.78	0.45
1:A:98:PRO:HD3	1:A:215:ALA:HB2	1.97	0.45
1:A:142:VAL:C	1:A:144:GLY:N	2.72	0.45
1:A:34:PHE:CE1	1:A:35:TRP:CZ3	3.04	0.45
1:A:59:TRP:C	1:A:61:GLY:N	2.75	0.45
1:A:46:LEU:HD12	1:A:46:LEU:C	2.40	0.45
1:A:56:THR:HG22	1:A:73:ILE:HG23	1.99	0.45
1:A:166:ILE:HB	1:A:212:MET:HE1	1.97	0.45
1:A:34:PHE:CE1	1:A:38:VAL:HG21	2.52	0.44
1:A:165:ILE:CG2	1:A:166:ILE:N	2.81	0.44
1:A:46:LEU:HD22	1:A:128:ILE:HD13	1.97	0.44
1:A:168:PHE:CD1	1:A:168:PHE:C	2.96	0.44
1:A:167:THR:O	1:A:171:VAL:CG2	2.61	0.44
1:A:195:PHE:N	1:A:195:PHE:CD1	2.85	0.44
1:A:66:LEU:C	1:A:68:VAL:H	2.25	0.43
1:A:142:VAL:O	1:A:144:GLY:N	2.51	0.43
1:A:36:LYS:H	1:A:36:LYS:HD2	1.84	0.43
1:A:141:VAL:O	1:A:142:VAL:C	2.61	0.43
1:A:97:ASN:O	1:A:98:PRO:C	2.60	0.43
1:A:164:LEU:HD12	1:A:240:GLY:CA	2.49	0.43
1:A:147:VAL:O	1:A:149:THR:N	2.51	0.43
1:A:34:PHE:CD2	1:A:114:LYS:HE3	2.54	0.43
1:A:171:VAL:O	1:A:175:PHE:CD1	2.71	0.43
1:A:178:CYS:O	1:A:179:ASP:C	2.62	0.42
1:A:81:ILE:O	1:A:82:ALA:C	2.61	0.42
1:A:163:GLU:HA	1:A:166:ILE:HD11	2.02	0.42
1:A:45:MET:HE2	1:A:216:ARG:N	2.35	0.42
1:A:188:SER:HB3	1:A:191:LEU:HB2	2.02	0.42
1:A:104:MET:CE	1:A:109:LYS:HD2	2.50	0.42
1:A:195:PHE:N	1:A:195:PHE:HD1	2.18	0.42
1:A:96:ILE:O	1:A:96:ILE:CG1	2.63	0.42
1:A:232:ILE:CA	1:A:235:VAL:HG22	2.49	0.42
1:A:234:TRP:O	1:A:238:ILE:HD12	2.20	0.42
1:A:125:GLY:HA2	1:A:128:ILE:CG2	2.50	0.41
1:A:179:ASP:HB3	1:A:248:TYR:HE2	1.85	0.41
1:A:135:LEU:HD13	1:A:135:LEU:O	2.20	0.41
1:A:168:PHE:CD2	1:A:244:ALA:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:ILE:HD13	1:A:58:ASN:HA	2.03	0.41
1:A:59:TRP:CE2	1:A:65:PRO:HB3	2.54	0.41
1:A:117:PHE:O	1:A:120:THR:CG2	2.65	0.41
1:A:229:ASN:O	1:A:229:ASN:CG	2.63	0.41
1:A:50:LEU:C	1:A:50:LEU:CD2	2.86	0.41
1:A:166:ILE:HG13	1:A:167:THR:N	2.36	0.41
1:A:228:GLU:HG3	1:A:229:ASN:ND2	2.35	0.41
1:A:235:VAL:CG2	1:A:236:GLY:H	2.32	0.41
1:A:173:THR:O	1:A:177:SER:HB2	2.21	0.41
1:A:199:ILE:O	1:A:200:GLY:C	2.63	0.41
1:A:45:MET:HE3	1:A:49:VAL:HG13	2.01	0.41
1:A:53:VAL:O	1:A:54:GLY:C	2.62	0.41
1:A:84:MET:HE3	1:A:87:CYS:SG	2.61	0.41
1:A:110:ILE:HD12	1:A:114:LYS:CE	2.51	0.41
1:A:117:PHE:O	1:A:118:TYR:C	2.61	0.40
1:A:141:VAL:HG13	1:A:142:VAL:N	2.35	0.40
1:A:216:ARG:HG2	1:A:216:ARG:HH11	1.86	0.40
1:A:168:PHE:HA	1:A:240:GLY:O	2.20	0.40
1:A:216:ARG:O	1:A:220:PRO:CD	2.70	0.40
1:A:54:GLY:O	1:A:58:ASN:HB2	2.22	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:142:VAL:CG1	1:A:142:VAL:CG1[8_667]	2.06	0.14

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 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	222/301 (74%)	177 (80%)	32 (14%)	13 (6%)	1 10

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	150	VAL
1	A	156	ALA
1	A	181	LYS
1	A	212	MET
1	A	142	VAL
1	A	148	THR
1	A	183	THR
1	A	250	TYR
1	A	251	VAL
1	A	179	ASP
1	A	60	GLY
1	A	96	ILE

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	176/243 (72%)	148 (84%)	28 (16%)	2 13

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	TRP
1	A	46	LEU
1	A	57	ILE
1	A	58	ASN
1	A	63	GLU
1	A	64	ASN
1	A	84	MET
1	A	88	PHE
1	A	90	HIS
1	A	91	ILE
1	A	98	PRO
1	A	119	ILE

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Mol	Chain	Res	Type
1	A	124	LEU
1	A	128	ILE
1	A	134	TYR
1	A	135	LEU
1	A	148	THR
1	A	154	LEU
1	A	160	LEU
1	A	169	GLN
1	A	177	SER
1	A	181	LYS
1	A	186	THR
1	A	208	THR
1	A	214	PRO
1	A	222	VAL
1	A	224	MET
1	A	232	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	169	GLN
1	A	213	ASN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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.